Simple Harmonic Oscillator

Note that HW problems refer Second Edition Textbook (not First Edition)

Oct. 13, 2016

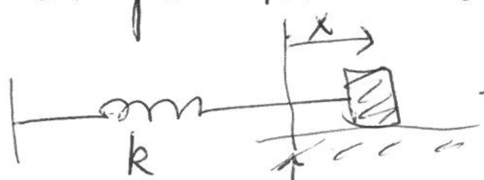
We have discussed both Schrödinger picture and Heisenberg picture as well as their corresponding equations, and concluded that the physical quantities (e.g. expectation values of observables) must be independent of which picture we may use to compute them.

We now apply this idea to (perhaps the best known) dynamical system: simple harmonic oscillator (SHO)

"so many different ways to solve SHO"

e.g.

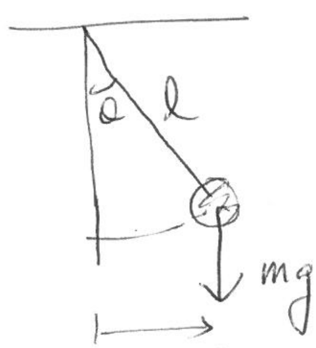
Spring:



equilibrium position

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2 \; ; \quad \omega^2 = \frac{k}{m} \quad (\text{or } k = m\omega^2)$$

Pendulum:



$$\begin{aligned} V &= mgl(1-\cos\theta) \\ &= 2mgl\sin^2\frac{\theta}{2} \\ &\approx \frac{1}{2}mgl\theta^2 = \frac{1}{2}m\underbrace{\left(\frac{g}{l}\right)}_{\omega^2}\underbrace{x^2}_{(l\theta)^2} \end{aligned}$$

$x \approx l\theta$ (for small angle oscillation)

SHO Hamiltonian is given by

$$\boxed{H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}}$$

Recall Schrödinger Equation (See lecture note on Sep. 29, 2016)

$$\boxed{i\hbar \frac{\partial}{\partial t}\psi(\vec{x}',t) = -\frac{\hbar^2}{2m}\vec{\nabla}'^2\psi(\vec{x}',t) + V(\vec{x}')\psi(\vec{x}',t)}$$

Time-Dependent Schrödinger Equation.

Here, $\psi(\vec{x}',t) = \langle \vec{x}' | \alpha, t \rangle$

and $|\alpha, t\rangle = e^{\frac{-iHt}{\hbar}} \underbrace{|\alpha, t=0\rangle}_{\sum_{a'} |a'\rangle\langle a' | \alpha, t=0\rangle}$

$$= \sum_{a'} |a'\rangle\langle a' | \alpha, t=0\rangle \, e^{\frac{-iE_{a'}t}{\hbar}}$$

from $H|a'\rangle = E_{a'}|a'\rangle$.

Base kets in Schrödinger picture are stationary.

Suppose $|\alpha, t=0\rangle = |a'\rangle$, then $|a', t\rangle = |a'\rangle e^{\frac{-iE_{a'}t}{\hbar}}$

$$\boxed{\langle \vec{x}' | a', t\rangle = \langle \vec{x}' | a'\rangle \, e^{\frac{-iE_{a'}t}{\hbar}}}$$

Time dependence of the energy eigenket is "trivial" $\left(e^{\frac{-iE_{a'}t}{\hbar}}\right)$ phase factor.

$$i\hbar \frac{\partial}{\partial t}\langle \vec{x}' | a', t\rangle = i\hbar\left(-\frac{i}{\hbar}E_{a'}\right)\langle \vec{x}' | a', t\rangle = E_{a'}\langle \vec{x}' | a', t\rangle$$

Thus, we get the time-independent (stationary) Schrödinger Equation.

$$-\left(\frac{\hbar^2}{2m}\right)\vec{\nabla}'^2\langle \vec{x}' | a'\rangle + V(\vec{x}')\langle \vec{x}' | a'\rangle = E_{a'}\langle \vec{x}' | a'\rangle$$

For the energy eigenfunction $u_E(\vec{x}')$; $\boxed{\begin{array}{c}\langle \vec{x}' | a'\rangle \rightarrow u_E(\vec{x}') \\ E_{a'} \rightarrow E\end{array}}$

$$\boxed{-\frac{\hbar^2}{2m}\vec{\nabla}'^2 u_E(\vec{x}') + V(\vec{x}')u_E(\vec{x}') = E\, u_E(\vec{x}')}$$

Eq. (2.4.11) p.98

SHO in 1-dim ;

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}u_E(x) + \frac{1}{2}m\omega^2 x^2 u_E(x) = E\,u_E(x)$$

Eq. (2.5.13) p. 105.

