Fick's law, equilibrium distribution and inhomogeneous space

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One of the theories

Langevin dynamics $\partial_t x = -\Gamma(x)\frac{\partial \mathcal{H}}{\partial x} + g(x)\eta(t),$ + extra term

Fokker-Planck dynamics $\partial_t P(x,t) = \frac{\partial}{\partial x} D(x)\left(\beta \frac{\partial \mathcal{H}}{\partial x} + \frac{\partial}{\partial x}\right) P(x,t),$

Extra term is $(1-\alpha)g(x)g'(x)$, Distribution is $P(x,t) \sim e^{-\mathcal{H}/(k_B T)}$

Corresponding Fick's law $J(x,t) = -D(x)\partial_x P(x,t).$

Lau and Lubensky, PHYSICAL REVIEW E 76, 011123 (2007)

Kramers-Moyal expansion

General dynamics $$\frac{\partial P(x,t)}{\partial t} = \sum_{n=1}^{\infty} \left(-\frac{\partial}{\partial x}\right)^n D^{(n)}(x,t)P(x,t),$$

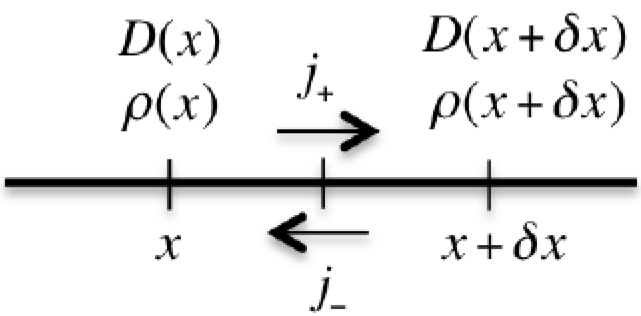
Where $$D^{(n)}(x,t) = \frac{1}{n!}\lim_{\tau\to\infty}\frac{1}{\tau} < [\xi(t+\tau)-x]^n >$$

- According to Pawula's theorem, when transition probability is positive definite, the dynamics can have either one term or two terms or infinitely many terms on the r.h.s.
- General Fokker-Planck equation obtained from this dynamics contains The first two terms.
- Fick's law turns out to be $j(x) = -\frac{\partial D(x)P(x)}{\partial x}$

Fick's law from first principle

Diffusivity $\mathrm{D} = \lim_{t \to \infty} \frac{1}{2t} < [x(t) - x(0)]^2 >,$

Local diffusivity $D(x(0)) = \frac{1}{2t} < [x(t) - x(0)]^2 >$



$$j_+ = \frac{\mathrm{D}(x)}{\delta x}\rho(x)$$

$$j_- = \frac{\mathrm{D}(x+\delta x)}{\delta x}\rho(x+\delta x).$$

$$j = j_+ - j_- = -\frac{\partial \mathrm{D}(x)\rho(x)}{\partial x} + O(\delta x)$$

$$\lim_{\delta x \to 0} j = -\frac{\partial \mathrm{D}(x)\rho(x)}{\partial x}$$

General equilibrium distribution

$$\frac{\partial \rho(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[\frac{\rho(x,t)}{\Gamma(x)}\frac{\partial \mathrm{U}(x)}{\partial x} + \frac{\partial \mathrm{D}(x)\rho(x,t)}{\partial x}\right] = -\frac{\partial}{\partial x} j(x,t).$$

$$\rho(x) = \frac{\mathrm{N}}{\mathrm{D}(x)} \exp \int \frac{\mathrm{F}(x)}{\mathrm{D}(x)\Gamma(x)} dx.$$

Potential in Boltzmann form $V(x) = \ln D(x) - \int dx F(x)/D(x)\Gamma(x)$

Conclusion

- Boltzmann distribution needs to get modified for equilibrium distribution of stochastic systems where there are other sources of inhomogeneity than a conservative force.

Thank You