Onsager's Regression Hypothesis and Fluctuation-Dissipation

le 27 avril 2007 slrhr ①/

The basic idea of Onsager's regression hypothesis is that near equilibrium, the relaxation from points prepared by nonequilibrium is indistinguishable from relaxation from spontaneous fluctuations to the same state.

With $\delta A(t) = A(t) - \langle A \rangle$ (the fluctuation from the equilibrium average)

$$C(t) = \langle \delta A(0)\, \delta A(t) \rangle = \langle (A(0) - \langle A \rangle)(A(t) - \langle A \rangle) \rangle = \langle A(0)A(t) - A(t)\langle A \rangle - A(0)\langle A \rangle + \langle A \rangle^2 \rangle$$

$$= \langle A(0)\, A(t) \rangle - (\langle A(t) \rangle + \langle A(0) \rangle)\langle A \rangle + \langle A \rangle^2 \qquad \langle A(t) \rangle = \langle A(0) \rangle = \langle A \rangle$$

$$= \langle A(0)\, A(t) \rangle - \langle A \rangle^2$$

Since the correlation function is really dependent on the difference between two times (at equilibrium) and not the absolute value of time, we have

$$C(t) = \langle \delta A(t')\, \delta A(t'') \rangle = \langle \delta A(0)\, \delta A(t) \rangle = \langle \delta A(-t)\, \delta A(0) \rangle$$

$$= \langle \delta A(0)\, \delta A(-t) \rangle = C(-t)$$

At small times $\quad C(0) = \langle \delta A(0)\, \delta A(0) \rangle = \langle (\delta A)^2 \rangle$

At large times $\quad C(t) \to \langle \delta A(0) \rangle \langle \delta A(t) \rangle \to 0 \qquad (\langle \delta A(0) \rangle = 0)$

Assuming we have an ergodic system, the time average on a very long trajectory will be the same as averaging over initial conditions:

$$\langle \delta A(0)\, \delta A(t) \rangle = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^{\tau} d\bar{t}\; \delta A(\bar{t} + t')\, \delta A(\bar{t} + t'') \qquad \text{w/ } t = t'' - t'$$

So defining $\Delta \bar{A}(t) = \bar{A}(t) - \langle A \rangle = \overline{\delta A}(t)$, Onsager's hypothesis says that, in the linear regime:

$$\frac{\Delta \bar{A}(t)}{\Delta \bar{A}(0)} = \frac{C(t)}{C(0)} = \frac{\langle \delta A(0)\, \delta A(t) \rangle}{\langle (\delta A)^2 \rangle}$$

Proof of Onsager's Regression Hypothesis

$$\langle A \rangle = \frac{Tr(e^{-\beta H} A)}{Tr(e^{-\beta H})}$$

perturb Hamiltonian w/ $\Delta H = -fA$

$$\bar{A}(0) = \frac{Tr(e^{-\beta(H+\Delta H)} A)}{Tr(e^{-\beta(H+\Delta H)})} \qquad \bar{A}(t) = \frac{Tr(e^{-\beta(H+\Delta H)} A(t))}{Tr(e^{-\beta(H+\Delta H)})}$$

Expanding $\bar{A}(t)$ in ΔH

$$\bar{A}(t) = \frac{Tr(e^{-\beta H}(1-\beta\Delta H) A(t))}{Tr(e^{-\beta H}(1-\beta\Delta H))}$$

(note that QM is harder... commutativity!)

$$= Tr\left(e^{-\beta H}(A(t) - (\beta\Delta H)A(t) + A(t)Tr(e^{-\beta H}\beta\Delta H)/Tr(e^{-\beta H}))\right)/Tr(e^{-\beta H})$$

$$= \langle A \rangle - \beta(\langle \Delta H\, A(t) \rangle - \langle A \rangle \langle \Delta H \rangle)$$

so $\boxed{\Delta\bar{A}(t) = \beta f \langle \delta A(0)\,\delta A(t) \rangle}$ (fluctuation-dissipation)

Since $\Delta\bar{A}(0) = \beta f \langle (\delta A)^2 \rangle$, we obtain Onsager's regression hypothesis.

Response Functions

$$\Delta\bar{A}(t) = \int_{\mathbb{R}} dt'\, \chi(t,t')\, f(t')$$

let $f(t)$ only applies at time t_0

$$\Delta\bar{A}(t) = f_0\, \chi(t,t_0) = f_0\, \chi(t-t_0)$$

(doesn't depend on absolute time)

Combining w/ fluctuation dissipation:

$$\chi(t) = -\beta \frac{d}{dt}\langle \delta A(0)\,\delta A(t) \rangle$$