That is 2nd order differential equation, and

Solutions are shown in pp. 105–108.

eigenvalue ; $E_n = (n+\frac{1}{2})\hbar\omega$,

eigenfunction ; $u_n(x) = 2^{-n/2}(n!)^{-1/2}\left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \underbrace{H_n\left(\sqrt{\frac{m\omega}{\hbar}}\,x\right)}_{\text{Hermite polynomials.}} e^{-\frac{m\omega}{2\hbar}x^2}$

$$\boxed{\xi \equiv \sqrt{\frac{m\omega}{\hbar}}\,x}$$

$H_0(\xi) = 1$, $H_1(\xi) = 2\xi$

$H_2(\xi) = -2 + 4\xi^2$, etc.

These solutions can be found by solving the 2nd order differential equation satisfying the boundary condition

$$u_E(x) \to 0 \text{ and } \frac{du_E(x)}{dx} \to 0 \quad \text{as } x \to \pm\infty$$

In the textbook, the properties of Hermite polynomials are summarised by using the "generating function" of the Hermite polynomials :

$$\boxed{g(x,t) \equiv e^{-t^2+2tx} = \sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!}}$$

See Eqs. (2.5.14) – (2.5.29)

Here, we solve SHO using entirely just commutation relations

This is so-called operator method or algebraic method in contrast to the usual method of solving differential equation.

Note that

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 = \hbar\omega\left\{\left(\sqrt{\frac{m\omega}{2\hbar}}\,x\right)^2 + \left(\frac{p}{\sqrt{2\hbar m\omega}}\right)^2\right\}$$

If we correspond

$$\sqrt{\frac{m\omega}{2\hbar}}\,x \sim \cos\theta = \frac{e^{i\theta}+e^{-i\theta}}{2}$$

$$\frac{p}{\sqrt{2\hbar m\omega}} \sim \sin\theta = \frac{e^{i\theta}-e^{-i\theta}}{2i}$$

then $H \sim \hbar\omega(\cos^2\theta + \sin^2\theta) \sim \hbar\omega$ (great simplification!).

Let's now correspond seriously $e^{i\theta} \to a$ and $e^{-i\theta} \to a^\dagger$, where a and $a^\dagger$ are ~~now~~ operators (non-Hermitian operators however).

Then, we get

$$\sqrt{\frac{m\omega}{2\hbar}}\,x = \frac{a+a^\dagger}{2} \quad \text{and} \quad \frac{p}{\sqrt{2\hbar m\omega}} = \frac{a-a^\dagger}{2i}$$

or

$$x = \sqrt{\frac{\hbar}{2m\omega}}\,(a+a^\dagger) \quad \text{and} \quad p = i\sqrt{\frac{m\hbar\omega}{2}}\,(-a+a^\dagger)$$

Note that $x^\dagger = x$ and $p^\dagger = p$ although a and $a^\dagger$ are non-Hermitian.

Inverse relations are given by

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{ip}{m\omega}\right) \quad \text{and} \quad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{ip}{m\omega}\right)$$

where $a^\dagger$ and a are known as the creation and annihilation operators respectively.

$$\boxed{[x,p] = i\hbar \longrightarrow [a,a^\dagger] = 1.}$$

$H^\dagger = H$ as it must be. $\boxed{a^\dagger a + a a^\dagger = \frac{2H}{\hbar\omega}}$

$\boxed{\text{or } H = \frac{\hbar\omega}{2}(a^\dagger a + a a^\dagger) = \hbar\omega(a^\dagger a + \tfrac{1}{2})}$

Denote $a^\dagger a = N$, then $H = (N + \frac{1}{2})\hbar\omega$,

where $N^\dagger = N$ (Hermitian).

Algebra of N, a and $a^\dagger$

$$[N, a] = -a \qquad (\because [a^\dagger a, a] = a^\dagger \cancel{[a,a]}^{\,0} + \underbrace{[a^\dagger, a]}_{-1} a)$$

$$[N, a^\dagger] = a^\dagger \qquad (\because [a^\dagger a, a^\dagger] = a^\dagger \underbrace{[a, a^\dagger]}_{1} + \cancel{[a^\dagger, a^\dagger]}^{\,0} a)$$

If we choose the base kets are the kets denoting the number of energy quanta, then we can understand the physical meaning of the Hamiltonian as the energy of the system with a certain number of quanta.

