Physics 210b

→ $\boxed{\text{Model Reduction}}$ ⟷ Statistical Dynamics
(Toward Renormalization)
[Phys. 217]

- Motivation:

- frequently of interest to reduce description of a system with many d-o-f's

- some notion of some d-o-f's $\left\{\begin{array}{l}\text{that}\\ \underline{\text{relevant}}\\ \text{of interest}\end{array}\right.$ (slow)
  some $\underline{\text{irrelevant}}$ (fast)

- often $\left\{\begin{array}{l}\text{relevance}\\ \text{irrelevance}\end{array}\right.$ based on
  $\underline{\text{space}}$ - $\underline{\text{time}}$ scales

$\underline{\text{e.g.}}$

complex turbulent flow
= large scales — relevant
$\underline{\text{i.e.}}$ determine flow pattern
macroscopics
+
small scales — irrelevant
$\underline{\text{i.e.}}$ don't need details (?)

Questions:

- statistical description of small scales
  explicit description of large scales

- how, systematically?

- how couple ranges?

Goal of Mori-Zwanzig Theory (Model Reduction) is to project irrelevant d-o-f's onto relevant d-o-f's, and derive model of relevant d-o-fs.

How?

- derive 'Langevin' equation for [redacted] relevant d-o-fs with (statistical) model of interaction with irrelevant d-o-fs

- Key elements:
  - memory kernel
  - noise

  $\Big\}$ products

→ Memory kernel can have extended width ⇒ Non-Markovian

Caveat Emptor : – Framework
– not universal, panacea.
– cumbersome
– continues in RG.

Sources : – Zwanzig } texts
– Serra, et. al. } texts
– Chorin } papers.
– Mori } papers.

also – Goldenfeld, – McComb texts.

Simple Examples

– (THE) Langevin Equation

$$\partial v + \frac{\beta}{m} v = \frac{\tilde{f}}{m}$$

$$\langle \tilde{f}(t)\tilde{f}(t')\rangle = |\tilde{f}|^2 \tau_{ac}\, \delta(t-t')$$

- d-o-fs : - thermal fluctuations
  τ_{ac}
- fluid dynamics β/m

dynamics on many time scales enter

- Brownian particle motion
  $t \gg (\beta/m)^{-1}$

simplest model !

$$\frac{dx}{dt} = \tilde{f}/\beta$$

$$\Rightarrow \quad \langle x^2 \rangle \sim 2Dt$$

$$D = T/\beta$$

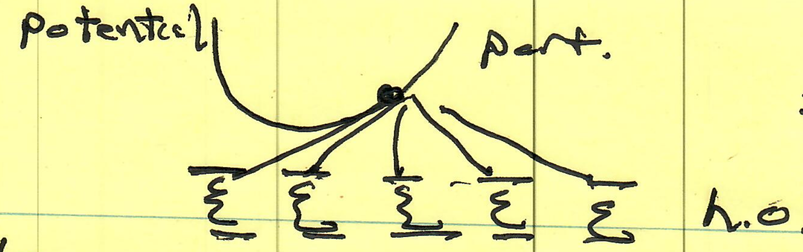
Obviously,

→ only particle motion is explicit

→ fast thermal d-o-fs ⇒ rndm forcing

fluid dynamics (memory) ⇒ drag coefficient

Recall : 'Mechanical' model of thermal bath (Zwanzig)



i.e. $\quad H = H_S + H_B$

$$H_S = \frac{p^2}{2m} + U(x) \quad \rightarrow \quad \text{'system'}$$

relevent

$$H_B = \sum_j \left[\frac{p_j^2}{2} + \frac{1}{2}\omega_j^2 \left(q_j - \frac{\gamma_j}{\omega_j^2} x \right)^2 \right]$$

→ 'bath' irrelevant

coupling of bath to system

simple!

- goal is to derive EOM for relevant variables in presence of bath

- * specify bath statistically

→ [~ coarse graining of irrelevant dynamics]

⇒ irreversibility !?

