restart

(a) Let's assume we know the function phi0(x), which we can get from the QHO worksheet:

```
ϕ0 := x→sqrt((sqrt(Pi) * beta))/Pi^(1/4) * exp(-beta^2 * x^2/(2));
```

$$x \to \frac{\sqrt{\sqrt{\pi}\,\beta}\, e^{-\frac{1}{2}\beta^2 x^2}}{\pi^{1/4}} \tag{1}$$

According to the differential equation, the form of phi1(x) can be obtained iteratively as

$$\phi 1 := x \to \frac{1}{\sqrt{2}} \cdot \left(\text{beta} \cdot x \cdot \phi 0(x) - \frac{1}{\text{beta}} \cdot \frac{d}{dx} \phi 0(x) \right)$$

$$x \to \frac{\beta\, x\, \phi 0(x) - \frac{\frac{d}{dx}\phi 0(x)}{\beta}}{\sqrt{2}} \tag{2}$$

This looks like the following function

$\phi 1(x)$

$$\frac{\sqrt{2}\,\beta\, x \sqrt{\sqrt{\pi}\,\beta}\, e^{-\frac{1}{2}\beta^2 x^2}}{\pi^{1/4}} \tag{3}$$

which seems ugly, but we can work with it! Similarly, we can define the n=2,3, and 4 functions as follows:

$$\phi 2 := x \to \frac{1}{\sqrt{2 \cdot 2}} \cdot \left(\text{beta} \cdot x \cdot \phi 1(x) - \frac{1}{\text{beta}} \cdot \frac{d}{dx} \phi 1(x) \right)$$

$$x \to \frac{\beta\, x\, \phi 1(x) - \frac{\frac{d}{dx}\phi 1(x)}{\beta}}{\sqrt{4}} \tag{4}$$

$$\phi 3 := x \to \frac{1}{\sqrt{2 \cdot 3}} \cdot \left(\text{beta} \cdot x \cdot \phi 2(x) - \frac{1}{\text{beta}} \cdot \frac{d}{dx} \phi 2(x) \right)$$

$$x \to \frac{\beta\, x\, \phi 2(x) - \frac{\frac{d}{dx}\phi 2(x)}{\beta}}{\sqrt{6}} \tag{5}$$

$$\phi 4 := x \rightarrow \frac{1}{\sqrt{2 \cdot 4}} \cdot \left(\mathrm{beta} \cdot x \cdot \phi 3(x) - \frac{1}{\mathrm{beta}} \cdot \frac{d}{dx} \phi 3(x) \right)$$

$$x \rightarrow \frac{\beta\, x\, \phi 3(x) - \frac{\frac{d}{dx} \phi 3(x)}{\beta}}{\sqrt{8}} \tag{6}$$

(b) Let's test them for normalization and orthogonality. First, we'll define our constants to be positive:

```
> assume(beta > 0)
```

$$\int_{-infinity}^{infinity} \phi 0(x)^2 \, dx$$

$$\sqrt{\pi} \tag{7}$$

$$\int_{-infinity}^{infinity} \phi 1(x)^2 \, dx$$

$$\sqrt{\pi} \tag{8}$$

$$\int_{-infinity}^{infinity} \phi 2(x)^2 \, dx$$

$$\sqrt{\pi} \tag{9}$$

$$\int_{-infinity}^{infinity} \phi 4(x)^2 \, dx$$

$$\sqrt{\pi} \tag{10}$$

Oops. Something is obviously a bit off, since we should expect this to be 1. However, that's nothing we can't overcome, since we can renormalize the wavefunction by dividing it by $\sqrt{\sqrt{\mathrm{pi}}}$.

