

Estudo sobre o papel do ruído em sistemas estocásticos fora do equilíbrio

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Resumo:

A partir das propriedades do ruído de Langevin podemos estudar o comportamento estacionário de vários modelos que representam sistemas fora do equilíbrio termodinâmico. Esta é uma técnica sistemática que pode ser utilizada para modelar sistemas econômicos ou biológicos.

Modelo e Distribuição Estacionária:

$$\dot{x}(t) = v(t),$$

$$M \dot{v}(t) = -k_0 v(t) - \gamma v(t) + \eta(t),$$

onde o ruído de Poisson é descrito por

$$\eta(t) = \sum_i \Phi_i \delta(t - t_i),$$

variando com frequência

$$\lambda(t) = \lambda_0 [1 + A \cos(\omega t)],$$

Os cumulantes do ruído são dados por

$$\langle \eta(t_1) \dots \eta(t_n) \rangle_c = \lambda(t_1) \Phi^n \delta(t_1 - t_2) \dots \delta(t_{n-1} - t_n).$$

Os cumulantes para os produtos das variáveis V e X são

$$\begin{aligned} \langle (x^n v^m) \rangle_c &= \lim_{z \rightarrow 0} z \int_0^\infty dt e^{-zt} \langle x^n(t) v^m(t) \rangle_c \\ &= \lim_{z \rightarrow 0} \lim_{\epsilon \rightarrow 0} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{dq_1}{2\pi} \frac{dq_2}{2\pi} \int_{-\infty}^{\infty} \frac{dp_1}{2\pi} \frac{dp_2}{2\pi} z^{-n} \frac{z}{\sum_{i=1}^n (i q_1 + \epsilon) + \sum_{j=1}^m (i p_1 + \epsilon)} \\ &\quad \times \prod_{k=1}^n \frac{1}{[M R(i q_k + \epsilon)]} \prod_{l=1}^m \frac{(i p_l + \epsilon)}{[M R(i p_l + \epsilon)]} \left\langle \prod_{k=1}^n \tilde{\eta}(i q_k + \epsilon) \prod_{l=1}^m \tilde{\eta}(i p_l + \epsilon) \right\rangle_c \end{aligned}$$

Podemos construir a distribuição de probabilidades estacionária:

$$P_{st}(x, v) = \int_{-\infty}^{\infty} \frac{dQ dP}{2\pi} e^{iQx + iPv} \exp \left\{ \sum_{n+m=0}^{\infty} \frac{(-iQ)^n (-iP)^m}{n! m!} \mathcal{P}_{n,m} \right\}.$$

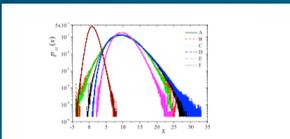


Figure 1. Numerically obtained probability density function $P(x, v)$ vs position x for various cases with $\lambda_0 = 10$, $\phi = 1$ and the noise defined by Eq. (5) with $\omega = 1$. Following the legend in the figure we have the respective cases: A: $M = 1, k_0 = 1, \gamma = 1, A = 0, B = 10, k_0 = 1, \gamma = 1, A = 0, C: M = 10, k_0 = 1, \gamma = 1, A = 1, D: M = 1, k_0 = 1, \gamma = 1, A = 0, E: M = 1, k_0 = 1, \gamma = 2, A = 0$ and F: $M = 1, k_0 = 10, \gamma = 1, A = 0$.

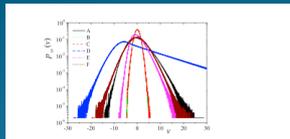


Figure 2. Numerically obtained probability density function $P(x, v)$ vs scalar velocity v for the same parameter sets of Fig. 1.