Recall:

$$\frac{dp}{dt} = -U'(x(t)) - \int_0^t ds\, K(s)\, \frac{p(t-s)}{m} + F_p(t)$$

$F_p(t)$ → noise

$K(s)$ → Memory Kernel

$$K(s) = \sum_j \frac{\gamma_j^2}{\omega_j^2} \cos(\omega_j t)$$

→ kernel set by Bath properties:

$\left\{\begin{array}{l}\text{couplings}\\ \text{freq.}\end{array}\right.$

→ ~ [self-energy

→ Contrast:

$$\frac{dv}{dt} = -\frac{\gamma}{m} v + \frac{\tilde{f}}{m}$$

$\frac{\gamma}{m}$ → local in time (Markovian)

$$\int_0^t K(s)\, \frac{p(t-s)}{m}$$

→ non-local (Non-Markovian)

NB: statistical Description of Bath

recall: $\sum_j \rightarrow \int d\omega\, g(\omega)$

$g(\omega)$ → density of states for bath

$$\gamma^2 = \gamma^2(\omega)$$

and if: $\rho(\omega) \sim \omega^2$
$\gamma^2 \sim \text{const.}$

$$k(t) = \gamma^2 \delta(t)$$

$\Downarrow$

Localized kernel → Markovian

→ Noise?

$$F_p(t) = \sum_j \gamma_j \, p_j(0) \, \frac{\sin \omega_j t}{\omega_j}$$

$$+ \sum_j \gamma_j \left(q_j(0) - \frac{\gamma_j}{\omega_j^2} x(0) \right) \cos \omega_j t$$

$p_j(0)$, $q_j(0)$ distributed according to:
$f_{eq} \cong \exp[-H_B/T]$ ⇒

$$\left\langle \left(q_j(0) - \frac{\gamma_j}{\omega_j^2} x(0) \right)^2 \right\rangle = \frac{T}{\omega_j^2} \quad \text{etc.}$$

and FDT → (description builds in)

$$\langle F_p(t) F_p(t') \rangle = T \, \underset{\uparrow}{k}(t-t')$$

memory kernel.

→ Why review?

MZT seeks to convert full problem to:

Non-Markovian 'Langevin Eqn.' for relevent variables in terms of

- memory kernel
- noise

for irrelevent variables

→ includes statistical representation of of irrelevent d-o-f's

⇒ reduced model.

→ Generic approach to model reduction ...

→ MST Formalism – General Theory

– N variables $\begin{cases} \text{modes} \\ \text{particles} \end{cases}$

$$q = (q_1, \ldots q_N)$$

$$\dot{q}_j = h_j(q) \quad \rightarrow \text{dynamical eqns.}$$

– then assume can linear transform EOM:

$$\dot{P}_j = -\gamma_j P_j + Z_j(P)$$

$$j = 1 \ldots N$$

(not always so clear)

– if concerned with evolution on time scale $\sim T$, then can classify variables

– $\gamma_i T > 1$ → "irrelevant"/fast variables i.e. have equilibrated on time scale T (analogous to terminal velocity)

$\gamma_i \tau \ll 1 \Rightarrow$ "a relevant"/slow variables
i.e. evolving, not equilibrated on τ

Idea: Project irrelevant variables onto relevant variables.

For fast variables:

$$\dot{P}_j = -\gamma_j P_j + Z_j(P), \quad j = M+1, \dots N$$
$$(M < N)$$

$$\dot{P}_j \cong 0 \Rightarrow P_j = \frac{Z_j(P)}{\gamma_j}$$

$$\boxed{P_{fast} = Z_{fast}(P) / \gamma_F}$$

[slaves fast eliminates variables to slow variables

Can use to obtain dynamical equations in terms slow variables, only.

Now, for pdf evolution →

[seek Master Eqn. for Non-Markovian system.

⇒ construct from Liouville

- variables
  - a → slow, relevent
  - b → fast, irrelevent

so for pdf:

$$\partial_t \rho(a,b,t) = L\,\rho(a,b,t)$$

L ↑ Liouville operator (differential) → i.e. Poisson bracket (recall Kubo)

Can define reduced pdf:

$$S(a,t) = \int db \;\rho(a,b,t)$$

↑ integrates out irrelevent, fast variables.

And, assume can decompose L as:

$$\underbrace{L}_{} = \underset{\substack{\downarrow\\ \text{slow}}}{L_a} + \underset{\substack{\downarrow\\ \text{fast}}}{L_b} + \underset{\substack{\downarrow\\ \text{interaction}\\ \text{(fast-slow coupling)}}}{L_i}$$

Now: - assume "equilibrium distribution" exists for b variables only.
[N.B. What does "equilibrium" mean?
Irreversibility?]