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$$\sqrt{\sqrt{\mathrm{pi}}}\,.$$

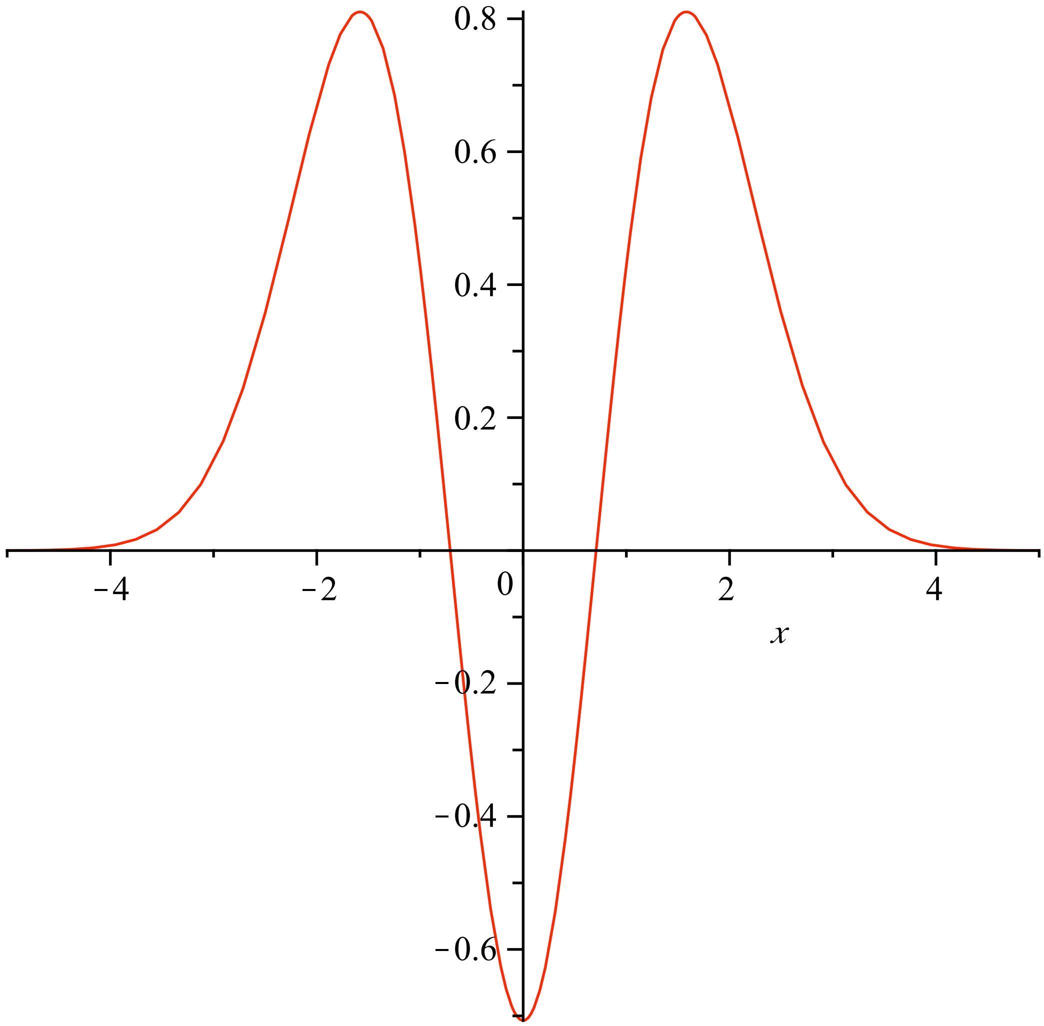
(b) Let's assume beta = 1:

