Infinite Potential Wall

The energy eigenfunctions and eigenvalues of the infinite potetial wall:

$$\psi[x\_, n\_] = \sqrt{\frac{2}{L}}\ \mathrm{Sin}\left[\frac{n\,\pi}{L}\,x\right];\ \mathrm{En}[n\_] = \frac{\hbar^2\,\pi^2}{2\,m\,L^2}\,n^2;$$

```
$Assumptions = n ∈ Integers && l ∈ Integers && n > 0 && m > 0 && L > 0 && ℏ > 0 && l > 0
```

```
n ∈ Integers && l ∈ Integers && n > 0 && m > 0 && L > 0 && ℏ > 0 && l > 0
```

Normalization:

$$\int_0^L \psi[x, n]\ \psi[x, n]\, dx$$

$$1$$

Calculate $< x >,\ < x^2 >,\ \Delta\ x$

$$\mathrm{xav}[n\_] = \int_0^L \psi[x, n]\ x\ \psi[x, n]\, dx$$

$$\frac{L}{2}$$

$$\mathrm{x2av}[n\_] = \int_0^L \psi[x, n]\ x^2\ \psi[x, n]\, dx$$

$$\frac{1}{6}\,L^2\left(2 - \frac{3}{n^2\,\pi^2}\right)$$

$$\Delta\,x[n\_] = \sqrt{\mathrm{x2av}[n] - (\mathrm{xav}[n])^2}\ \ //\ \mathrm{Simplify}$$

$$\frac{\sqrt{L^2\left(1 - \frac{6}{n^2\,\pi^2}\right)}}{2\,\sqrt{3}}$$

Calculate $< p >,\ < p^2 >,\ \Delta\ p$

```
pav[n_] = ∫_0^L ψ[x, n] (-ⅈ ℏ) ∂_x ψ[x, n] ⅆx
```

```
0
```

```
p2av[n_] = ∫_0^L ψ[x, n] (- ℏ^2) ∂_xx ψ[x, n] ⅆx
```

$$\frac{n^2 \pi^2 \hbar^2}{L^2}$$

```
Δ p[n_] = Sqrt[p2av[n] - (pav[n])^2] // Simplify
```

$$n \pi \sqrt{\frac{\hbar^2}{L^2}}$$

Heisenberg Uncertainty principle:

```
Δ x[n] Δ p[n] // Simplify
```

$$\frac{\sqrt{-6 + n^2 \pi^2}\ \hbar}{2 \sqrt{3}}$$

The product is always larger than $\hbar/2$:

```
Table[Δ x[n] Δ p[n] // Simplify // N, {n, 1, 10}]
```

```
{0.567862 ℏ, 1.67029 ℏ, 2.6272 ℏ, 3.55802 ℏ,
 4.47903 ℏ, 5.39526 ℏ, 6.30879 ℏ, 7.22066 ℏ, 8.13141 ℏ, 9.04139 ℏ}
```

Problem 1:

Consider the particle in the initial state $\phi(x, 0) = A\, x\, (L - x)$. Compute the state $\phi(x, t)$ and the corresponding average values of position , momentum etc.

Solution:

Consider the expression of the wave function interms of the energy eigenfunctions:

$$\phi(x, 0) \equiv \phi(x) = \sum_{n=1}^{\infty} c_n\, \psi_n(x), \quad c_n = \int_0^L \psi_n^*(x)\, \phi(x)\, dx$$

$$\phi(x, t) = \sum_{n=1}^{\infty} c_n\, \psi_n(x)\, e^{-i E_n t/\hbar}$$

$$< x > (t) = \sum_{n,m=1}^{\infty} c_m^*\, c_n\, e^{-i (E_n - E_m) t/\hbar} \int_0^L \psi_m^*(x)\, x\, \psi_n(x)\, dx$$

$$< x^2 > (t) = \sum_{n,m=1}^{\infty} c_m^*\, c_n\, e^{-i (E_n - E_m) t/\hbar} \int_0^L \psi_m^*(x)\, x^2\, \psi_n(x)\, dx$$