$P_{eq}(b)$

- $L_b P_{eq}(b) = 0$

$\int db\, P_{eq}(b) = 1$

- can define projection $\underline{\underline{P}}$ onto a variables via:

$$\underline{\underline{P}}\, \rho(a,b,t) \equiv P_{eq}(b) \int db\, \rho(a,b,t)$$

$$= P_{eq}(b)\, \sigma(a,t)$$

Now, for projection, need:

$$\underline{\underline{P}}\,\underline{\underline{P}}\,\rho = \underline{\underline{P}}\,\rho \qquad \text{(idempotency)}$$

$$\underline{\underline{P}}^2 \rho(a,b,t) = \underline{\underline{P}}\,\rho_{eq}(b)\,\sigma(a,t)$$

$$= \rho_{eq} \int db\, \rho_{eq}(b)\,\sigma(a,t)$$

$$= \rho_{eq}\,\sigma(a,t) = \underline{\underline{P}}\,\rho(a,b,t)$$

$\underline{\underline{P}}$ is projection ✓

– And can further define:

$$\rho_1 = \underline{\underline{P}}\,\rho(a,b,t)$$

$$\rho_2 = (\underline{\underline{1}} - \underline{\underline{P}})\,\rho(a,b,t) = \underline{\underline{Q}}\,\rho(a,b,t)$$

so

$$\frac{\partial}{\partial t}\rho = L\rho$$

and

$$\frac{\partial}{\partial t}\rho_1 = \underline{P}\, L(\rho_1+\rho_2) \qquad (\text{oper. } \underline{P})$$

$\to$ slow

$$\frac{\partial}{\partial t}\rho_2 = \underline{Q}\, L(\rho_1+\rho_2)$$

$\to$ fast

Solving ρ_2 equation $\Rightarrow$

$$\rho_2(t) = e^{\underline{Q}Lt}\rho_2(0) + e^{\underline{Q}Lt}\int_0^t ds\, e^{-\underline{Q}Ls}\,\underline{Q}L\rho_1(s)$$

$\underline{Q} \to Q$

$$= e^{QLt}\rho_2(0) + \int_0^t e^{QLs}\, QL\rho_1(t-s)\, ds$$

then can substitute into ρ_1 eqn. to eliminate ρ_2.

$\Rightarrow$

$\to$ prop i.c.   a $\to$ slow, b $\to$ fast

$$\frac{\partial}{\partial t}\rho_1(t) = PLP\rho(t) + PLe^{QLt}Q\rho(0)$$

$\to$ fast $\to$ slow

$$+\int_0^t \underbrace{PLe^{QLs}QLP}_{\phi(s)}\,\rho_1(t-s)$$

$\phi(s)$ – memory kernel

→ similar structure to bath problem (not surprisingly)

Salient features:

- memory kernel $\phi(s)$ → from elimination of fast b's in terms slow a's

- has form ↦ time propagator

$$\underbrace{PL\,e^{QLs}\,QLP}_{\text{2 Liouville operators}}$$

Key physics: what controls time history in memory kernel?

- recall form of non-Markovian renormalized Vlasov eqn.

$$-i(\omega - kv) f_{k,\omega} - \partial_v D_{k,\omega} \partial_v f_{k,\omega} = -\frac{q}{m} E_{k,\omega} \frac{\partial \langle f \rangle}{\partial v}.$$

$$L e^{QLs} L \to \partial_v D_{k,\omega} \partial_v$$

[similar structure]

$\leftrightarrow \tau_c \quad k'+k,\ \omega'+\omega$

→ Simplifying the Non-Markovian Master Eqn.

$$\frac{\partial}{\partial t} P_1 = PLP\rho(t) + PLe^{QLt} Q\rho(0) + \int_0^t \underbrace{\phi(s)}_{\text{kernel}} \rho(t-s)\, ds$$

$$L = L_a + L_b + L_i$$

$$= \underbrace{L_0}_{\substack{\text{zeroth order} \\ \text{decoupled Liouvillian} \\ \text{operator}}} + L_i$$

L_i → a, b interacting Liouville operator

Then, like Schroedinger → Heisenberg
(Zwanzig → states) (Mori → follows Kubo)

$$\rho \equiv e^{-L_0} \rho(a,b,t)$$

$$L_0 = L_a + L_b$$

$$L_i(t) = e^{-L_0 t} L_i e^{L_0 t}$$

$$\boxed{\partial_t \, \rho(t) = L_i(t) \, \rho(t)}$$

i.e.