$$\mathrm{beta} := 1$$

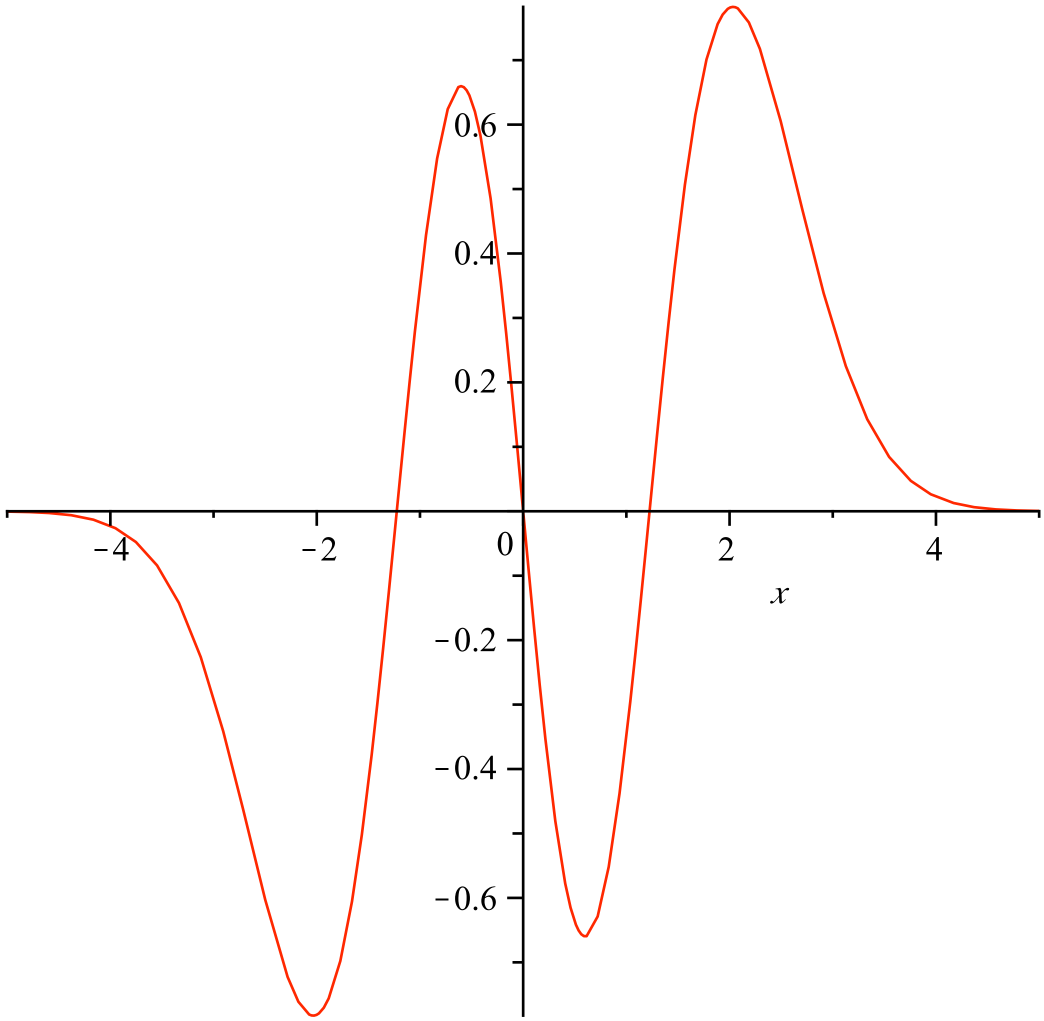
$$1 \tag{11}$$

We can now plot these as follows:

