Microscopic Foundation of GENERIC

A. DONEV

The Mori-Zwanzig formalism provides the microscopic justification for the coarse-grained Langevin equations we have been discussing.

Let us focus on closed systems and choose energy as one of the coarse-grained variables $\Leftrightarrow$ GENERIC

A. Doner <u>GENERIC</u> equation for $X(z)$: (2)

kinetic

$$\dot{x} = L \cdot \frac{\partial E}{\partial x} + M \cdot \frac{\partial S}{\partial x} + \sqrt{2k_B}\ \tilde{M} \boxdot W(t)$$

or Ito + DRIFT!

reversible (conservative)

irreversible (dissipative)

$$\boxed{\tilde{M}\tilde{M}^* = M}$$

fluctuation-dissipation balance

$L^* = -L$

(skew-adjoint)

$M^* = M$

(self-adjoint)

$$\boxed{L \cdot \frac{\partial S}{\partial x} = 0}$$

$$\boxed{M \cdot \frac{\partial E}{\partial x} = 0}$$

<u>degeneracy</u> conditions

<u>Fokker-Planck</u>

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial x} \cdot \left\{ \left[L \cdot \frac{\partial E}{\partial x} + M \cdot \frac{\partial S}{\partial x} \right] P - k_B\ M \cdot \frac{\partial}{\partial x} P \right\}$$

$$\boxed{\partial_x \cdot L = 0}$$

which preserves $\exp[S/k_B]$

In the **Markovian** approximation, the Zwanzig procedure gives:

$$S(a) = \ln \Omega(a) = \ln \int dz\, \delta[A(z) - a]$$

$$\overset{|||}{X}$$

Let us define the **constrained** equilibrium average

$$\langle F \rangle^{x} = \frac{1}{\Omega(x)} \int dz\, \delta[A(z) - a]\, F(z)$$

then one can show that the drift

$$L \cdot \frac{\partial E}{\partial x} = \vartheta(x) = \left\langle i L \bar{\underline{X}} \right\rangle^{x}$$

and in fact

$$\boxed{L_{\mu\nu}(a) = \left\langle \frac{\partial A_\mu}{\partial z} J_0 \frac{\partial A_\nu}{\partial z} \right\rangle^{a}}$$

where $$iL = -\frac{\partial H}{\partial z} J_0 \frac{\partial}{\partial z}$$

symplectic matrix

$$J_0 = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}$$

The diffusion matrix is

$$\boxed{M_{\mu\nu}(a) = \int_0^\infty d\tau \left\langle (\delta\dot{A}_\nu)\, e^{-iL\tau} (\delta\dot{A}_\mu) \right\rangle^a}$$

Green - Kubo integral

where

$$\boxed{\delta\dot{A}_\nu = iLA_\nu - v_\nu(a)}$$

is the fluctuation of the "velocity" of $A(t)$ around the mean.

$$M_{\mu\nu}(a) = \int_0^\infty d\tau \left\langle (\delta\dot{A}_\nu)(\tau)\,(\delta\dot{A}_\nu)(0) \right\rangle^a$$

One can also show from these expressions that

$$\boxed{M \cdot \frac{\partial E}{\partial x} = 0}$$ identically

and also it is obviously true that $\boxed{L^* = -L}$ and $\boxed{M^* = M}$

From the microscopic expressions one can also show

ASSUME

$$\boxed{L \cdot \frac{\partial S}{\partial x} = k_B \frac{\partial}{\partial x} \cdot L} \simeq 0$$

which ensures the Einstein Distribution $P_{eq} \sim e^{S/k_B}$