$$\partial_t \left(e^{-L_0 t} \rho(q, p, t) \right) =$$

$$e^{-L_0 t} \left(-L_0 \rho + \frac{\partial \rho}{\partial t} \right) =$$

$$\left(e^{-L_0 t} L_i e^{L_0 t} \right) \left(e^{-L_0 t} \rho \right)$$

$$-L_0 \rho + \frac{\partial \rho}{\partial t} = L_i \rho$$

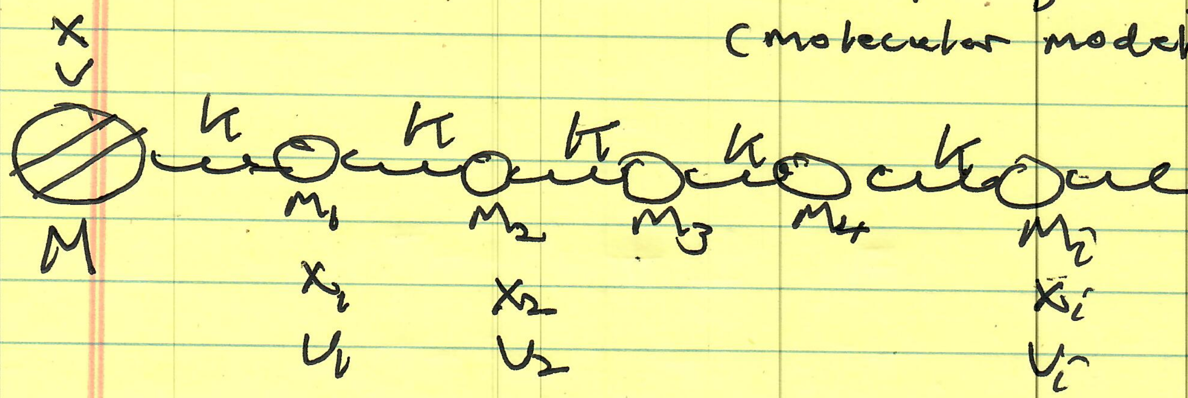
$$\frac{\partial \rho}{\partial t} = (L_0 + L_i) \rho$$

Note: Understood that exponential to be calculated ala'

$$\overleftarrow{\exp} \left[\int_0^t A(s) \, ds \right] = 1 + \sum_{r=1}^{\infty} \frac{(-1)^r}{r!} \int_0^t ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{r-1}} ds_r \, \overleftarrow{T} \left[A(s_1) \cdots A(s_r) \right]$$

→ Linear Chain → A Case Study

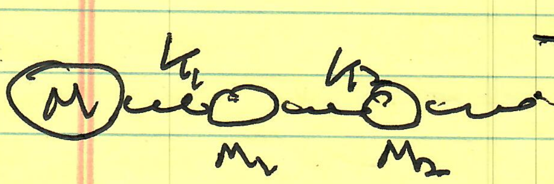
- Chain of springs with constant k and masses $M \gg m_1, m_2, \dots m_N$ (molecular model)



$$\omega^2_{\substack{\text{end}\\\text{mass}}} = \frac{k}{M} \ll \omega_i^2 = \frac{k}{m}$$

slow, relevant — fast irrelevant

- Application – Linear Chain



→ thermal noise (real case entropic)

Now → tweak with a laser

⇒ output is spectra ⇒ mode frequencies.

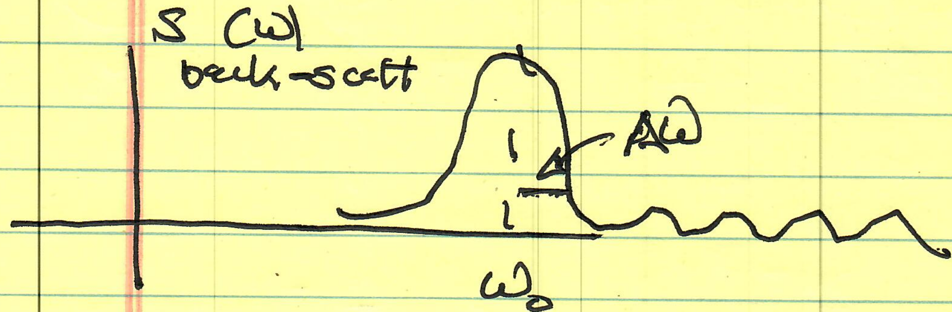
but recall:

$$\omega_0^2 = \frac{k}{M} \ll \omega_i^2$$

ω_0^2: relevant, slow

ω_i^2: fast irrelevant

→ suggests small masses motion constitute noise for slow mode



→ What is $\Delta\omega_0$? → relaxation rate of of low frequency mode

→ But relaxation rate set by kicks due fast modes ⟺ background effective noise.
calculate

⇒ MZT useful in calculating relaxation rates for slow modes in complex systems.

