Notes on Linear Response Theory   Michael Cross — *April 13, 2006*

Useful references are Callen and Greene [1], and Chandler [2], chapter 16.

Task

To calculate the change in a measurement $\langle B(t)\rangle$ due to the application of a small "field" $F(t)$ that gives a perturbation to the Hamiltonian $\Delta H = -F(t)\,A$. Here both A and B are determined by the phase space coordinates denoted $\vec{r}^N(t), \vec{p}^N(t)$ (e.g. B might be the electric current $\sum_{i=1}^N (e/m)\,\vec{p}_i$). The time dependence is given by the evolution of $\vec{r}^N(t), \vec{p}^N(t)$ according to Hamilton's equations. In statistical mechanics we deal with an ensemble of systems given for example by a known distribution $\rho\left(\vec{r}^N, \vec{p}^N\right)$ at $t = 0$. The expectation value at a later time t is then

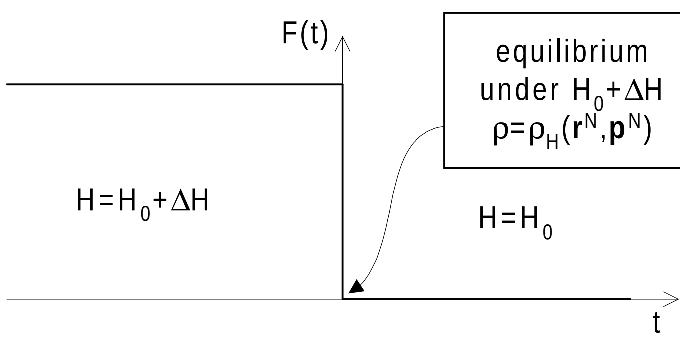
$$\langle B(t)\rangle = \int d\vec{r}^N d\vec{p}^N \rho\left(\vec{r}^N, \vec{p}^N\right) B\left(\vec{r}^N(t) \leftarrow \vec{r}^N, \vec{p}^N(t) \leftarrow \vec{p}^N\right) \tag{1}$$

where the cumbersome notation $\vec{r}^N(t) \leftarrow \vec{r}^N$ means we must evaluate B at the phase space coordinate that evolves from the value $\vec{r}^N$ at $t = 0$. For shorthand this will be denoted $B(t)$. We could equivalently follow the time evolution of ρ through Liouville's equation and instead evaluate

$$\langle B(t)\rangle = \int d\vec{r}^N d\vec{p}^N \rho\left(\vec{r}^N, \vec{p}^N, t\right) B\left(\vec{r}^N, \vec{p}^N\right) \tag{2}$$

but the first form is more convenient.

Onsager regression



First consider the special case of a force $F(t)$ switched on to the value F in the distant past, and then switched off at $t = 0$. We are interested in measurements in the system for $t > 0$ as it relaxes to equilibrium.

For $t \le 0$ the distribution is the equilibrium one for the *perturbed* Hamiltonian $H\left(\vec{r}^N, \vec{p}^N\right) = H_0 + \Delta H$, with H_0 the unperturbed Hamiltonian, i.e. (for a canonical distribution)

$$\rho\left(\vec{r}^N, \vec{p}^N\right) = \frac{e^{-\beta(H_0+\Delta H)}}{\int d\vec{r}^N d\vec{p}^N e^{-\beta(H_0+\Delta H)}} \tag{3}$$

so that introducing a convenient notation for the integral over phase space $Tr \equiv \int d\vec{r}^N d\vec{p}^N$

$$\langle B(0)\rangle = \frac{Tr e^{-\beta(H_0+\Delta H)} B\left(\vec{r}^N, \vec{p}^N\right)}{Tr e^{-\beta(H_0+\Delta H)}} \quad . \tag{4}$$

For $t \geq 0$ we let $\vec{r}^N(t)$, $\vec{p}^N(t)$ for each member of the ensemble evolve under the Hamiltonian, now H_0 from its value $\vec{r}^N$, $\vec{p}^N$ at $t = 0$,so that

$$\langle B(t) \rangle = \frac{Tr e^{-\beta(H_0+\Delta H)} B\left(\vec{r}^N(t) \leftarrow \vec{r}^N, \vec{p}^N(t) \leftarrow \vec{p}^N\right)}{Tr e^{-\beta(H_0+\Delta H)}} \quad . \tag{5}$$

Note that the integral is over $\vec{r}^N$, $\vec{p}^N$ which we can denote $\vec{r}^N(0)$, $\vec{p}^N(0)$, and $\Delta H = \Delta H\left(\vec{r}^N, \vec{p}^N\right)$ etc.