We compute the normalization factor A and define the wave function at t=0

```
A = 1/Sqrt[∫_0^L (x (L - x))^2 dx]
```

$$\frac{\sqrt{30}}{\sqrt{L^5}}$$

```
ϕ[x_, 0] = A x (L - x); ∫_0^L ϕ[x, 0]^2 dx
```

1

We compute the coeeficients c_n:

```
cn[n_] = ∫_0^L ψ[x, n] ϕ[x, 0] dx /. {Cos[n π] → (-1)^n, Sin[n π] → 0}
```

$$\frac{2\sqrt{15}\,(2-2\,(-1)^n)}{n^3\,\pi^3}$$

Even order n coefficients are zero. Odd eigenfunctions are absent since $\phi(x, 0)$ is even.

```
cn[2 n] // Simplify
```

0

```
cm[n_] = cn[2 n + 1] // Simplify
```

$$\frac{8\sqrt{15}}{(\pi + 2\,n\,\pi)^3}$$

Of course $M \to \infty$ but we will use it as a cutoff:

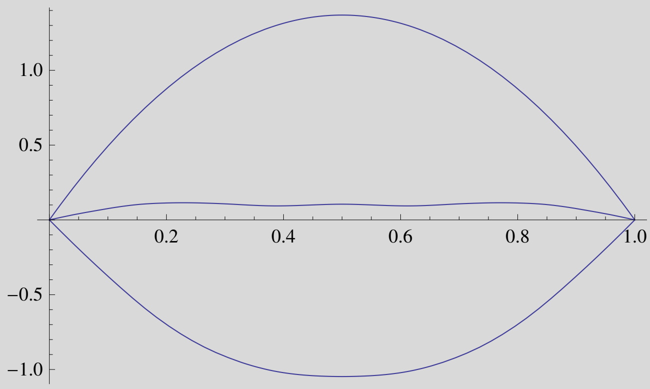
```
ϕ[x_, t_, M_] := Sum[cm[l] ψ[x, 2 l + 1] e^(-i En[2 l+1] t/ħ), {l, 0, M}]
```

These are the periods $T_n = \frac{2\pi}{\omega_n} = \frac{2\pi}{E_n/\hbar} = \frac{4\,m\,L^2}{\pi\,\hbar\,n^2}$

$$\frac{4\,m\,L^2}{\pi\,\hbar\,n^2} \text{ /. \{L → 1, m → 1, ℏ → 1\} // N}$$

$$\frac{1.27324}{n^2}$$

```
Plot[Re[{ϕ[x, 0, 20], ϕ[x, 0.3, 20], ϕ[x, 0.5, 20]}] /. {L → 1, m → 1, ℏ → 1}, {x, 0, 1}]
```



We compute the coefficients $x_{nm} = \int_0^L \psi_n\square\,(x)\, x\, \psi_m(x)\, dx$ and $x^2{}_{nm} = \int_0^L \psi_n\square\,(x)\, x^2\, \psi_m(x)\, dx$

$$\text{xnm[n\_, l\_] } = \int_0^L \psi[x, n]\, x\, \psi[x, l]\, dx$$

$$\frac{4\left(-1 + (-1)^{1+n}\right) l\, L\, n}{\left(l^2 - n^2\right)^2 \pi^2}$$