Injeção de Energia e Balanço Energético

$$\sum W_{F_{ext,t}} = \Delta E_m$$

$$\int \eta dx - \gamma \int v dx = \frac{1}{2} M v(t)^2 + \frac{1}{2} k_0 x(t)^2$$

Forma de v(t) e cumulantes via transformadas de Laplace do ruído

$$v(t)^2 = \int \int v(t_1) v(t_2) \delta(t - t_1) \delta(t - t_2) dt_1 dt_2$$

$$= \lim_{\epsilon \rightarrow 0} \int \int e^{i(q_1 t_1 + q_2 t_2) + \epsilon t} \tilde{v}(i q_1 + \epsilon) \tilde{v}(i q_2 + \epsilon) \frac{dq_1 dq_2}{2\pi 2\pi}$$

$$\langle v(t)^2 \rangle - \langle v(t) \rangle^2 = \lim_{\epsilon \rightarrow 0} \frac{1}{M^2} \int \int e^{i(q_1 t_1 + q_2 t_2) + \epsilon t} (i q_1 + \epsilon) (i q_2 + \epsilon) \times \frac{\tilde{\eta}(i q_1 + \epsilon) \tilde{\eta}(i q_2 + \epsilon)}{R(i q_1 + \epsilon) R(i q_2 + \epsilon)} \frac{dq_1 dq_2}{2\pi 2\pi}$$



Desenvolvimento assintótico de v(t) e x(t)

$$\langle v(t)^2 \rangle_{asy} - \langle v(t) \rangle_{asy}^2 = \frac{\lambda_0 \Phi^2}{\gamma M} + 8 \frac{A^2 (\omega^2 \Phi^2 + \theta \omega_0^4) \cos(\omega t) + \omega^2 \theta^2 \sin(\omega t) \lambda_0 \Phi^2}{M^2 (4\theta^2 + \omega^2) (\omega_0^2 - \omega^2)^2 + 4\theta^2 \omega^2} + 4 \frac{A [2\theta (\omega^4 - 3\omega_0^2 \omega^2) \cos(\omega t) - 3\omega_0^2 \omega^2 \sin(\omega t)] \lambda_0 \Phi^2}{M^2 (4\theta^2 + \omega^2) (\omega_0^2 - \omega^2)^2 + 4\theta^2 \omega^2} + 2 \frac{A (\omega^2 + 8\omega_0^2 \omega) \lambda_0 \Phi^2 \sin(\omega t)}{M^2 (4\theta^2 + \omega^2) (\omega_0^2 - \omega^2)^2 + 4\theta^2 \omega^2},$$

and

$$\langle x(t)^2 \rangle_{asy} - \langle x(t) \rangle_{asy}^2 = \Phi^2 \frac{\lambda_0}{\gamma k_0} + \frac{4\omega (\omega^2 - 4\omega_0^2 - 8\theta^2) A \Phi^2 \lambda_0 \sin(\omega t)}{(\omega^4 - 8\omega_0^2 \omega^2 + 16\theta^2 \omega^2 + 16\omega_0^4) (4\theta^2 + \omega^2) M^2} + \frac{8(3\theta \omega^2 - 2\theta \omega_0^2) A \Phi^2 \lambda_0 \cos(\omega t)}{(\omega^4 - 8\omega_0^2 \omega^2 + 16\theta^2 \omega^2 + 16\omega_0^4) (4\theta^2 + \omega^2) M^2}.$$

$$\langle v(t) \rangle_{asy} = \frac{A [(\omega^2 - \omega_0^2) \sin(\omega t) + 2\omega \theta \cos(\omega t)] \omega \lambda_0 \Phi}{M [(\omega_0^2 - \omega^2)^2 + 4\theta^2 \omega^2]},$$

$$\langle x(t) \rangle_{asy} = \frac{\Phi \lambda_0}{\omega_0^2 M} - \frac{A [(\omega^2 - \omega_0^2) \cos(\omega t) - 2\theta \omega \sin(\omega t)] \lambda_0 \Phi}{M [(\omega_0^2 - \omega^2)^2 + 4\theta^2 \omega^2]},$$

$$\sqrt{\langle x(t)^2 \rangle_{asy}} = \frac{\Phi \lambda_0}{\omega_0^2 M} \sqrt{1 + A^2 \frac{\omega_0^2}{2 [4\theta^2 \omega^2 + (\omega_0^2 - \omega^2)^2]}}$$

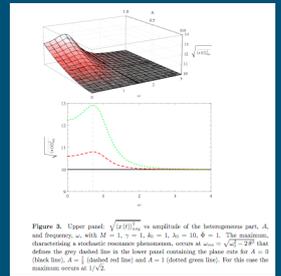


Figure 3. Upper panel: $\sqrt{\langle x(t)^2 \rangle_{asy}}$ vs magnitude of the homogeneous part, A , and frequency, ω , with $M = 1, \gamma = 1, \lambda_0 = 1, k_0 = 10, \phi = 1$. The maximum, denoting a stochastic resonance phenomenon, occurs at $\omega_0 = \sqrt{2} - 2\theta$ that defines the grey dotted line in the lower panel concerning the phase case. In A = 0 (black line), $A = 1$ (dashed red line) and $A = 1$ (dotted green line). For this case the maximum occurs at $\omega = 0$.

