

The Simple Harmonic Oscillator

The deterministic simple harmonic oscillator is governed by the equation

$$\ddot{x} + \gamma \dot{x} + \omega^2 x = f(t)$$

or equivalently

$$\begin{aligned} \frac{dv}{dt} &= -\omega^2 x - \gamma v + f(t) \\ &= -\omega^2 x - \gamma v + f(t) \end{aligned}$$

$$\Rightarrow dv = -\omega^2 x dt - \gamma v dt + f(t) dt$$

and

$$\begin{aligned} \frac{dx}{dt} &= v \\ \Rightarrow dx &= v dt \end{aligned}$$

Assuming that the forcing is being caused by the surrounding molecules and the damping is also due to the surrounding molecules; we can model

the stochastic forcing due to surrounding molecules by

$$f(t) dt = \sqrt{\beta^2 dt} N_t^{++dt} (0,1)$$

and thus,

$$dV = -\omega^2 x - \gamma V + \sqrt{\beta^2 dt} N_t^{++dt} (0,1)$$

and $dx = V dt$.

Clearly as in earlier cases; assuming that

$x(0)$ and $v(0)$ are deterministic we

have that

$$V(dt) = -\omega^2 x(0) - \gamma V(0) + \sqrt{\beta^2 dt} N_0^{++dt} (0,1) + v(0) \in \text{Span} \{ N_0^{++dt} (0,1) \}$$

$$x(dt) = V(0) dt + x(0) \in$$

$$V(2dt) = -\omega^2 x(dt) - \gamma V(dt) + \sqrt{\beta^2 dt} N_{dt}^{++2dt} (0,1) + v(dt)$$

Normality

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$$\therefore V(2dt) \in \text{Span} \left\{ N_0^{dt} (0,1), N_{dt}^{2dt} (0,1) \right\}$$

$$\text{||} \text{y, } X(2dt) \in \text{Span} \left\{ N_0^{dt} (0,1) \right\}.$$

and in general

$$V(ndt) \in \text{Span} \left\{ N_0^{dt} (0,1), \dots, N_{(n-1)dt}^{dt} (0,1) \right\}$$

$$X(ndt) \in \text{Span} \left\{ N_0^{dt} (0,1), \dots, N_{(n-2)dt}^{(n-1)dt} (0,1) \right\}$$

Letting $ndt = t$

$$\Rightarrow V(t) \in \text{Span} \left\{ N_0^{dt} (0,1), \dots, N_{t-dt}^{+} (0,1) \right\}$$

$$X(t) \in \text{Span} \left\{ N_0^{dt} (0,1), \dots, N_{t-2dt}^{+dt} (0,1) \right\}.$$

Thus, both $V(t)$ and $X(t)$ are linear combinations of the same set of independent normals and therefore jointly Gaussian. Therefore their joint pdf is completely determined by

Jointly Gaussianity of X and V

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$$\langle x(t) \rangle; \quad \langle v(t) \rangle; \quad \langle x^2(t) \rangle; \quad \langle v^2(t) \rangle$$

and $\omega_{\{x(t), v(t)\}}$.

We will determine these now.

Mean of X and V

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Note that

$$v(t+dt) - v(t) = -\omega^2 x(t) - \gamma v(t) dt + \sqrt{\beta^2 dt} N(t)$$

$$\Rightarrow \langle v(t+dt) \rangle - \langle v(t) \rangle = -\omega^2 \langle x(t) \rangle - \gamma \langle v(t) \rangle dt$$

and $\langle x(t+dt) \rangle - \langle x(t) \rangle = \langle v(t) \rangle dt$

$$\Rightarrow \lim_{dt \rightarrow 0} \frac{\langle v(t+dt) \rangle - \langle v(t) \rangle}{dt} = [-\omega^2 \quad -\gamma] \begin{bmatrix} \langle x(t) \rangle \\ \langle v(t) \rangle \end{bmatrix}$$

$$\Rightarrow \frac{d\langle v(t) \rangle}{dt} = [-\omega^2 \quad -\gamma] \begin{bmatrix} \langle x(t) \rangle \\ \langle v(t) \rangle \end{bmatrix}$$

$$\frac{d\langle x(t) \rangle}{dt} = [0 \quad 1] \begin{bmatrix} \langle x(t) \rangle \\ \langle v(t) \rangle \end{bmatrix}$$

$$\Rightarrow \begin{bmatrix} \frac{d\langle x(t) \rangle}{dt} \\ \frac{d\langle v(t) \rangle}{dt} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -\omega^2 & -\gamma \end{bmatrix} \begin{bmatrix} \langle x(t) \rangle \\ \langle v(t) \rangle \end{bmatrix}$$

with initial conditions

$$\langle x(0) \rangle = X_0 \text{ and}$$

$$\langle v(0) \rangle = V_0.$$

Mean of X and V

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Letting $A = \begin{bmatrix} 0 & 1 \\ -\omega^2 & \gamma \end{bmatrix}$

and letting $\delta = \begin{bmatrix} \langle x(b) \rangle \\ \langle v(b) \rangle \end{bmatrix}$

we have

$$\frac{d\delta}{dt} = A\delta \quad \text{with} \quad \delta(0) = \begin{bmatrix} \langle x(0) \rangle \\ \langle v(0) \rangle \end{bmatrix}$$

and this has a solution

$$\delta(t) = e^{At} \delta(0)$$

where

$$\begin{aligned} e^{At} &:= \left(\mathbf{I} + At + \frac{A^2 t^2}{2!} + \dots \right) \\ &= \sum_{n=0}^{\infty} \frac{(At)^n}{n!} \end{aligned}$$