The $n = m$ case must be treated differently:

$$\text{xnm[n\_, n\_] } = \int_0^L \psi[x, n]\, x\, \psi[x, n]\, dx$$

$$\frac{L}{2}$$

```
Table[xnm[i, j], {i, 1, 10}, {j, 1, 10}] // MatrixForm
```

$$\begin{pmatrix}
\frac{L}{2} & -\frac{16 L}{9 \pi^2} & 0 & -\frac{32 L}{225 \pi^2} & 0 & -\frac{48 L}{1225 \pi^2} & 0 & -\frac{64 L}{3969 \pi^2} & 0 & -\frac{80 L}{9801 \pi^2} \\
-\frac{16 L}{9 \pi^2} & \frac{L}{2} & -\frac{48 L}{25 \pi^2} & 0 & -\frac{80 L}{441 \pi^2} & 0 & -\frac{112 L}{2025 \pi^2} & 0 & -\frac{144 L}{5929 \pi^2} & 0 \\
0 & -\frac{48 L}{25 \pi^2} & \frac{L}{2} & -\frac{96 L}{49 \pi^2} & 0 & -\frac{16 L}{81 \pi^2} & 0 & -\frac{192 L}{3025 \pi^2} & 0 & -\frac{240 L}{8281 \pi^2} \\
-\frac{32 L}{225 \pi^2} & 0 & -\frac{96 L}{49 \pi^2} & \frac{L}{2} & -\frac{160 L}{81 \pi^2} & 0 & -\frac{224 L}{1089 \pi^2} & 0 & -\frac{288 L}{4225 \pi^2} & 0 \\
0 & -\frac{80 L}{441 \pi^2} & 0 & -\frac{160 L}{81 \pi^2} & \frac{L}{2} & -\frac{240 L}{121 \pi^2} & 0 & -\frac{320 L}{1521 \pi^2} & 0 & -\frac{16 L}{225 \pi^2} \\
-\frac{48 L}{1225 \pi^2} & 0 & -\frac{16 L}{81 \pi^2} & 0 & -\frac{240 L}{121 \pi^2} & \frac{L}{2} & -\frac{336 L}{169 \pi^2} & 0 & -\frac{16 L}{75 \pi^2} & 0 \\
0 & -\frac{112 L}{2025 \pi^2} & 0 & -\frac{224 L}{1089 \pi^2} & 0 & -\frac{336 L}{169 \pi^2} & \frac{L}{2} & -\frac{448 L}{225 \pi^2} & 0 & -\frac{560 L}{2601 \pi^2} \\
-\frac{64 L}{3969 \pi^2} & 0 & -\frac{192 L}{3025 \pi^2} & 0 & -\frac{320 L}{1521 \pi^2} & 0 & -\frac{448 L}{225 \pi^2} & \frac{L}{2} & -\frac{576 L}{289 \pi^2} & 0 \\
0 & -\frac{144 L}{5929 \pi^2} & 0 & -\frac{288 L}{4225 \pi^2} & 0 & -\frac{16 L}{75 \pi^2} & 0 & -\frac{576 L}{289 \pi^2} & \frac{L}{2} & -\frac{720 L}{361 \pi^2} \\
-\frac{80 L}{9801 \pi^2} & 0 & -\frac{240 L}{8281 \pi^2} & 0 & -\frac{16 L}{225 \pi^2} & 0 & -\frac{560 L}{2601 \pi^2} & 0 & -\frac{720 L}{361 \pi^2} & \frac{L}{2}
\end{pmatrix}$$