$N = a^\dagger a$ plays the role of Number Operator.

$\boxed{N|n\rangle = n|n\rangle}$ $\{|n\rangle\}$ set of base kets $\{|0\rangle, |1\rangle, |2\rangle, \ldots\}$

Then, $H|n\rangle = (n + \frac{1}{2})\hbar\omega\, |n\rangle$.

This means that the energy eigenvalues are given by

$$E_n = (n + \tfrac{1}{2})\hbar\omega.$$

Let's consider the physical meaning of $a^\dagger$ and a.

From
$$N(a^\dagger|n\rangle) = (\underbrace{[N, a^\dagger]}_{a^\dagger} + a^\dagger N)|n\rangle = (n+1)(a^\dagger|n\rangle),$$

we see that $a^\dagger|n\rangle \sim |n+1\rangle$, i.e. "creation" of a quanta.

Similarly,
$$N(a|n\rangle) = (\underbrace{[N, a]}_{-a} + aN)|n\rangle = (n-1)(a|n\rangle)$$

i.e. $a|n\rangle \sim |n-\rangle$, "annihilation of a quanta".

Thus, it deems appropriate to call $a^\dagger$ and a as creation and annihilation operators, respectively.

To fix the coefficient, let's set
$a|n\rangle = c|n-1\rangle$. Then $\langle n|\underbrace{a^\dagger a}_{N}|n\rangle = |c|^2 = n \geq 0$

or $c = \sqrt{n}$.

So,
$$a|n\rangle = \sqrt{n}\,|n-1\rangle$$
$$a^2|n\rangle = \sqrt{n(n-1)}\,|n-2\rangle$$
$$\vdots$$
$$a^n|n\rangle = \sqrt{n(n-1)(n-2)\cdots 1}\,|0\rangle$$
$$\boxed{a|0\rangle = 0} \leftarrow \text{null ket}$$

Note that, if we start with a noninteger n, then the sequence won't terminate leading to eigenkets with a negative value of n.
As the sequence must terminate with $n=0$, n must be non-negative integer.

Similarly, $a^\dagger|n\rangle = d|n+1\rangle$ and

$$\langle n|aa^\dagger|n\rangle = |d|^2 = \langle n|\underbrace{a^\dagger a}_{N}|n\rangle + 1$$

$$= n+1$$

or $d = \sqrt{n+1}$

So, $a^\dagger|0\rangle = |1\rangle$

$$(a^\dagger)^2|0\rangle = \sqrt{2}\,|2\rangle$$

$$\vdots$$

$$(a^\dagger)^n|0\rangle = \sqrt{\underbrace{n(n-1)(n-2)\cdots 1}_{n!}}\,|n\rangle = \sqrt{n!}\,|n\rangle$$

Position space representation of energy eigenkets

To find $\psi_n(x') = \langle x'|n\rangle$, let's first find $\psi_0(x') = \langle x'|0\rangle$

$$0 = \langle x'|a|0\rangle = \sqrt{\frac{m\omega}{2\hbar}}\langle x'|\,x + \frac{ip}{m\omega}\,|0\rangle$$

$$= \sqrt{\frac{m\omega}{2\hbar}}\underbrace{\langle x'|x|0\rangle}_{x'\langle x'|0\rangle = x'\psi_0(x')} + i\sqrt{\frac{1}{2m\omega\hbar}}\underbrace{\langle x'|p|0\rangle}_{\frac{\hbar}{i}\frac{d}{dx'}\langle x'|0\rangle = \frac{\hbar}{i}\frac{d}{dx'}\psi_0(x')}$$

Thus, we find the following equation that $\psi_0(x')$ must satisfy,

$$\sqrt{\frac{m\omega}{2\hbar}}\,x'\psi_0(x') + i\sqrt{\frac{1}{2m\omega\hbar}}\,\frac{\hbar}{i}\frac{d}{dx'}\psi_0(x') = 0$$

or $\left(x' + \frac{\hbar}{m\omega}\frac{d}{dx'}\right)\psi_0(x') = 0.$

Define $x_0^2 \equiv \frac{\hbar}{m\omega}$ or $x_0 = \sqrt{\frac{\hbar}{m\omega}}$

which provides the length scale of the oscillator.

$$\boxed{\left(x' + x_0^2 \frac{d}{dx'}\right) \psi_0(x') = 0}$$

Solution; $\psi_0(x') = \frac{1}{\pi^{1/4}\sqrt{x_0}} e^{-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2}$

$E_0 = \frac{1}{2}\hbar\omega$; See Appendix B.4 p.527

Eq. (2.3.30) p.92.