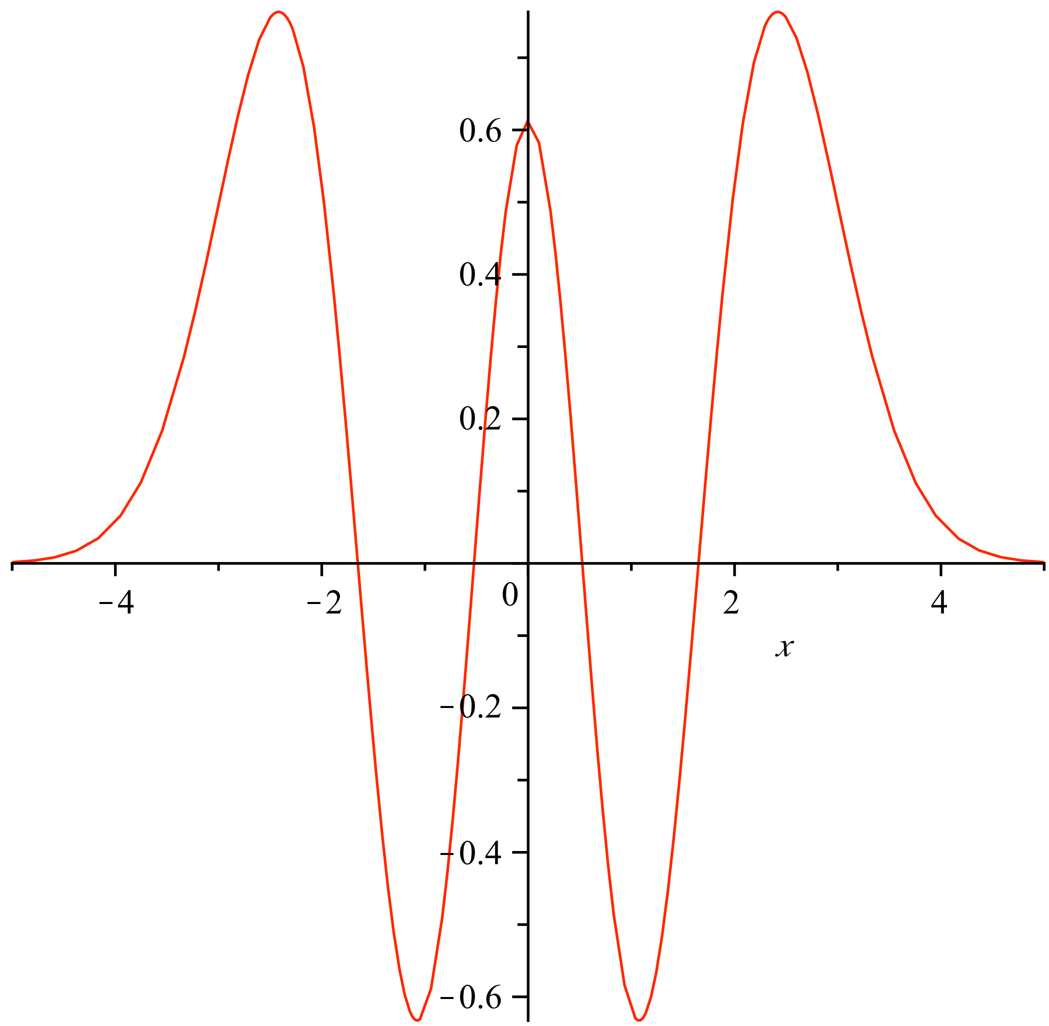
$$plot(\phi 2(x), x=-5..5)$$



plot($\phi 3(x)$, x=-5 ..5)



$plot(\phi 4(x), x=-5..5)$



which is what we would find with the pre-defined versions (in terms of the Hermite polynomials).

2 (a) We need to use the functions from question 1, so let's continue on the same worksheet. The wavefunction in question is a superposition of phi0 and phi4. These states will have energies

$$E := n \rightarrow \left(n + \frac{1}{2}\right) \cdot hbar \cdot \text{omega}$$

$$n \rightarrow \left(n + \frac{1}{2}\right) hbar\, \omega \quad \textbf{(12)}$$

where we will set n=0 and n=4, respectively. The time-dependent wavefunction is then

$$\text{qho} := (x, t) \rightarrow \frac{1}{\sqrt{2}} \cdot \left(\phi 0(x) \cdot \exp\left(-\frac{I \cdot E(0) \cdot t}{hbar}\right) + \phi 4(x) \cdot \exp\left(-\frac{I \cdot E(4) \cdot t}{hbar}\right)\right)$$