Aside: How calculate line width ?

→ Then, write down equations of motion, each mass:

{all k same

$\dot{x} = v$
$\dot{v} = -\frac{k}{M}(x - x_1)$

$\dot{x}_1 = v_1$
$\dot{v}_1 = -\frac{k}{m_1}(x_1 - x_2) - \frac{k}{m}(x_1 - x)$

$\vdots$

$x_i = v_i \quad , \quad \dot{v}_i = -\frac{k}{m_{i+1}}(x_i - x_{i-1}) - \frac{k}{m_{i+1}}(x_i - x_{i+1})$

To simplify, work in relative coordinates only:

$\delta x_0 = x - x_1$
$\delta x_1 = x_1 - x_2$
$\delta x_i = x_i - x_{i+1}$

so, EOMs in simplest form:

$\delta \dot{x}_0 = v$
$\delta \dot{x}_i = v_i - v_{i+1}$
$\delta \dot{x}_1 = v - v_1$

$\dot{v} = -\frac{k}{M}\delta x_0$

$\dot{v}_1 = \frac{k}{m_1}\delta x_0 - \frac{k}{m_1}\delta x_1$

+ from $-(x_1 - x)$

$\dot{v}_i = \frac{k}{m_i}\delta x_{i-1} - \frac{k}{m_i}\delta x_i$

so now construct Liouvillian:

$$L = \underbrace{\frac{dx}{dt}\frac{\partial}{\partial x} + \frac{dv}{dt}\frac{\partial}{\partial v}}_{M} + \sum_j \left(\frac{d}{dt}\delta x_j \frac{\partial}{\partial \delta x_j} + \frac{dv_j}{dt}\frac{\partial}{\partial v_j} \right).$$

where: $\Rightarrow \frac{d}{dt}\delta x_j = (v_j - v_{j+1})$

$$\frac{dv_j}{dt} = \frac{k}{m_j}\delta x_{j-1} - \frac{k}{m}\delta x_j$$

$$\rightarrow \dot{v} = -\frac{k}{M}\delta x_0$$

x variable absorbed into δx_0

so

$$L = \left[-\frac{k}{M}\delta x_0 \frac{\partial}{\partial v} + \left[(v - v_1)\frac{\partial}{\partial \delta x_0} \right] \right]$$

$$+ \left[\left(\frac{k}{m}\delta x_0 - \frac{k}{m}\delta x_1 \right) \frac{\partial}{\partial v_1} \right] + \left(v_1 - v_2 \right) \frac{\partial}{\partial \delta x_1} \Bigg]$$

$$+ \left(\frac{k}{m_1}\delta x_1 - \frac{k}{m}\delta x_2 \right) \frac{\partial}{\partial v_2}$$

$+ \ldots$

$$+ (v_i - v_{i+1}) \frac{\partial}{\partial \delta x_i} + \left(\frac{k_i}{m_i} \delta x_{i-1} - \frac{k_i}{m_i} \delta x_i \right) \frac{\partial}{\partial v_{i+1}}$$

This yields Liouville equation:

$$\frac{\partial}{\partial t} \rho + \nabla_\Gamma \cdot \left[V_\Gamma \rho \right] = 0$$

$\nabla \cdot V_\Gamma = 0$ Hamiltonian

$$\frac{\partial \rho}{\partial t} + L\rho = 0 , \qquad L = V_\Gamma \cdot \nabla_\Gamma$$

remains to decompose L

As before:

- need decompose into $\begin{cases} \text{relevant (a) (slow)} \\ \text{irrelevant (b) (fast)} \\ \text{interaction (c)} \end{cases}$ parts

- $\omega_0^2 = \frac{k}{M} \ll \omega_j^2 = \frac{k}{m_j}$

slow (variable) frequency

but

- using relative coordinates ⇒ no isolated slow variables i.e.

$$\delta x_0 = \underset{\text{slow}}{x_0} - \underset{\text{fast}}{x_1}$$

- $L_a \equiv 0$

$$L_i = -\frac{k}{m}\,\delta x_0 \frac{\partial}{\partial V} + V \frac{\partial}{\partial \delta x_0}$$