It is now a simple matter to expand the exponentials to first order in ΔH (F small!) to give

$$\langle B(t) \rangle = \langle B \rangle_0 - \beta\left[\langle \Delta H\, B(t) \rangle_0 - \langle B \rangle_0 \langle \Delta H \rangle_0\right] + O(\Delta H)^2 \tag{6}$$

where $<>_0$denotes the average over the ensemble for a system for which no perturbation was applied i.e. $\rho_0 = e^{-\beta H_0}/Tr e^{-\beta H_0}$. Note in this unperturbed system the Hamiltonian remains H_0 for all time, so that one-time averages such as $\langle B(t) \rangle_0$ are in fact time independent. Finally putting in the form of ΔH, writing $\delta B(t) = B(t) - \langle B \rangle_0$ etc., and noticing that $A(\vec{r}^N, \vec{p}^N)$ is equivalent to $A(0)$,

$$\Delta H = -FA\left(\vec{r}^N, \vec{p}^N\right) = -FA\left(\vec{r}^N(0) \leftarrow \vec{r}^N, \vec{p}^N(0) \leftarrow \vec{p}^N\right) = -FA(0), \tag{7}$$

gives for the change in the measurement $\Delta \langle B(t) \rangle = \langle B(t) \rangle - \langle B \rangle_0$

$$\Delta \langle B(t) \rangle = \beta F\ \langle \delta A(0)\, \delta B(t) \rangle_0 \quad , \tag{8}$$

where we have written the result in terms of $\delta A = A - \langle A \rangle_0$.

This result which equates the time dependence of the decay of a prepared perturbation to the time dependence of a correlation function in the unperturbed system proves the **Onsager regression hypothesis**.

Kubo formula

For a general $F(t)$ we write the linear response as

$$\Delta \langle B(t) \rangle = \int_{-\infty}^{\infty} \chi_{AB}\left(t, t'\right) F\left(t'\right) dt' \tag{9}$$

with χ_{AB} the susceptibility or response function with the properties

$$\begin{array}{cc} \chi_{AB}\left(t, t'\right) = \chi_{AB}\left(t - t'\right) & \text{stationarity of unperturbed system} \\ \chi_{AB}\left(t - t'\right) = 0 \text{ for } t < t' & \text{causality} \\ \tilde{\chi}_{AB}(-f) = \tilde{\chi}^*_{AB}(f) & \chi_{AB}\left(t, t'\right) \text{ real} \end{array} \quad . \tag{10}$$

The causality condition leads to interesting properties in the complex f plane ($\tilde{\chi}(f)$ must be analytic (no poles) in the upper half plane), but we will not need this here.

For the step function force turned off at $t = 0$

$$\Delta \langle B(t) \rangle = F \int_{-\infty}^{0} \chi_{AB}\left(t - t'\right) dt' \tag{11a}$$

$$= F \int_{t}^{\infty} \chi_{AB}(\tau)\, d\tau \quad . \tag{11b}$$

Differentiating then gives the **classical Kubo expression**

$$\chi_{AB}(t) = \begin{cases} -\beta \frac{d}{dt} \langle \delta A(0)\, \delta B(t) \rangle_0 & t \geq 0 \\ 0 & t < 0 \end{cases} \quad . \tag{12}$$

Connection with energy absorption: fluctuation-dissipation

Consider a sinusoidal force $F(t) = \mathrm{Re}\, F_f e^{2\pi i f t} = \frac{1}{2}(F_f e^{2\pi i f t} + c.c.)$. The rate of doing work on the system is "force $\times$ velocity" $W = F\dot{A}$ i.e.

$$W = F(t) \frac{d}{dt} \int_{-\infty}^{\infty} \chi\left(t, t'\right) F\left(t'\right) dt' \tag{13}$$

writing simply χ for χ_{AA}. Substituting in the sinusoidal form for the force we recognize the integral as giving us the Fourier transform of χ so that the average rate of working is

$$W(f) = \tfrac{1}{4} 2\pi i f \left|F_f\right|^2 \left[\tilde{\chi}(f) - \tilde{\chi}(-f)\right] \tag{14a}$$

$$= \pi f \left|F_f\right|^2 \left(-\tilde{\chi}''(f)\right) \tag{14b}$$

where $\tilde{\chi}''$ is Im $\tilde{\chi}$ and terms varying as $e^{\pm 4\pi i f t}$ which average to zero have been ignored. Thus the imaginary part of $\tilde{\chi}$ tells us about the energy absorption or dissipation.

