Lecture 10. Near equilibrium theory I

1 Introduction

In general, systems close to equilibrium are better understood at this time than those much removed. In this lecture and the next we discuss two important and practical results/theories which have had widespread practical application in recent years.

2 Fluctuation-Dissipation Theorems

If a statistical system in equilibrium is subjected to a small external force then the mean values of various random variables for the system exhibit a well defined response to this forcing. It turns out that such responses may be related to the equilibrium time lagged correlations of certain random variables within the system. This is of practical significance because often the equilibrium system may be observed over an extended period and so the time lag correlations of any observable random variables easily calculated. The Fluctuation-Dissipation theorem may then be used to deduce the response of the statistical system to an arbitrary but small perturbation. There exist a variety of such theorems for different models of non-equilibrium systems. In this lecture[1] we shall confine our attention to those which we discussed in Lecture 8 namely those of a conventional stochastic differential equation.

2.1 General result for a stochastic differential equation

Recall that we can write stochastic differential equations rigorously as

$$dx_i = A_i(\boldsymbol{x}, t)dt + B_{ij}(\boldsymbol{x}, t)dW_j \tag{1}$$

and derive a Fokker Planck equation for the probability density of the generic form

$$\begin{aligned} \partial_t p &= L_{FP}(\boldsymbol{x}, t)p \\ L_{FP} &\equiv -\sum_{i=1}^{N} \partial_i A_i + \frac{1}{2}\sum_{i,j=1}^{N} \partial_i \partial_j C_{ij} \\ C_{ij} &\equiv B_{ki}B_{kj} \end{aligned} \tag{2}$$

where L_{FP} is a differential operator. Suppose now we perturb this system by adding small terms to both A (called the drift) and C (called the diffusion).

[1] In the next lecture when we discuss other results we consider somewhat more general stochastic systems.

This corresponds to a direct determinstic perturbation to equation (1) and a small modification of the statistics of the stochastic forcing. We obtain therefore

$$\begin{aligned} A'_i &= A_i + A_i^{ext} \\ C'_{ij} &= C_{ij} + C_{ij}^{ext} \end{aligned} \tag{3}$$

where the *ext* superscript indicates an externally imposed small perturbation. We shall further assume for simplicity that these external forcings are separable in time i.e.

$$\begin{aligned} A_i^{ext} &= A_i^{ext}(\boldsymbol{x})F^i(t) \\ C_{ij}^{ext} &= C_{ij}^{ext}(\boldsymbol{x})F^{ij}(t) \end{aligned}$$

(summation convention not used). Assume now that the system is initially in equilibrium with density q which we assume we are able to write down explicitly. It follows that

$$L_{FP}q = 0$$

Once the small external forcing is imposed the differential operator L has an additional term L^{ext} added. This is easily deduced from equation (3)):

$$L^{ext} = -\sum_{i=1}^{N} F_i \partial_i A_i^{ext}(\boldsymbol{x}) + \frac{1}{2}\sum_{i,j=1}^{N} F_{ij}\partial_i\partial_j C_{ij}^{ext}(\boldsymbol{x}) \equiv \boldsymbol{F}(t) \bullet \boldsymbol{L}^{ext}(\boldsymbol{x}) \tag{4}$$

Moreover the density is modified by the addition of a small (time dependent) p. We have therefore

$$\begin{aligned} p_t &= \left(L_{FP} + L^{ext}\right)(q+p) \\ &\approx L_{FP}p + L^{ext}q \end{aligned} \tag{5}$$

where we are neglecting the second order term due to the smallness of the perturbation. The PDE (5) may be formally solved as follows:

$$p(\boldsymbol{x},t) = \int_{-\infty}^{t} \exp\left(L_{FP}\left(t-t'\right)\right) L^{ext} q dt' \tag{6}$$

The reader may care to verify this with elementary calculus. Note that the exponential in the integrand is a differential operator defined in the obvious way from it's differential operator exponent.