Mean of X and V

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One can solve for e^{At} in closed form

to obtain

$$\langle X(t) \rangle = e^{-\gamma t/2} \left[x_0 \cos(\omega' t) + \left(\gamma_0 + \frac{\gamma x_0}{2} \right) \frac{\sin \omega' t}{\omega'} \right]$$

(9.1.9)

and

$$\langle V(t) \rangle = e^{-\gamma t/2} \left[v_0 \cos \omega' t - \left(x_0 \omega^2 + \frac{\gamma v_0}{2} \right) \frac{\sin \omega' t}{\omega'} \right]$$

(9.1.10)

where $\omega' = \sqrt{\omega^2 - \gamma^2/4}$; $X(0) = x_0$

$V(0) = v_0$.

Variance of V

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Note that

$$dV = -\omega^2 x dt - rV dt + \sqrt{\beta^2 dt} N_+^{++dt} (0,1)$$

and therefore

$$dV^2 = V^2(t+dt) - V^2(t)$$

$$\begin{aligned} &= (V+dV)^2 - V^2 = V^2 + 2VdV + (dV)^2 - V^2 \\ &= 2VdV + (dV)^2 \end{aligned}$$

$$\therefore d\langle V^2 \rangle = \langle dV^2 \rangle = 2\langle VdV \rangle + \langle (dV)^2 \rangle$$

$$= 2\langle -\omega^2 xV dt - rV^2 dt + \sqrt{\beta^2 dt} V N_+^{++dt} (0,1) \rangle$$

$$+ \langle (-\omega^2 x)^2 dt^2 + (rV dt)^2 + (\sqrt{\beta^2 dt} N_+^{++dt} (0,1))^2 \rangle$$

$$+ 2\langle (-\omega^2 x)(-rV) \rangle dt^2$$

$$+ 2\langle -\omega^2 x \sqrt{\beta^2 dt} N_+^{++dt} (0,1) \rangle dt$$

$$+ 2\langle -rV \sqrt{\beta^2 dt} N_+^{++dt} (0,1) \rangle dt$$

$$= -2\omega^2 \langle xV \rangle dt - 2r \langle V^2 \rangle dt + 0$$

$$+ \langle -\omega^2 x \rangle dt^2 + \langle r^2 V \rangle dt^2 + \beta^2 dt$$

$$- 2\omega^2 r \langle xV \rangle dt^2 + 0 + 0$$

Ode for $\text{var}\{V\}$

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$$\therefore \frac{d\langle V^2 \rangle}{dt} = -2\omega^2 \langle x, y \rangle - 2\gamma \langle V^2 \rangle + \beta^2$$

We already have

$$\frac{d\langle V \rangle^2}{dt} = 2\langle V \rangle \frac{d\langle V \rangle}{dt}$$

$$= 2\langle V \rangle [-\omega^2 \langle x \rangle - \gamma \langle V \rangle]$$

$$= -\omega^2 2\langle V \rangle \langle x \rangle - \gamma \langle V \rangle^2$$

$$\therefore \frac{d\langle V^2 \rangle - \langle V \rangle^2}{dt} = -2\omega^2 \text{Cov}\{x, V\} - 2\gamma \text{Var}\{V\} + \beta^2$$

$$\therefore \frac{d\text{Var}\{V\}}{dt} = -2\omega^2 \text{Cov}\{x, V\} - 2\gamma \text{Var}\{V\} + \beta^2.$$

Now.

Ode for $\text{Var}\{X\}$

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$$\begin{aligned} dx^2 &:= x(t+dt)^2 - x(t)^2 \\ &= (x+dx)^2 - x^2 \\ &= x^2 + (dx)^2 + 2x dx - x^2 \\ &= (dx)^2 + 2x dx \\ &= (v dt)^2 + 2x dx \\ &= v^2 dt^2 + 2x dx. = \ominus v^2 dt^2 + 2x v dt \end{aligned}$$

$$\therefore \langle dx^2 \rangle = \langle v^2 dt^2 \rangle + 2 \langle x v \rangle dt$$

$$\frac{d\langle x^2 \rangle}{dt} = 2 \langle x v \rangle$$

$$\frac{d\langle x \rangle^2}{dt} = 2 \langle x \rangle \frac{d\langle x \rangle}{dt} = 2 \langle x \rangle \langle v \rangle$$

$$\begin{aligned} \therefore \frac{d(\langle x^2 \rangle - \langle x \rangle^2)}{dt} &= 2(\langle x v \rangle - \langle x \rangle \langle v \rangle) \\ &= 2 \text{cov}(x, v). \end{aligned}$$