How about excited states?

$$\begin{aligned}
\psi_1(x') &= \langle x' | 1 \rangle \\
&= \langle x' | a^\dagger | 0 \rangle \\
&= \sqrt{\frac{m\omega}{2\hbar}} \langle x' | X - \frac{iP}{m\omega} | 0 \rangle \\
&= \sqrt{\frac{m\omega}{2\hbar}} x' \langle x' | 0 \rangle - \sqrt{\frac{m\omega}{2\hbar}} \frac{i}{m\omega} \frac{\hbar}{i} \frac{d}{dx'} \langle x' | 0 \rangle \\
&= \frac{1}{\sqrt{2}\, x_0} \left(x' - x_0^2 \frac{d}{dx'}\right) \psi_0(x') \\
&= \frac{\sqrt{2}}{\pi^{1/4}\sqrt{x_0}} \left(\frac{x'}{x_0}\right) e^{-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2} \quad \text{with } E_1 = \frac{3}{2}\hbar\omega,
\end{aligned}$$

etc.

In general,

$$\varphi_n(x') = \langle x'|n\rangle = \langle x'| \frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle$$

$$= \frac{1}{\sqrt{n!}} \left(\frac{1}{\sqrt{2}\,x_0}\right)^n \left(x' - x_0^2 \frac{d}{dx'}\right)^n \varphi_0(x')$$

$$= \frac{1}{\pi^{1/4}\sqrt{x_0}} \frac{1}{\sqrt{2^n n!}} H_n\!\left(\frac{x'}{x_0}\right) e^{-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2}$$

Hermite polynomial

with

$$E_n = \left(n + \tfrac{1}{2}\right)\hbar\omega.$$

This is exactly the same solution obtained by solving the second order differential equation with the boundary condition,

Heisenberg base kets are time-dependent

$$|n,t\rangle_H = \mathcal{U}^\dagger(t)\,|n\rangle \quad \left(i\hbar\frac{\partial}{\partial t}|n,t\rangle_H = -H\,|n,t\rangle_H\right)$$

$$= e^{\frac{iHt}{\hbar}}|n\rangle = e^{\frac{iE_nt}{\hbar}}|n\rangle \qquad i\hbar\frac{\partial}{\partial t}\left(e^{\frac{iHt}{\hbar}}\right)$$

Let's compute operators as outerproducts of bras & kets in Heisenberg picture.

$$a|n\rangle = \sqrt{n}\,|n-1\rangle$$

$$a|n\rangle\langle n| = \sqrt{n}\,|n-1\rangle\langle n|$$

$$a = \sum_n \sqrt{n}\,|n-1\rangle\langle n| \quad \text{as} \quad \sum_n |n\rangle\langle n| = I,$$

closure.

Thus,

$$a(t) = \sum_n \sqrt{n}\,\underbrace{|n-1,t\rangle_H}_{e^{\frac{iE_{n-1}t}{\hbar}}|n-1\rangle}\ \underbrace{{}_H\langle n,t|}_{e^{-\frac{iE_nt}{\hbar}}\langle n|}$$

$$= \sum_n e^{\frac{i(E_{n-1}-E_n)t}{\hbar}}\sqrt{n}\,|n-1\rangle\langle n| \qquad E_{n-1}-E_n = (n-\tfrac{1}{2})\hbar\omega - (n+\tfrac{1}{2})\hbar\omega = -\hbar\omega$$

$$= e^{-i\omega t}\underbrace{\sum_n \sqrt{n}\,|n-1\rangle\langle n|}_{a(0)}$$

Similarly, $a^\dagger(t) = e^{+i\omega t}a^\dagger(0)$

Therefore, we find

$$X(t) = \sqrt{\frac{\hbar}{2m\omega}}\left(a(t)+a^\dagger(t)\right)$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left[\underset{\substack{\uparrow \\ \cos\omega t - i\sin\omega t}}{e^{-i\omega t}}a(0) + \underset{\substack{\uparrow \\ \cos\omega t + i\sin\omega t}}{e^{i\omega t}}a^\dagger(0)\right]$$