But from the definition of the Fourier transform

$$\tilde{\chi}''(f) = \int_{-\infty}^{\infty} \chi(t) \sin(2\pi f t)\, dt \tag{15a}$$

$$= -\beta \int_0^{\infty} \frac{d}{dt} \langle \delta A(0)\, \delta A(t) \rangle_0 \sin(2\pi f t)\, dt \tag{15b}$$

$$= \beta (2\pi f) \int_0^{\infty} \langle \delta A(0)\, \delta A(t) \rangle_0 \cos(2\pi f t)\, dt \tag{15c}$$

where we have used the fluctuation-dissipation expression for $\chi = \chi_{AA}$ and then integrated by parts. Finally we recognize the integral as giving the spectral density of A fluctuations, so that (including necessary factors)

$$G_A(f) = 4kT \frac{-\tilde{\chi}''(f)}{2\pi f} \tag{16}$$

relating the spectral density of fluctuations to the susceptibility component giving energy absorption, i.e. the **classical fluctuation-dissipation theorem**.

Langevin Force

If we suppose the fluctuations in A derive from a fluctuating Langevin contribution F' to the force F we can write

$$\delta A(t) = \int_{-\infty}^{\infty} \chi\left(t, t'\right) F'\left(t'\right) dt' \quad . \tag{17}$$

Since the Fourier transform of a convolution is just the product of the Fourier transforms the spectral density of A is given by

$$G_A(f) = \left|\tilde{\chi}(f)\right|^2 G_F(f) \quad , \tag{18}$$

and using the expression for G_A derived above leads to

$$G_F(f) = 4kT \frac{1}{2\pi f} \mathrm{Im}\left[\frac{1}{\tilde{\chi}(f)}\right] \quad . \tag{19}$$

Instead of the susceptibility we can introduce the *impedance* $Z = F/\dot{A}$ so that

$$\tilde{Z}(f) = \frac{1}{2\pi i f} \frac{1}{\tilde{\chi}(f)} \quad . \tag{20}$$

Then defining the “resistance” $\tilde{R}(f) = \mathrm{Re}\,\tilde{Z}(f)$ we can write the spectral density of the fluctuating force as

$$G_F(f) = 4kT\,\tilde{R}(f) \quad . \tag{21}$$

The analogy with the Johnson noise expression should be apparent.

Note that the derivations have been classical, so we arrive at the classical version of the fluctuation-dissipation theorem, the force expression etc. In a quantum treatment A and B, as well as H are *operators* that may not commute, so that we have to be more careful in the expansion of the exponentials. Thus Eq.(12) will involve commutators of operators. The sismplest form of the expression is to define a slightly different susceptibility $\chi''(t) = (2i)^{-1}[\chi(t) - \chi(-t)]$ (the Fourier inverse of the dissipative part $\chi''(\omega)$) which is then related to the commutator-correlation function

$$\chi''_{AB}(t) = \frac{1}{2\hbar}\langle[A(0), B(t)]\rangle_0\,, \tag{22}$$

where A, B are Heisenberg (time dependent) operators. The change to Eq.(16) is quite simple: make the replacement

$$kT \to \frac{hf}{2}\coth\left(\frac{hf}{2kT}\right) \tag{23}$$

which can be interpreted as taking into account the Bose occupation factor of the modes. The quantum approach was pioneered by Kubo [3], and the set of ideas are often called the Kubo formalism.

References

[1] H.B. Callen and R.F. Greene, Phys. Rev. **86**, 702 (1952)

[2] D. Chandler, *Introduction to modern statistical mechanics* (Oxford University Press, 1987)

[3] R. Kubo, J. Phys. Soc. Japan **12**, 570 (1957)