$$\text{x2nm[n\_, l\_]} = \int_0^L \psi[x, n]\, x^2\, \psi[x, l]\, dx$$

$$\frac{8\,(-1)^{l+n}\, l\, L^2\, n}{\left(l^2 - n^2\right)^2 \pi^2}$$

$$\text{x2nm[n\_, n\_]} = \int_0^L \psi[x, n]\, x^2\, \psi[x, n]\, dx$$

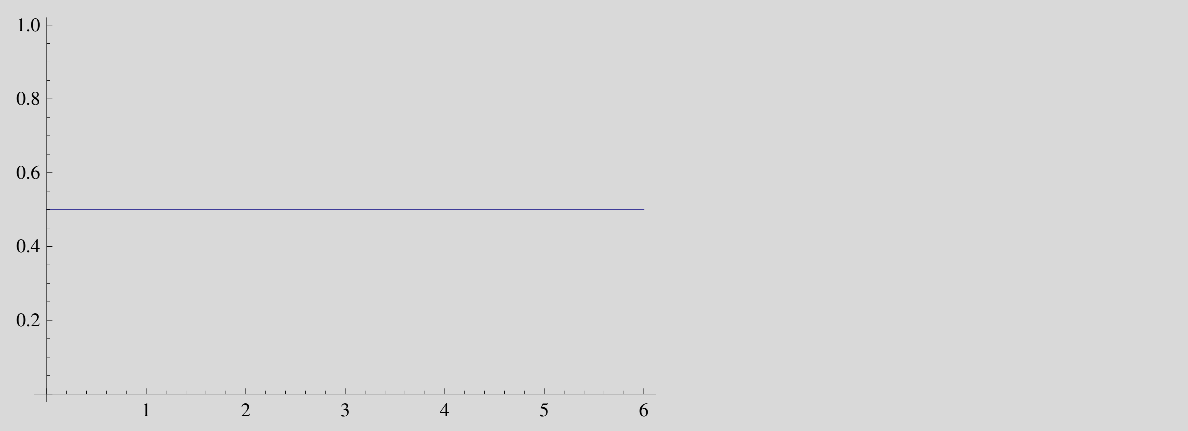
$$\frac{1}{6} L^2 \left(2 - \frac{3}{n^2 \pi^2}\right)$$

```
Table[x2nm[i, j], {i, 1, 10}, {j, 1, 10}] // MatrixForm
```

$\frac{1}{6} L^2 \left(2 - \frac{3}{\pi^2}\right)$	$-\frac{16 L^2}{9 \pi^2}$	$\frac{3 L^2}{8 \pi^2}$	$-\frac{32 L^2}{225 \pi^2}$	$\frac{5 L^2}{72 \pi^2}$	$-\frac{48 L^2}{1225 \pi^2}$	[illegible]
$-\frac{16 L^2}{9 \pi^2}$	$\frac{1}{6} L^2 \left(2 - \frac{3}{4 \pi^2}\right)$	$-\frac{48 L^2}{25 \pi^2}$	$\frac{4 L^2}{9 \pi^2}$	$-\frac{80 L^2}{441 \pi^2}$	$\frac{3 L^2}{32 \pi^2}$	[illegible]
$\frac{3 L^2}{8 \pi^2}$	$-\frac{48 L^2}{25 \pi^2}$	$\frac{1}{6} L^2 \left(2 - \frac{1}{3 \pi^2}\right)$	$-\frac{96 L^2}{49 \pi^2}$	$\frac{15 L^2}{32 \pi^2}$	$-\frac{16 L^2}{81 \pi^2}$	[illegible]
$-\frac{32 L^2}{225 \pi^2}$	$\frac{4 L^2}{9 \pi^2}$	$-\frac{96 L^2}{49 \pi^2}$	$\frac{1}{6} L^2 \left(2 - \frac{3}{16 \pi^2}\right)$	$-\frac{160 L^2}{81 \pi^2}$	$\frac{12 L^2}{25 \pi^2}$	[illegible]
$\frac{5 L^2}{72 \pi^2}$	$-\frac{80 L^2}{441 \pi^2}$	$\frac{15 L^2}{32 \pi^2}$	$-\frac{160 L^2}{81 \pi^2}$	$\frac{1}{6} L^2 \left(2 - \frac{3}{25 \pi^2}\right)$	$-\frac{240 L^2}{121 \pi^2}$	[illegible]
$-\frac{48 L^2}{1225 \pi^2}$	$\frac{3 L^2}{32 \pi^2}$	$-\frac{16 L^2}{81 \pi^2}$	$\frac{12 L^2}{25 \pi^2}$	$-\frac{240 L^2}{121 \pi^2}$	$\frac{1}{6} L^2 \left(2 - \frac{1}{12 \pi^2}\right)$	[illegible]
$\frac{7 L^2}{288 \pi^2}$	$-\frac{112 L^2}{2025 \pi^2}$	$\frac{21 L^2}{200 \pi^2}$	$-\frac{224 L^2}{1089 \pi^2}$	$\frac{35 L^2}{72 \pi^2}$	$-\frac{336 L^2}{169 \pi^2}$	$\frac{1}{6} L^2 ($
$-\frac{64 L^2}{3969 \pi^2}$	$\frac{8 L^2}{225 \pi^2}$	$-\frac{192 L^2}{3025 \pi^2}$	$\frac{L^2}{9 \pi^2}$	$-\frac{320 L^2}{1521 \pi^2}$	$\frac{24 L^2}{49 \pi^2}$	[illegible]
$\frac{9 L^2}{800 \pi^2}$	$-\frac{144 L^2}{5929 \pi^2}$	$\frac{L^2}{24 \pi^2}$	$-\frac{288 L^2}{4225 \pi^2}$	$\frac{45 L^2}{392 \pi^2}$	$-\frac{16 L^2}{75 \pi^2}$	[illegible]
$-\frac{80 L^2}{9801 \pi^2}$	$\frac{5 L^2}{288 \pi^2}$	$-\frac{240 L^2}{8281 \pi^2}$	$\frac{20 L^2}{441 \pi^2}$	$-\frac{16 L^2}{225 \pi^2}$	$\frac{15 L^2}{128 \pi^2}$	[illegible]