Consider now the perturbation effect of the external forcing on the expectation of a general random variable $Q(\boldsymbol{x})$ at time t:

$$\begin{aligned} \delta\langle Q\rangle(t) &= \int d^n x Q(\boldsymbol{x}) p(\boldsymbol{x},t) = \int_{-\infty}^{\infty} \boldsymbol{R}_Q(t-t') \bullet \boldsymbol{F}(t')dt' \\ \boldsymbol{R}_Q(t) &\equiv \int d^n x Q \exp\left(L_{FP}t\right) \boldsymbol{L}^{ext}(\boldsymbol{x}) q \quad t \geqq 0 \\ &= 0 \quad t < 0 \end{aligned} \tag{7}$$

where we have used (6) and $\boldsymbol{R}_Q$ is called the response function for the system and the random variable Q. Note that this perturbation effect is time dependent. In the case that the forcing is applied as an impulse at time zero then $\boldsymbol{F}$ is a Dirac delta "function" in t and we obtain the simple expression

$$\delta \langle Q \rangle (t) = \boldsymbol{R}_Q(t)$$

other choices for the time dependency of the forcing obviously give a convolution of the forcing time dependency with the response function.

Consider now the second moment of two functions of the basic random variables $F(\boldsymbol{x}(t))$ and $G(\boldsymbol{x}(t'))$ at different times in an equilibrium stochastic system. Since the system is an equilibrium one we can set $t' = 0$ and $t > 0$ without loss of generality (the moments need to be time invariant). Now we have

$$\langle FG \rangle (t) = \iint d^n x d^n x' p_{eq}(\boldsymbol{x}(t); \boldsymbol{x}'(0)) F(\boldsymbol{x}(t)) G(\boldsymbol{x}'(0))$$

where the function p in the integrand is the (equilibrium) **joint** distribution of the basic system random variables at two different times. To evaluate this we return to the Fokker Planck equation (2) and observe that time translations can be implemented as follows using a Taylor expansion

$$r(t+a) = \exp(a\frac{\partial}{\partial t}) r(t) = \exp\left(aL_{FP}\right) r(t) \tag{8}$$

Now the joint distribution is given by

$$p_{eq}(\boldsymbol{x}(t); \boldsymbol{x}'(0)) = p(\boldsymbol{x}(t)|\boldsymbol{x}'(0)) p_{eq}(\boldsymbol{x}'(0))$$

where the first function on the right is the conditional probability of $\boldsymbol{x}$ at time t given that at time 0 we know the basic variable takes with certainty the value $\boldsymbol{x}'$. Using (8) we deduce therefore that[2]

$$p(\boldsymbol{x}(t)|\boldsymbol{x}'(0)) = \exp\left(tL_{FP}\right) \delta\left(\boldsymbol{x} - \boldsymbol{x}'\right)$$

where L_{FP} is a differential operator involving $\boldsymbol{x}$. Hence we obtain

$$\langle FG \rangle (t) = \iint d^n x d^n x' F(\boldsymbol{x}(t)) (\exp\left(tL_{FP}\right) \delta\left(\boldsymbol{x} - \boldsymbol{x}'\right)) G(\boldsymbol{x}'(0)) p_{eq}(x'(0))$$

and hence carrying out the integrations of $\boldsymbol{x}$'(0) that

$$\langle FG \rangle (t) = \int d^n x F(\boldsymbol{x}) \exp\left(tL_{FP}\right) p_{eq}(\boldsymbol{x}) G(\boldsymbol{x}) \tag{9}$$

Now if we choose a vector random variable $\boldsymbol{G}$ in a certain way we get an interesting result:

$$\boldsymbol{G} = p_{eq}^{-1} \boldsymbol{L}_{ext} p_{eq} \tag{10}$$

[2]To make this rigorous one could set the delta function to be a Gaussian probability of standard deviation ε and then take the limit as $\varepsilon \rightarrow 0$ below