$$= \cos\omega t\,\sqrt{\frac{\hbar}{2m\omega}}\left(a(0)+a^\dagger(0)\right) + \sin\omega t\; i\sqrt{\frac{\hbar}{2m\omega}}\left(-a(0)+a^\dagger(0)\right)$$

$$= \cos\omega t\,\boxed{X(0)} + \sin\omega t\,\boxed{\frac{P(0)}{m\omega}}.$$

$$p(t) = i\sqrt{\frac{m\hbar\omega}{2}}\left(-a(t) + a^{\dagger}(t)\right)$$

$$= i\sqrt{\frac{m\hbar\omega}{2}}\left(-\underset{\substack{\uparrow \\ \cos\omega t - i\sin\omega t}}{e^{-i\omega t}}\, a(0) + \underset{\substack{\uparrow \\ \cos\omega t + i\sin\omega t}}{e^{i\omega t}}\, a^{\dagger}(0)\right)$$

$$= -m\omega \underbrace{\boxed{\sqrt{\frac{\hbar}{2m\omega}}\left(a(0) + a^{\dagger}(0)\right)}}_{\times \sin\omega t} + \underbrace{\boxed{i\sqrt{\frac{m\hbar\omega}{2}}\left(-a(0) + a^{\dagger}(0)\right)}}_{\times \cos\omega t}$$

$$= -m\omega X(0)\sin\omega t + p(0)\cos\omega t$$

In summary,

$$X(t) = X(0)\cos\omega t + \frac{p(0)}{m\omega}\sin\omega t$$

$$p(t) = -m\omega X(0)\sin\omega t + p(0)\cos\omega t.$$

This can be also found by using Baker–Hausdorff Lemma.

$$X(t) = e^{\frac{iHt}{\hbar}} X(0)\, e^{-\frac{iHt}{\hbar}}$$

$$= X(0) + \frac{it}{\hbar}\underbrace{[H, X(0)]}_{-i\hbar\frac{p(0)}{m}} + \frac{1}{2!}\left(\frac{it}{\hbar}\right)^2 \underbrace{[H, \overbrace{[H, X(0)]}^{-i\hbar\frac{p(0)}{m}}]}_{\substack{-\frac{i\hbar}{m}[H,\, p(0)] \\ \shortparallel \\ -\frac{i\hbar}{m}(i\hbar m\omega^2 X(0))}} + \cdots$$

$$= X(0)\left(1 - \frac{\omega^2 t^2}{2!} + \cdots\right) + \frac{p(0)}{m\omega}\left(\omega t - \frac{\omega^3 t^3}{3!} + \cdots\right)$$

$$= X(0)\cos\omega t + \frac{p(0)}{m\omega}\sin\omega t.$$

$x(t)$ and $p(t)$ also satisfy Heisenberg Eqs.

$$\frac{dp(t)}{dt} = \frac{1}{i\hbar}\left[p(t), H\right]$$

$$= \frac{1}{i\hbar}\left[p(t), \frac{m\omega^2 x^2(t)}{2}\right]$$

$$= \frac{1}{i\hbar}\frac{m\omega^2}{2}\underbrace{\left[p(t), x^2(t)\right]}_{\frac{\hbar}{i}\frac{\partial}{\partial x}(x^2) = \frac{\hbar}{i}2x}$$

$$[p, x^2] = px^2 - x^2 p$$
$$= px^2 - xpx + xpx - x^2 p$$
$$= [p, x]x + x[p, x]$$
$$= -2i\hbar x$$

$$= -m\omega^2 x(t)$$

(Hooke's law)

$$\frac{dx(t)}{dt} = \frac{1}{i\hbar}\left[x(t), H\right]$$

$$= \frac{1}{i\hbar}\underbrace{\left[x(t), \frac{p^2(t)}{2m}\right]}_{i\hbar\frac{\partial}{\partial p}\left(\frac{p^2}{2m}\right)}$$