$$\text{xav}\phi[\text{t\_}, \text{NN\_}, \text{MM\_}] := \sum_{n=0}^{NN} \sum_{l=0}^{MM} \text{cm}[n]\, \text{cm}[l]\, \text{xnm}[2n+1, 2l+1]\, e^{-i\,(\text{En}[2l+1]-\text{En}[2n+1])\,t/\hbar}$$

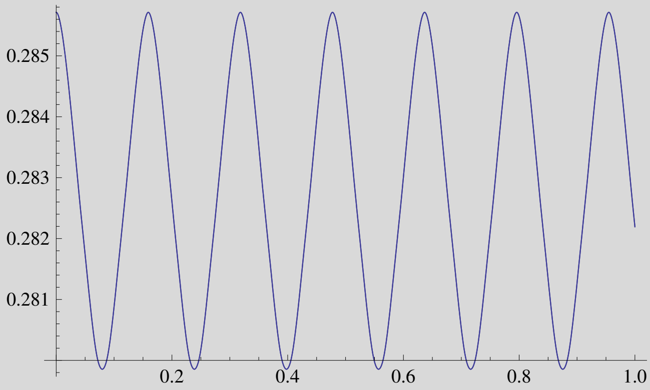
```
Plot[xavϕ[t, 6, 6] /. {L → 1, m → 1, ℏ → 1}, {t, 0, 6}]
```



$$\text{x2av}\phi[\text{t\_}, \text{NN\_}, \text{MM\_}] := \sum_{n=0}^{NN} \sum_{l=0}^{MM} \text{cm}[n]\, \text{cm}[l]\, \text{x2nm}[2n+1, 2l+1]\, e^{-i\,(\text{En}[2l+1]-\text{En}[2n+1])\,t/\hbar}$$

One should choose some values of the cutoff in order to compute. 6→ 10makes no visible difference

```
Plot[{x2avϕ[t, 6, 6]} /. {L → 1, m → 1, ℏ → 1}, {t, 0, 1}]
```



Momenta now:

```
pnm[n_, l_] = ∫_0^L ψ[x, n] (-ⅈ ℏ) ∂_x ψ[x, l] ⅆx /. Cos[l π] → (-1)^l
```

$$\frac{2\,i\left(-1+(-1)^{l+n}\right) l\, n\, \hbar}{L\left(-l^2+n^2\right)}$$

```
pnm[n_, n_] = ∫_0^L ψ[x, n] (-ⅈ ℏ) ∂_x ψ[x, n] ⅆx
```