Ode for Cov{X,V}

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$$\begin{aligned}
 d(xv) &= x(t+dt)v(t+dt) - x(t)v(t) \\
 &= (x+dx)(v+dv) - xv \\
 &= xv + xdv + vdx + dx dv - xv \\
 &= xdv + vdx + dx dv \\
 &= xdv + v^2 dt + v dv dt
 \end{aligned}$$

$$d\langle xv \rangle = \langle dxv \rangle = \langle xdv \rangle + \langle v^2 dt \rangle$$

$$\begin{aligned}
 &+ \langle v dv dt \rangle \\
 &= \langle x(-\omega^2 x dt - r v dt + N_{\uparrow}^{t+dt}(0,1)) \rangle \\
 &+ \langle v^2 \rangle dt + \langle v(-\omega^2 x dt - r v dt + N_{\uparrow}^{t+dt}(0,1)) \rangle
 \end{aligned}$$

$$\begin{aligned}
 &= -\omega^2 \langle x^2 \rangle dt - r \langle x, v \rangle dt + 0 + \langle v^2 \rangle dt \\
 &+ 0(dt^2)
 \end{aligned}$$

$$\begin{aligned}
 \therefore \frac{d\langle xv \rangle}{dt} &= -\omega^2 \langle x^2 \rangle - r \langle x, v \rangle + \langle v^2 \rangle \\
 \frac{d\langle x \rangle \langle v \rangle}{dt} &= \langle x \rangle \frac{d\langle v \rangle}{dt} + \langle v \rangle \frac{d\langle x \rangle}{dt}
 \end{aligned}$$

Solution for second order statistics

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$$= \langle x \rangle (-\omega^2 \langle x \rangle - \gamma \langle y \rangle) + \langle y \rangle \langle y \rangle$$

$$= -\omega^2 \langle x^2 \rangle - \gamma \langle x \rangle \langle y \rangle + \langle y \rangle^2$$

$$\Rightarrow \frac{d}{dt} \text{Cov}\{x, y\} = -\omega^2 \text{Var}\{x\} - \gamma \text{Cov}\{x, y\} + \alpha \text{Var}\{y\}$$

The three differential equations are

$$\frac{d}{dt} \text{Cov}\{x, y\} = -\omega^2 \text{Var}\{x\} - \gamma \text{Cov}\{x, y\} + \alpha \text{Var}\{y\} \quad (*)$$

$$\frac{d}{dt} \text{Var}\{x\} = 2 \text{Cov}\{x, y\} \quad \dots \quad (**)$$

$$\frac{d}{dt} \text{Var}\{y\} = -2\gamma \text{Var}\{y\} - 2\omega^2 \text{Cov}\{x, y\} + \beta^2 \quad (***)$$

From (*), (**) and (***) we obtain

$$\frac{d^3}{dt^3} \text{Var}\{x\} + 3\gamma \frac{d^2}{dt^2} \text{Var}\{x\} + (4\omega^2 + 2\gamma^2) \frac{d}{dt} \text{Var}\{x\} + 4\gamma\omega^2 (\text{Var}\{x\} - \beta^2 / 2\gamma\omega^2) = 0$$

Solution for second order statistics

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Defining $y = \text{Var}\{x\} - \frac{\beta^2}{2r\omega^2}$

$$\frac{d^3 y}{dt^3} + 3r \frac{d^2 y}{dt^2} + (4\omega^2 + 2r^2) \frac{dy}{dt} + 4r\omega^2 y = 0.$$

which can be solved to obtain.

$$\text{Var}\{x\} = \frac{\beta^2}{2r\omega^2} + e^{-rt} \left(\frac{\beta^2}{8r\omega^2\omega'^2} \right) \times$$

$$\left\{ -4\omega^2 + r^2(\omega \cos(2\omega't) - 2r\omega' \sin(2\omega't)) \right\}$$

$$\text{Cov}\{x, y\} = e^{-rt} \left(\frac{\beta^2}{4\omega'^2} \right) [1 - \cos(2\omega't)]$$

$$\text{Var}\{y\} = \frac{\beta^2}{2r} + e^{-rt} \frac{\beta^2}{8r\omega'^2} \left[-4\omega^2 + r^2 \cos(2\omega't) \right]$$

$$+ 2r\omega' \sin(2\omega't)]$$

Thermal Equilibrium

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$$\text{As } \gamma t \rightarrow \infty \quad \text{Var}\{v\} \rightarrow \frac{\beta^2}{2\gamma}$$

$$\text{and } \frac{1}{2} M \text{Var}\{v\} = \frac{1}{2} \frac{kT}{\beta}$$

$$\Rightarrow \boxed{\frac{\beta^2}{2\gamma} = \frac{kT}{\beta M}}$$