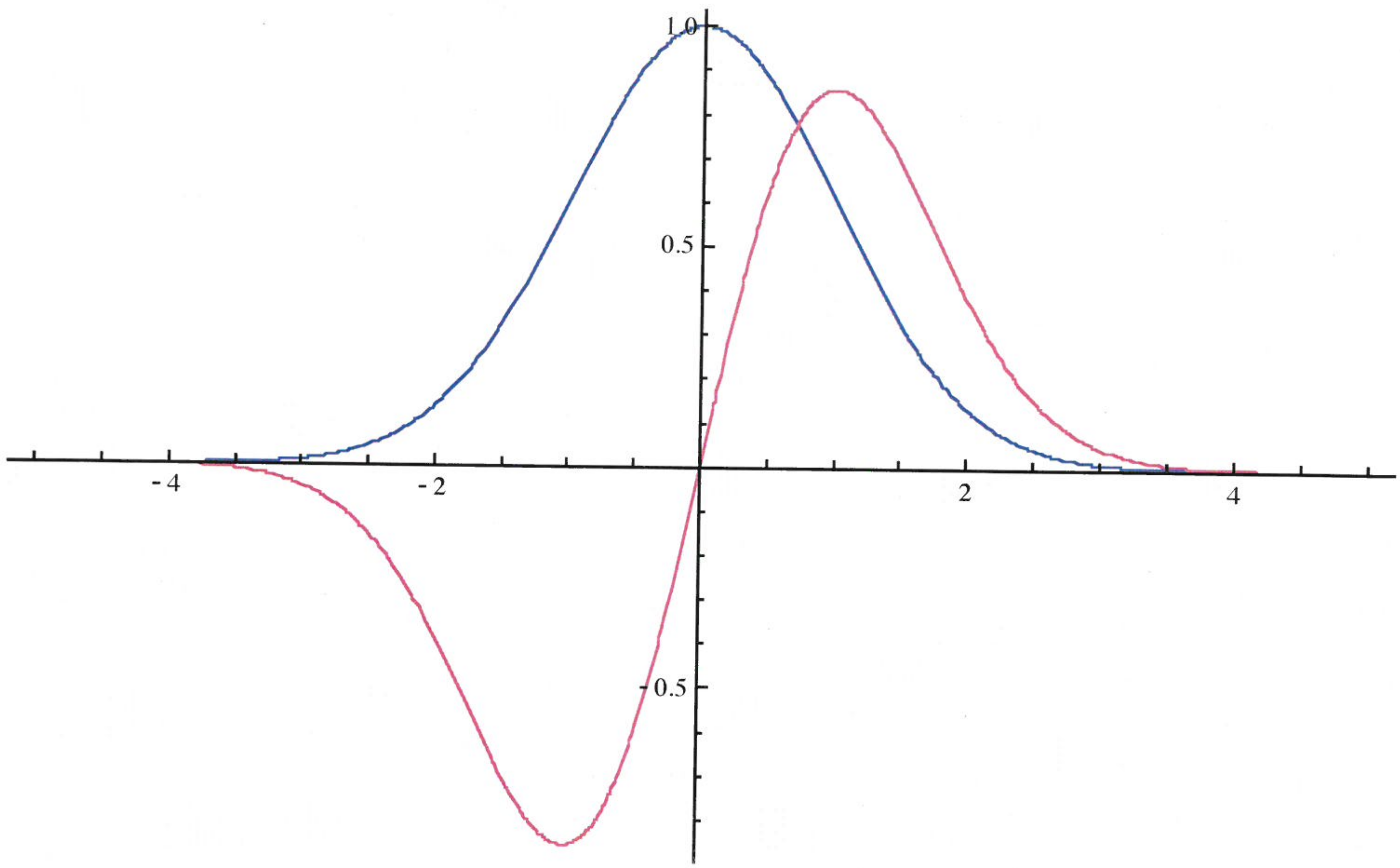
$$= \frac{p(t)}{m}.$$

In summary, $\dfrac{dp(t)}{dt} = -m\omega^2 x(t)$, $\dfrac{dx(t)}{dt} = \dfrac{p(t)}{m}$.

Decoupling $x(t)$ by raising the order of differentiation, we get

$$\frac{d^2 x(t)}{dt^2} = \frac{1}{m}\frac{dp(t)}{dt} = -\omega^2 x(t) \quad \text{or} \quad \frac{d^2 x(t)}{dt^2} + \omega^2 x(t) = 0.$$

Ehrenfest theorem works, i.e. Classical Correspondence: $\dfrac{d^2\langle x(t)\rangle}{dt^2} + \omega^2\langle x(t)\rangle = 0$



1.0
0.5
-0.5
-4
-2
2
4