0

```
Table[pnm[i, j], {i, 1, 10}, {j, 1, 10}] // MatrixForm
```

$$\begin{pmatrix}
0 & \frac{8 i \hbar}{3 L} & 0 & \frac{16 i \hbar}{15 L} & 0 & \frac{24 i \hbar}{35 L} & 0 & \frac{32 i \hbar}{63 L} & 0 & \frac{40 i \hbar}{99 L} \\
-\frac{8 i \hbar}{3 L} & 0 & \frac{24 i \hbar}{5 L} & 0 & \frac{40 i \hbar}{21 L} & 0 & \frac{56 i \hbar}{45 L} & 0 & \frac{72 i \hbar}{77 L} & 0 \\
0 & -\frac{24 i \hbar}{5 L} & 0 & \frac{48 i \hbar}{7 L} & 0 & \frac{8 i \hbar}{3 L} & 0 & \frac{96 i \hbar}{55 L} & 0 & \frac{120 i \hbar}{91 L} \\
-\frac{16 i \hbar}{15 L} & 0 & -\frac{48 i \hbar}{7 L} & 0 & \frac{80 i \hbar}{9 L} & 0 & \frac{112 i \hbar}{33 L} & 0 & \frac{144 i \hbar}{65 L} & 0 \\
0 & -\frac{40 i \hbar}{21 L} & 0 & -\frac{80 i \hbar}{9 L} & 0 & \frac{120 i \hbar}{11 L} & 0 & \frac{160 i \hbar}{39 L} & 0 & \frac{8 i \hbar}{3 L} \\
-\frac{24 i \hbar}{35 L} & 0 & -\frac{8 i \hbar}{3 L} & 0 & -\frac{120 i \hbar}{11 L} & 0 & \frac{168 i \hbar}{13 L} & 0 & \frac{24 i \hbar}{5 L} & 0 \\
0 & -\frac{56 i \hbar}{45 L} & 0 & -\frac{112 i \hbar}{33 L} & 0 & -\frac{168 i \hbar}{13 L} & 0 & \frac{224 i \hbar}{15 L} & 0 & \frac{280 i \hbar}{51 L} \\
-\frac{32 i \hbar}{63 L} & 0 & -\frac{96 i \hbar}{55 L} & 0 & -\frac{160 i \hbar}{39 L} & 0 & -\frac{224 i \hbar}{15 L} & 0 & \frac{288 i \hbar}{17 L} & 0 \\
0 & -\frac{72 i \hbar}{77 L} & 0 & -\frac{144 i \hbar}{65 L} & 0 & -\frac{24 i \hbar}{5 L} & 0 & -\frac{288 i \hbar}{17 L} & 0 & \frac{360 i \hbar}{19 L} \\
-\frac{40 i \hbar}{99 L} & 0 & -\frac{120 i \hbar}{91 L} & 0 & -\frac{8 i \hbar}{3 L} & 0 & -\frac{280 i \hbar}{51 L} & 0 & -\frac{360 i \hbar}{19 L} & 0
\end{pmatrix}$$

```
p2nm[n_, l_] = ∫_0^L ψ[x, n] (- ℏ^2) ∂xx ψ[x, l] ⅆx
```