Energia no regime assintótico (média temporal)

$$E_{\bar{v}} = \frac{1}{2} M \langle v(t)^2 \rangle_{asy} + \frac{1}{2} k_0 \langle x(t)^2 \rangle_{asy}$$

$$= \lambda_0 \frac{\Phi^2}{\gamma} + \frac{\lambda_0^2 \Phi^2}{2 M \omega_0^2} + \frac{\lambda_0^2 \Phi^2 A^2 (\omega^2 + \omega_0^2)}{4 M [(\omega_0^2 - \omega^2)^2 + 4\theta^2 \omega^2]}.$$

Injeção e Dissipação de Energia:

$$J_{IT} = \int_0^T dt v(t) \eta(t), \quad \text{e} \quad J_{DT} = -\gamma \int_0^T dt v^2(t).$$

$$J_{DT} = -\gamma \int_0^T dt \int_0^\infty dt_1 \delta(t - t_1) \int_0^\infty dt_2 \delta(t - t_2) v(t_1) \eta(t_2),$$

$$= \lim_{\epsilon \rightarrow 0} \int_{-\infty}^{\infty} \frac{dq_1}{2\pi} \int_{-\infty}^{\infty} \frac{dq_2}{2\pi} e^{i(q_1 t_1 + q_2 t_2) + \epsilon t} \tilde{v}(i q_1 + \epsilon) \tilde{v}(i q_2 + \epsilon),$$

$$= \lim_{\epsilon \rightarrow 0} \int_{-\infty}^{\infty} \frac{dq_1}{2\pi} \int_{-\infty}^{\infty} \frac{dq_2}{2\pi} e^{i(q_1 t_1 + q_2 t_2) + \epsilon t} \times \frac{(i q_1 + \epsilon) (i q_2 + \epsilon)}{[M R(i q_1 + \epsilon) M R(i q_2 + \epsilon)]} \tilde{\eta}(i q_1 + \epsilon) \tilde{\eta}(i q_2 + \epsilon),$$

onde

$$R(s) \equiv s^2 + \frac{\gamma}{M} s + \frac{k_0}{M} = (s - \kappa_+) (s - \kappa_-),$$

$$\begin{aligned} J_{DT}(T) &= - \left(\frac{\Phi^2 \lambda_0}{M} + \frac{A^2 \omega^2 \theta^2 \lambda_0^2}{[\omega^2 (\omega^2 - 2\omega_0^2 + 4\theta^2) + \omega_0^2] M} \right) T, \\ &\text{an oscillating term,} \\ J_{DT}(T) &= - \frac{A [2\theta \omega^2 \omega^2 - 4\theta \omega_0^2 - 2\theta \omega^2 - 4\theta^2 \omega^2] \Phi^2 \lambda_0 \sin(\omega T)}{M \omega (4\theta^2 + \omega^2) (\omega^2 - 16\theta^2 \omega^2 + 16\omega_0^2 - 8\omega_0^4)} \\ &\quad - \frac{2 A [2\omega_0^2 (\omega^4 - 4\theta^2 \omega^2 - \omega_0^2 - 4\omega_0^2 \omega^2) \Phi^2 \lambda_0 \cos(\omega T)]}{M \omega (\omega^2 + 4\theta^2) (\omega^2 + 16\omega_0^2 + 16\omega_0^4 - 8\omega_0^2 \omega^2)} \\ &\quad - \frac{A [\omega^2 \sin(2\omega T) + (\omega^2 - \omega_0^2) \cos(2\omega T)] \Phi^2 \lambda_0^2}{M [\omega^2 (\omega^2 - 2\omega_0^2 + 4\theta^2) + \omega_0^2]} \\ &\quad - \frac{A^2 [\omega^2 (\omega^2 + 2\omega_0^2) + \omega_0^2] \Phi^2 \lambda_0^2 \sin(2\omega T)}{2 M [\omega^2 (\omega^2 - 2\omega_0^2 + 4\theta^2) + \omega_0^2]}, \end{aligned}$$