↓
interaction

$$\delta x_0 = \underbrace{x}_{s} - \underbrace{x_1}_{f}$$

- $L_b \equiv$ irrelevant (fast) Liouvillian; fast variable

above

$$L_b \equiv (\cancel{V} - V_1)\frac{\partial}{\partial \delta x_0} + \left(\frac{k}{m_1}\delta x_0 - \frac{k}{m}\delta x_1\right)\frac{\partial}{\partial V_1}$$

$$+ (V_1 - V_2)\frac{\partial}{\partial \delta x_1} + \left(\frac{k}{m_1}\delta x_1 - \frac{k}{m_2}\delta x_2\right)\frac{\partial}{\partial V_2}$$

$$\vdots$$

$$(V_i - V_{i+1})\frac{\partial}{\partial \delta x_i} + \left(\frac{k}{m_i}\delta x_{i-1} - \frac{k}{m}\delta x_i\right)\frac{\partial}{\partial V_{i+1}}$$

so $L = \cancel{L_a} + L_i + L_b$

$$\frac{\partial \rho}{\partial t} = L\rho$$

$$\Rightarrow \quad \frac{\partial \rho}{\partial t} + \underline{V}_\Gamma \cdot \underline{\nabla}_\Gamma \, \rho = 0 \qquad \text{as} \qquad \underline{\nabla} \cdot \underline{V}_\Gamma = 0$$

(Hamiltonian)

Now:

→ integrate out the fast variables

→ need $\rho_{eq}(b)$ → fast equilibrium distribution

→ recall $\underline{P} = \rho_{eq}(b) \int db$

⇒ can write:

$$\rho_{eq}(\delta x_i; v_i) = \prod_{i=1}^{N} \exp\left[-\delta x_i^2 / 2\Delta_i^2\right] * \exp\left[-v_i^2 / 2\langle v_i^2 \rangle\right]$$

factorize, for each d.o.f.

Gaussian convenient (moments converge)

→ thermalization assumption

For eqbrm:

- $L_b \, P_{eq}(b) = 0$ $\Leftrightarrow$ explicit FDT (noise + damping)
- Form: CLT

Then,

$$L_b \, P_{eq}(b) = 0$$

then

$$(v - v_1)\frac{\delta x_0}{\Delta_0^2} + \left(\frac{k}{m_1}\delta x_0 - \frac{k}{m_1}\delta x_1\right)\frac{v_1}{\langle v_1^2\rangle}$$

$$+ (v_1 - v_2)\frac{\delta x_1}{\Delta_1^2} + \left(\frac{k}{m_2}\delta x_1 - \frac{k}{m_1}\delta x_2\right)\frac{v_2}{\langle v_2^2\rangle}$$

if $\quad \dfrac{1}{\Delta_0^2} = \dfrac{k}{m_1 \langle v_1\rangle^2} \quad \Rightarrow \quad \dfrac{m\langle v_1^2\rangle}{2} = \dfrac{k\Delta_0^2}{2}$

$$v_1 \frac{\cancel{\delta x_1}}{\Delta_1^2} = \frac{k}{m_1}\frac{\cancel{\delta x_1}}{\langle v_1^2\rangle} \qquad \frac{m\langle v_2^2\rangle}{2} = \frac{k\Delta_1^2}{2}$$

$\vdots$ $\qquad\qquad$ $\vdots$

⇒ "sequential equipartition thru chain"!

$$\boxed{\frac{k}{2}\Delta_j^2 = \frac{m}{2}\langle v_{j+1}^2\rangle}$$

needed

then $\boxed{L_0\, \rho_{eq}(b) = 0}$

Recall: $L_i = -\frac{k}{m} dx_0 \frac{\partial}{\partial v} + v\frac{\partial}{\partial dx_0}$

For total equilibrium:

$$\rho = C \exp\left[-v^2/2\langle v^2\rangle\right]\rho_{eq}(b)$$

$$M\langle V^2\rangle = k\langle\Delta_0^2\rangle = \ldots m\langle v_i^2\rangle$$

so, for projection,

$$\underline{P}\,\rho(v, b, t) = \rho_{eq}(b)\int db\, \rho(v, b, t)$$

→ Now, to construct Master equation:

$\mathcal{L} = L_i$

– recall derived:

i.c.

