Fluctuation-Dissipation Theorem

Consider a stationary ensemble characterized by k random variables $\vec{a}(t)$.

Assume the single-time average of $\vec{a}$ vanishes; or define new variables $\vec{a}(t)-\langle\vec{a}(t)\rangle$ ⋯

The variables $\vec{a}(t)$ satisfy a Langevin-like equation

$$\frac{d\vec{a}}{dt}=\hat{H}\vec{a}+\vec{f}$$

$\hat{H}$: a matrix whose eigenvalues have negative real parts (to make the stochastic process bounded).

$\vec{f}(t)$: a white noise so that $\langle\vec{f}(t)\rangle=\vec{0}$ and $\langle\vec{f}(t')\vec{f}(t)\rangle=\gamma\delta(t-t')$, where γ is a positive semi-definite matrix.

Solving the system of ODEs.

First, solve the homogenous part $\frac{d\vec{a}^h}{dt}=\hat{H}\vec{a}^h \Rightarrow \vec{a}^h(t)=\exp(\hat{H}t)\vec{a}(0)$. where $\exp(\hat{H}t)=\sum_{n=0}^{\infty}\frac{(\hat{H}t)^n}{n!}$.

Then, use the method of variation of the constant (ansatz), set $\vec{a}(t)=\exp(\hat{H}t)\vec{g}(t)$ and plug in $\frac{d\vec{a}}{dt}=\hat{H}\vec{a}+\vec{f}$.

Easily we get $\vec{a}(t)=\exp(\hat{H}t)\vec{a}(0)+\int_0^t\exp[\hat{H}(t-\tau)]\vec{f}(\tau)\,d\tau$.

Set $\vec{a}(0)=\vec{a}^0$, then $\langle\vec{a}(t)\rangle^0=\exp(\hat{H}t)\vec{a}^0+\int_0^t\exp[\hat{H}(t-\tau)]\langle\vec{f}(\tau)\rangle\,d\tau=\exp(\hat{H}t)\vec{a}^0$. (1.8.7)

The covariance of the conditional fluctuation, $\delta\vec{a}=\vec{a}(t)-\langle\vec{a}(t)\rangle^0$, is calculated to be

$$\hat{\sigma}(t)\equiv\langle\delta\vec{a}(t)\delta\vec{a}^T(t)\rangle^0=\exp(\hat{H}t)\left(\int_0^t d\tau\int_0^t d\tau'\exp(-\hat{H}\tau)\langle\vec{f}(\tau)\vec{f}(\tau')\rangle\exp(-\hat{H}^T\tau')\right)\exp(\hat{H}^Tt)$$

$$=\exp(\hat{H}t)\left(\int_0^t d\tau\exp(-\hat{H}\tau)\gamma\exp(-\hat{H}^T\tau)\right)\exp(\hat{H}^Tt) \quad (1.8.8)$$

Easily we get $\frac{d\hat{\sigma}(t)}{dt}=\hat{H}\hat{\sigma}(t)+\hat{\sigma}(t)\hat{H}^T+\hat{\gamma}$. with $\hat{\sigma}(0)\equiv\hat{0}$.

Changing variables to $s=t-\tau$, $\hat{\sigma}(t)=\int_0^t\exp(\hat{H}s)\gamma\exp(\hat{H}^Ts)\,ds$. (1.8.10)

$\hat{\sigma}\equiv\lim_{t\to\infty}\hat{\sigma}(t)=\int_0^\infty\exp(\hat{H}s)\gamma\exp(\hat{H}^Ts)\,ds$ (1.8.11) exists because the eigenvalues of $\hat{H}$ have negative real parts.

(1.8.11) − (1.8.10), $\tau=s-t \Rightarrow \hat{\sigma}(t)=\hat{\sigma}-\exp(\hat{H}t)\,\hat{\sigma}\exp(\hat{H}^Tt)$ (1.8.12)

We assume that $\vec{a}(t)$ is a stationary Gaussian process, then (1.8.7) and (1.8.8) are enough to determine the conditional probability density.

$$P_2(\vec{a},t\,|\,\vec{a}^0)=\frac{1}{\sqrt{(2\pi)^k\det\hat{\sigma}(t)}}\exp\left[-\frac{1}{2}(\vec{a}-\exp(\hat{H}t)\vec{a}^0)^T\hat{\sigma}^{-1}(t)(\vec{a}-\exp(\hat{H}t)\vec{a}^0)\right]$$

$$W_1(\vec{a})=\frac{1}{\sqrt{(2\pi)^k\det\hat{\sigma}(t)}}\exp\left[-\frac{1}{2}\vec{a}^T\hat{\sigma}^{-1}\vec{a}\right] \quad (1.8.5)$$

$\lim_{t\to\infty}P_2(\vec{a},t\,|\,\vec{a}^0)=W_1(\vec{a})$, becomes independent of $\vec{a}^0$.

(1.8.5) and (1.8.12) implies that $\lim_{t\to\infty}\sigma(t)=\sigma=\langle\vec{a}(0)\vec{a}^T(0)\rangle$, and $\frac{d\hat{\sigma}}{dt}=\hat{0}$.

Therefore, $\hat{H}\hat{\sigma}+\hat{\sigma}\hat{H}^T=-\gamma$. Fluctuation-dissipation theorem.