This choice gives immediately from (7) and (9) that

$$\begin{aligned} \boldsymbol{R}_F(t) &= \langle F\boldsymbol{G}\rangle(t) \quad t \geqq 0 \\ &= 0 \quad t < 0 \end{aligned} \tag{11}$$

In other words the response function and hence mean random variable perturbations can be deduced from the time lagged moments of this random variable with another random variable given by equation (10). This latter random variable can be deduced from a knowledge of the equilibrium density of the system. The lagged moments are then able to be calculated from a long term observation of the equilibrium system. Results of the kind (11) are known generically as Fluctuation-Dissipation theorems and have wide application to near equilibrium statistical systems.

2.2 Simple example: Ornstein-Uhlenbeck process.

The multivariate Ornstein-Uhlenbeck process corresponds physically with finite dimensional damped oscillators with additive stochastic forcing and with prescribed constant statistics. Physical systems are frequently modelled using such a random process in many different fields (an example is climate). Without the forcing such systems are simply linear systems, which because they are damped, approach zero as $t \to \infty$ albeit in a possibly oscillatory manner. In terms of equation (1) we have (with the summation convention):

$$A = -\gamma_{ij} x_j$$

with γ constant and positive definite. Moreover the matrix C is also constant. Because of the linearity of the unforced deterministic system complete closed form solutions are often possible for the time dependent density p for such a system (see e.g. [1] Section 4.4.6). More particularly from the viewpoint of the present application the equilibrium density is known to be Gaussian and of the form

$$p_{eq} = D \exp\left(-\frac{1}{2}\sigma_{ij}^{-1} x_i x_j\right) \tag{12}$$

where the matrix σ is the covariance matrix for the equilibrium system and is a solution of the following matrix equation known as the continuous Lyupanov equation:

$$\sigma\gamma^T + \gamma\sigma = C$$

It is left as a (moderately difficult) exercise to verify that p_{eq} is not time dependent.

Now suppose we introduce a small perturbation in the $k'th$ equation only of the damped oscillator with time dependency $F(t)$. We are therefore modifying A only not C. It follows easily from equations (1), (2) and (4) that the perturbation Fokker Planck operator is simply

$$L_j^{ext}(\boldsymbol{x}) = -\frac{\partial}{\partial x_k} \quad j = k \tag{13}$$

$$= 0 \quad j \neq k \tag{14}$$

We can now calculate the vector function $\boldsymbol{G}$ using (10) and (12) obtaining that the only non-zero component is

$$G_k = \sigma_{kj}^{-1} x_j$$

The response function for a general x_l is now easily calculated using the fluctuation dissipation theorem i.e. equation (11) and we obtain

$$R_{x_l}(t) = \sigma_{kj}^{-1} \langle x_l(t) x_j(0) \rangle$$

Since the means of x are zero this is simply the time lagged correlation of the appropriate system variables multiplied by the inverse of the equilibrium covariance matrix. Both of these matrices are easily calculatable from the equilibrium statistical system and if we form the convolution with F we can obtain the mean response of any variable to a small perturbation.

3 Final remarks

A fluctuation dissipation theorem can be deduced for many different statistical system not just the stochastic differential equations of the previous section. It has many powerful applications for near equilibrium systems. One example has been it's recent extensive successful application by Branstator to the atmosphere with the forcing perturbation being diabatic heating (see [2]). Extensive further applications to stochastic systems can be found in Chapter 7 of Risken (see [3]) from which these notes were prepared.

References

[1] C. W. Gardiner. *Handbook of Stochastic Methods for Physics, Chemistry and the Natural Sciences*, volume 13 of *Springer Series in Synergetics*. Springer, 2004.

[2] A. Gritsun and G. Branstator. Climate response using a three-dimensional operator based on the fluctuation–dissipation theorem. *J. Atmos, Sci.*, 64(7), 2007.

[3] H. Risken. *The Fokker-Plank Equation*. Springer Verlag, Berlin, 2nd edition, 1989.