$$(x, t) \rightarrow \frac{\phi 0(x)\, \mathrm{e}^{-\frac{\mathrm{I}\, E(0)\, t}{hbar}} + \phi 4(x)\, \mathrm{e}^{-\frac{\mathrm{I}\, E(4)\, t}{hbar}}}{\sqrt{2}} \quad \textbf{(13)}$$

which looks like

$qho(x, t)$

$$\frac{1}{2}\sqrt{2}\left(e^{-\frac{1}{2}x^2} e^{-\frac{1}{2}I t} + \frac{1}{4}\sqrt{2}\left(\frac{1}{6}x\sqrt{6}\left(x\left(\sqrt{2}\,x^2 e^{-\frac{1}{2}x^2} - \frac{1}{2}\sqrt{2}\,e^{-\frac{1}{2}x^2}\right) - \frac{5}{2}\sqrt{2}\,x\,e^{-\frac{1}{2}x^2} + \sqrt{2}\,x^3 e^{-\frac{1}{2}x^2}\right) - \frac{1}{6}\sqrt{6}\left(\frac{13}{2}\sqrt{2}\,x^2 e^{-\frac{1}{2}x^2} - 3\sqrt{2}\,e^{-\frac{1}{2}x^2} + x\left(\frac{5}{2}\sqrt{2}\,x\,e^{-\frac{1}{2}x^2} - \sqrt{2}\,x^3 e^{-\frac{1}{2}x^2}\right) - \sqrt{2}\,x^4 e^{-\frac{1}{2}x^2}\right)\right) e^{-\frac{9}{2}I t}\right) \quad \textbf{(14)}$$

(b) In order to define the probability density, we need to write down the complex conjugate of the wavefunction:

$$qhostar := (x, t) \rightarrow \frac{1}{\sqrt{2}}\cdot\left(\phi0(x)\cdot\exp\left(+\frac{I\cdot E(0)\cdot t}{hbar}\right) + \phi4(x)\cdot\exp\left(+\frac{I\cdot E(4)\cdot t}{hbar}\right)\right)$$

$$(x, t) \rightarrow \frac{\phi0(x)\, e^{\frac{I E(0)\, t}{hbar}} + \phi4(x)\, e^{\frac{I E(4)\, t}{hbar}}}{\sqrt{2}} \quad \textbf{(15)}$$

so we have

$assume(\text{omega} > 0);$
$\text{rho} := (x, t) \rightarrow qho(x, t)\cdot qhostar(x, t)$

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Error, (in assume) cannot assume on a constant object
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$$(x, t) \rightarrow qho(x, t)\; qhostar(x, t) \quad \textbf{(16)}$$

$\text{rho}(x, t)$

$$\frac{1}{2}\left(e^{-\frac{1}{2}x^2} e^{-\frac{1}{2}I t} + \frac{1}{4}\sqrt{2}\left(\frac{1}{6}x\sqrt{6}\left(x\left(\sqrt{2}\,x^2 e^{-\frac{1}{2}x^2} - \frac{1}{2}\sqrt{2}\,e^{-\frac{1}{2}x^2}\right) - \frac{5}{2}\sqrt{2}\,x\,e^{-\frac{1}{2}x^2} + \sqrt{2}\,x^3 e^{-\frac{1}{2}x^2}\right) - \frac{1}{6}\sqrt{6}\left(\frac{13}{2}\sqrt{2}\,x^2 e^{-\frac{1}{2}x^2} - 3\sqrt{2}\,e^{-\frac{1}{2}x^2} + x\left(\frac{5}{2}\sqrt{2}\,x\,e^{-\frac{1}{2}x^2} - \sqrt{2}\,x^3 e^{-\frac{1}{2}x^2}\right) - \sqrt{2}\,x^4 e^{-\frac{1}{2}x^2}\right)\right) e^{-\frac{9}{2}I t}\right)\left(e^{-\frac{1}{2}x^2} e^{\frac{1}{2}I t} + \frac{1}{4}\sqrt{2}\left(\frac{1}{6}x\sqrt{6}\left(x\left(\sqrt{2}\,x^2 e^{-\frac{1}{2}x^2} - \frac{1}{2}\sqrt{2}\,e^{-\frac{1}{2}x^2}\right) - \frac{5}{2}\sqrt{2}\,x\,e^{-\frac{1}{2}x^2} + \sqrt{2}\,x^3 e^{-\frac{1}{2}x^2}\right) - \frac{1}{6}\sqrt{6}\left(\frac{13}{2}\sqrt{2}\,x^2 e^{-\frac{1}{2}x^2} - 3\sqrt{2}\,e^{-\frac{1}{2}x^2} + x\left(\frac{5}{2}\sqrt{2}\,x\,e^{-\frac{1}{2}x^2} - \sqrt{2}\,x^3 e^{-\frac{1}{2}x^2}\right) - \sqrt{2}\,x^4 e^{-\frac{1}{2}x^2}\right)\right) e^{\frac{9}{2}I t}\right) \quad \textbf{(17)}$$