$$\frac{\partial}{\partial t} P\rho = P\mathcal{L}_i(t)\,P\rho(t) + P\mathcal{L}_i\,\overleftarrow{\exp}\left[\int_0^t ds\, Q\mathcal{L}_i(s)\right] Q\rho(0)$$

$$+\int_0^t ds\, \underbrace{P\mathcal{L}_i(t)\,\overleftarrow{\exp}\left[\int_s^t ds_1\, Q\mathcal{L}_i(s_1)\right] Q\mathcal{L}_i(s)\, P\rho(s)}_{\text{Memory kernel}}$$

higher order interaction effect

Now – ignore h.o. interactions, implicit in exponential

$\exp[\;\;] \approx 1$. → short τ_{c}

so

$$\frac{\partial}{\partial t}\rho_1 = \int_0^t ds\, P\mathcal{L}_i(t)\,\mathcal{L}_i(s)\,P\rho(s)$$

$$\frac{\partial}{\partial t}\tilde{\rho}_1(t) = \int_0^t ds\; \underline{\underline{P}}\; \mathcal{L}_i(t)\, \mathcal{L}_i(s)\, \tilde{\rho}_1(s)$$

$$\left\{ \begin{array}{l} \rho_1 = \rho/\rho_{eq}(v) \\ \text{absorb } \rho_{eq}(v) \\ \text{in } \rho_{eq}(b) \end{array} \right.$$

or

$$\overset{\text{Kernel}}{\downarrow}$$

$$\Phi = e^{-\mathcal{L}_0(t-s)}\; \underset{\text{truncate (slow)}}{\Phi_B(t-s)}$$

$$\Phi_B(t-s) = \underline{P}\,\mathcal{L}_1\, e^{(\cancel{\mathcal{L}_a} + \mathcal{L}_b)(t-s)}\,\mathcal{L}_1\, P$$

Thus can finally write non-Markovian Master equation for reduced system as:

$$\boxed{\begin{aligned} \frac{\partial \rho(y,t)}{\partial t} &= \underbrace{\frac{1}{\rho_{eq}(b)}}_{\text{to cancel piece of } \underline{P}} \int_0^t \underbrace{\Phi_B(t-s)}_{\text{Kernel}}\, \rho_{eq}(b)\, \rho(y,s)\, ds \\[2ex] \Phi_B &= \underline{P}\,\mathcal{L}_i\, e^{-\mathcal{L}_b(t-s)}\,\mathcal{L}_i\, \underline{P} \end{aligned}}$$

Now:

- time scale for $\rho(V,t)$

$$\frac{1}{\rho}\frac{\partial \rho}{\partial t} \sim \frac{1}{\tau_{slow}}$$

$\tau_{slow} \gg \tau_{slow-fast}$ memory $\rightarrow$ characteristic time of memory kernel

- so, take Markovian limit -

$$\boxed{\begin{aligned} &\frac{\partial \rho}{\partial t} = \mathcal{L}_{eff}\,\rho \quad * \qquad \rho = \rho(V,t) \\ &\mathcal{L}_{eff} = \frac{1}{\rho_{eq}(b)} \int_0^\infty ds\, \Phi_B(s)\, \rho_{eq}(b) \\ &\Phi_B = P\mathcal{L}_i\, \underbrace{e^{-\mathcal{L}_b(t-s)}}_{\text{kernel}}\, \mathcal{L}_i P \end{aligned}}$$

i.e. $\frac{\partial \rho}{\partial t} = \frac{-1}{\tau_{eff}}\rho$ $\qquad 1/\tau_{eff} \equiv |\mathcal{L}_{eff}|$ *

→ An Explicit Evaluation

$$\mathcal{L}_i = -\frac{k}{M}\,\delta x_0 \frac{\partial}{\partial v} + v\frac{\partial}{\partial \delta x_0}$$

$$\underline{P} = \rho_{eq}(b)\int db\ \rho(a, b, t)$$

b includes δx_0 → relative separation

Also useful to recall:

$$\rho_{eq}(b) = (\text{const})\prod_{i=1}^{N} \exp\left[-\delta x_{i-1}^2/2\Delta_i^2\right]\exp\left[-V_{i-1}^2/2\langle V_{i-1}^2\rangle\right]$$

so

$$\underline{P}\ v\frac{\partial}{\partial \delta x_0} = \int dx_0\ v\frac{\partial}{\partial \delta x_0}$$

$$= 0$$

so only $\partial/\partial v$ pieces $\mathcal{L}_i$ survive!