0

```
p2nm[n_, n_] = ∫_0^L ψ[x, n] (- ℏ^2) ∂xx ψ[x, n] ⅆx
```

$$\frac{n^2 \pi^2 \hbar^2}{L^2}$$

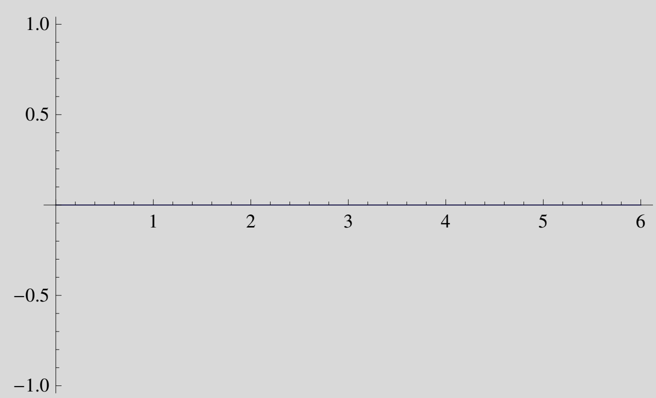
```
Table[p2nm[i, j], {i, 1, 10}, {j, 1, 10}] // MatrixForm
```

$$\begin{pmatrix} \frac{\pi^2 \hbar^2}{L^2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{4 \pi^2 \hbar^2}{L^2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{9 \pi^2 \hbar^2}{L^2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{16 \pi^2 \hbar^2}{L^2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{25 \pi^2 \hbar^2}{L^2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{36 \pi^2 \hbar^2}{L^2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{49 \pi^2 \hbar^2}{L^2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{64 \pi^2 \hbar^2}{L^2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{81 \pi^2 \hbar^2}{L^2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{100 \pi^2 \hbar^2}{L^2} \end{pmatrix}$$

```
pavϕ[t_, NN_, MM_] := Sum_{n=0}^{NN} Sum_{l=0}^{MM} cm[n] cm[l] pnm[2 n + 1, 2 l + 1] ⅇ^(-ⅈ (En[2 l+1]-En[2 n+1]) t/ℏ)
```

As can be seen by inspection all coefficients are 0:

```
Plot[pavϕ[t, 6, 6] /. {L → 1, m → 1, ℏ → 1}, {t, 0, 6}]
```

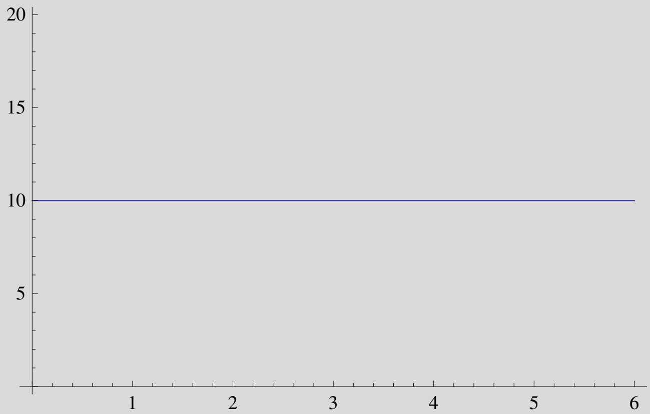


Since $p_{n m}$ are non zero only at the diagonal, $< p > (t)$ does not change with time:

```
p2avϕ[t_, NN_, MM_] := Sum[Sum[cm[n] cm[l] p2nm[2 n + 1, 2 l + 1] e^(-i (En[2 l+1]-En[2 n+1]) t/ℏ), {l, 0, MM}], {n, 0, NN}]
```

$$\text{p2av}\phi[t\_,\ NN\_,\ MM\_] := \sum_{n=0}^{NN} \sum_{l=0}^{MM} \text{cm}[n]\, \text{cm}[l]\, \text{p2nm}[2 n + 1, 2 l + 1]\, e^{-i\, (\text{En}[2 l+1]-\text{En}[2 n+1])\, t/\hbar}$$

```
Plot[p2avϕ[t, 6, 6] /. {L → 1, m → 1, ℏ → 1}, {t, 0, 6}]
```



Compare with the exact formula for $< p^2 > (0)$:

$$\int_0^L \phi[x, 0]\, \left(-\hbar^2\right) \partial_{xx} \phi[x, 0]\, dx$$

$$\frac{10\, \hbar^2}{L^2}$$