$expand(\%)$

$$\frac{1}{2}\left(e^{-\frac{1}{2}x^2}\right)^2 e^{-\frac{1}{2}It} e^{\frac{1}{2}It} + \frac{1}{6}\left(e^{-\frac{1}{2}x^2}\right)^2 e^{-\frac{1}{2}It} e^{\frac{9}{2}It} x^4\sqrt{6}$$
$$-\frac{1}{2}\left(e^{-\frac{1}{2}x^2}\right)^2 e^{-\frac{1}{2}It} e^{\frac{9}{2}It} x^2\sqrt{6} + \frac{1}{8}\left(e^{-\frac{1}{2}x^2}\right)^2 e^{-\frac{1}{2}It} e^{\frac{9}{2}It}\sqrt{6}$$
$$+\frac{1}{6}e^{-\frac{9}{2}It}x^4\sqrt{6}\left(e^{-\frac{1}{2}x^2}\right)^2 e^{\frac{1}{2}It} + \frac{1}{3}e^{-\frac{9}{2}It}x^8\left(e^{-\frac{1}{2}x^2}\right)^2 e^{\frac{9}{2}It}$$
$$-2\,e^{-\frac{9}{2}It}x^6\left(e^{-\frac{1}{2}x^2}\right)^2 e^{\frac{9}{2}It} + \frac{7}{2}e^{-\frac{9}{2}It}x^4\left(e^{-\frac{1}{2}x^2}\right)^2 e^{\frac{9}{2}It}$$
$$-\frac{1}{2}e^{-\frac{9}{2}It}x^2\sqrt{6}\left(e^{-\frac{1}{2}x^2}\right)^2 e^{\frac{1}{2}It} - \frac{3}{2}e^{-\frac{9}{2}It}x^2\left(e^{-\frac{1}{2}x^2}\right)^2 e^{\frac{9}{2}It}$$
$$+\frac{1}{8}e^{-\frac{9}{2}It}\sqrt{6}\left(e^{-\frac{1}{2}x^2}\right)^2 e^{\frac{1}{2}It} + \frac{3}{16}e^{-\frac{9}{2}It}\left(e^{-\frac{1}{2}x^2}\right)^2 e^{\frac{9}{2}It} \quad \textbf{(18)}$$

simplify(%)

$$\frac{1}{48}e^{-x^2}\left(16\cos(4t)\sqrt{6}\,x^4 - 48\cos(4t)\,x^2\sqrt{6} + 12\cos(4t)\sqrt{6} + 33 - 96x^6 + 168x^4 - 72x^2 + 16x^8\right) \quad \textbf{(19)}$$

The time dependence boils down to a cosine function. So, the probability density varies periodically, as we would expect.