→ should recall $\partial/\partial v$ acts on
$\rho_{eq}(v, b)$

$$\rho = \rho_{eq} \frac{\rho}{\rho_{eq}}$$

from ρ_{eq}

$$\mathcal{L}_i = \frac{k}{M} \delta x_0 \left(\frac{\partial}{\partial v} + \frac{v}{v_T^2} \right) - v \left(\cancel{\frac{\partial}{\partial \delta x_0}} + \frac{k \delta x_0}{T} \right)$$

so on absorbed in $\mathcal{L}_i^2$!

so for $\mathcal{L}_{eff}$:

$$\mathcal{L}_{eff} = \frac{1}{\rho_{eq}(b)} \left(\int_0^\infty ds \, P \, \mathcal{L}_i \, e^{-\mathcal{L}_0 (t-s)} \mathcal{L}_i P \right) \rho_{eq}(b)$$

$$= \frac{1}{\rho_{eq}(b)} \left[\int_0^\infty ds \, \rho_{eq}(b) \int db \left(\frac{k}{M} \delta x_0 \left(\frac{\partial}{\partial v} + \frac{v}{v_T^2} \right) - v \frac{k \delta x_0}{T} \right) e^{-\mathcal{L}_0 (t-s)} \left(\frac{k}{M} \delta x_0 \left(\frac{\partial}{\partial v} + \frac{v}{v_T^2} \right) - \frac{v k \delta x_0}{T} \right) \times \right.$$

$$\rho_{eq} \int db \, \rho_{eq}(b)$$

As: $\langle \delta x_0 \rangle = 0$

$P \mathcal{L}_t P = 0$ (obv.)

Have: $$\mathcal{L}_{eff} = \left(\frac{k}{M}\right) \Phi(0) \left(\langle v^2 \rangle \frac{\partial^2}{\partial v^2} + \frac{\partial}{\partial v} v \right)$$

$$\Phi(z) = \int_0^\infty dt\, e^{-zt} \frac{\langle \delta x_0 \, \delta x_0(t) \rangle_{eq}}{T}$$

$$\Phi(0) = \frac{k}{M} \Phi(z) \Big|_{z=0}$$ → Kubo!

and

times v

$$\frac{\partial}{\partial t} \rho(v,t) = \mathcal{L}_{eff}\, \rho(v,t)$$
$$= \frac{k}{M} \Phi(0) \left\{ \langle v^2 \rangle \frac{\partial^2}{\partial v^2} + \frac{\partial}{\partial v} v \right\} \rho(v,t)$$

→ as Markovian ↔ Fokker-Planck form!

→ Note can re-write in Fokker-Planck Form:

$$\frac{\partial \rho}{\partial t} = \frac{\partial^2}{\partial v^2}(D\rho) - \frac{\partial}{\partial v}(\beta v \rho)$$

where

$$D \equiv \int_0^\infty \rho_{eq}(h)\, \frac{k^2}{M^2}\, \rho\, \delta x_0\, e^{L_0(t-\tau)}\, \delta x_0\, \rho_{eq}(h)\, d(t-\tau)$$

$$\beta = T \int_0^\infty \rho_{eq}^{-1}(h)\, \frac{k}{M}\, \delta x_0\, e^{L_0(t-\tau)}\, \frac{\partial}{\partial \delta x_0}\, \rho_{eq}\, d(t-\tau)$$

Some observations:

- F-P eqn recovered in

  → weak interaction limit $\exp[\;] \approx 1$

  → Markovian

→ predictable

→ could go directly, by Kubo formalism approach

→ simplification of complex problem.

→ Major assumption:

- ρ_{eq} thermal distribution
- i.e. eq. for irrelevant

→ $D_{eff} = \frac{k}{M} \Phi(0) \langle V^2 \rangle$ $\left\{ \text{velocity space diffn} \right.$

$$\Phi(0) = \lim_{z \to 0} \int_0^\infty dt \, e^{-zt} \frac{\langle \delta X_0 \delta X(t) \rangle_{eq}}{\langle \delta X(0)^2 \rangle_{eq}}$$

a la' Kubo.

- Questions:
  - higher order → D_{eff} renormalized

$$\frac{k}{M} \Phi(0) = \underbrace{\gamma_v}_{\text{friction}} \Rightarrow \gamma_v + \delta\gamma_v$$

i.e. consider simple case

$$\Phi(t) = \frac{\langle \delta X_0 \delta X_0(t) \rangle}{\langle \delta X_0^2 \rangle} = e^{-\gamma_0 t}$$

(usual)

i.e. $\gamma_v = \frac{k/M}{\gamma_c}$

$\delta\gamma_v \sim \frac{(k/M)^2}{\gamma_c^3}$

⇒ Left out ?

- time scale separation arbitrary ⇒ scalings, etc
- adiabatic variation of fast variables

adiabatic elimination ⇒ adiabatic evolution

also feedback in modulations.

etc.