$$\text{and a constant term,}$$

$$J_{DT} = \frac{\Phi^2 \lambda_0}{2 M} + \frac{\Phi^2 \lambda_0}{2 M} \frac{A^2 \lambda_0^2 (\omega^2 - \omega_0^2)}{[\omega^2 (\omega^2 - 2\omega_0^2 + 4\theta^2) + \omega_0^2]} + \frac{A^2 [2\omega^2 (\omega^2 + 2\theta^2) - \omega_0^2] + 8\omega_0^2 (\theta^2 - \omega^2) \Phi^2 \lambda_0^2}{2 M [\omega^2 (\omega^2 - 2\omega_0^2 + 4\theta^2) + \omega_0^2]}$$

where $J_{DT} = J_{DT}(T) + J_{DT}(T) + J_{DT}$.

Then finally, we write the contributions for the injection of energy as

$$J_{IT}(T) = \left(\frac{\lambda_0 \Phi^2}{M} + \frac{A^2 \omega^2 \theta^2 \lambda_0^2 \Phi^2}{[\omega^2 (\omega^2 - 2\omega_0^2 + 4\theta^2) + \omega_0^2]} \right) T,$$

and

$$J_{IT}(T) = \frac{\lambda_0 \Phi^2 A \sin(\omega T)}{M \omega} + \frac{A [A (\omega^2 - \omega_0^2) \cos(2\omega T) + 4\omega_0^2 \cos(\omega T)] \lambda_0^2 \Phi^2}{4 M [\omega^2 (\omega^2 - 2\omega_0^2 + 4\theta^2) + \omega_0^2]} + \frac{A [2\theta \omega (\omega^2 + 4\theta^2) + 4\omega_0^2 \cos(\omega T)] \lambda_0^2 \Phi^2}{4 M [\omega^2 (\omega^2 - 2\omega_0^2 + 4\theta^2) + \omega_0^2]} \quad (47)$$

and

$$J_{IT} = \frac{\lambda_0^2 \Phi^2}{M \omega_0^2} + \frac{A \lambda_0^2 \Phi^2 (\omega^2 - \omega_0^2)}{M [\omega^2 (\omega^2 - 2\omega_0^2 + 4\theta^2) + \omega_0^2]} + \frac{[\omega^2 (\omega^2 - 12\theta^2) + \omega_0^2 (3\omega_0^2 - 5\omega_0^2 \omega^2 + \omega^2 - 4\theta^2)] A^2 \lambda_0^2 \Phi^2}{4 M [\omega^2 (\omega^2 - 2\omega_0^2 + 4\theta^2) + \omega_0^2]} \quad (48)$$

Somando tudo:

$$J_E^{no} = \frac{\Phi^2 \lambda_0 (2 M \omega_0^2 + \lambda_0 \gamma)}{2 \gamma M \omega_0^2} + \frac{(\omega^2 + \omega_0^2) A^2 \Phi^2 \lambda_0^2}{4 M [\omega^2 (\omega^2 - 2\omega_0^2 + 4\theta^2) + \omega_0^2]}$$

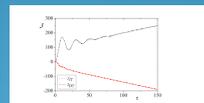


Figure 4. Upper panel: Plot of the injection of energy, J_{IT} , and dissipation of energy, J_{DT} , vs time T . The injection of energy, J_{IT} , is plotted in the upper panel and the dissipation of energy, J_{DT} , is plotted in the lower panel. The inset shows the oscillating component of the injection of energy, J_{IT} , and the dissipation of energy, J_{DT} .

Conclusões:

Temos uma metodologia que permite uma análise detalhada e exata da ação do ruído sobre sistemas pequenos. Este tipo de abordagem pode ser estendido para tratarmos do comportamento térmico de proteínas e moléculas idealizadas.