>

(c) We can study the motion of the QHO solution with animate:

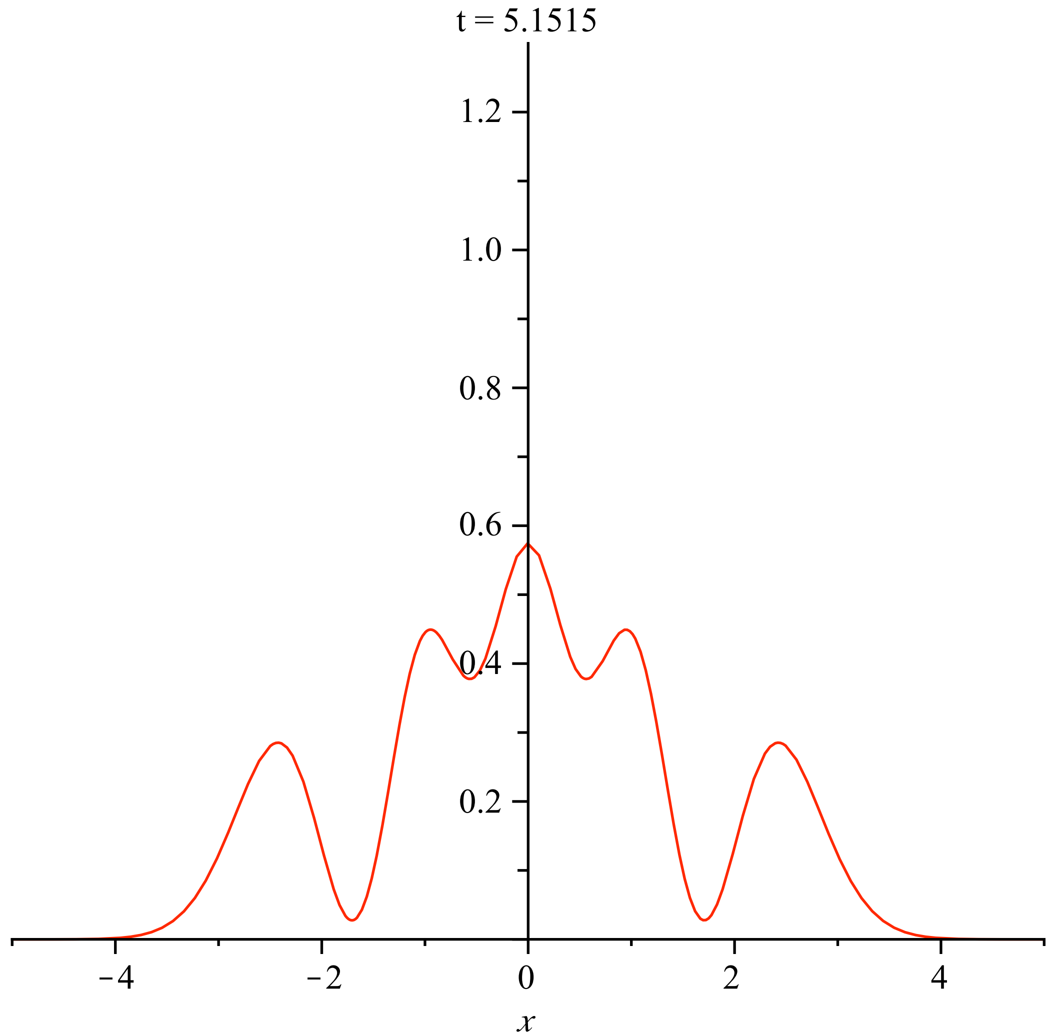
with(*plots*) : omega := 1; *hbar* := 1; *m* := 1;

1

1

1 **(20)**

animate(*plot*, [rho(*x*, *t*), *x*=-5 ..5], *t*=0 ..10, *frames*=100);



The majority of the oscillatory motion is confined to switching between the ground state (at the center) and the n=4 state to either side. The harmonic oscillator resonates between the x=0 position and about x=+/-1.