II.1.E Projection Operators

Short-time expansion of correlation functions tedious and limited in scope

different approach: projection of full dynamics into subspaces of relevant and irrelevant variables

Definitions:

n fluctuating variables $|A_i\rangle$, $i=1..n$

matrix of correlation functions

$$C_{ij}(t) = \langle A_i(t) | A_j\rangle = \langle e^{i\mathcal{L}t} A_i | A_j\rangle$$
$$= \langle A_i | e^{-i\mathcal{L}t} | A_j\rangle$$

Hilbert space spanned by kets $|A_i\rangle$, $i=1, \dots n, n+1, .. n+m$

correlators in Fourier-Laplace domain

$$\hat{C}_{ij}(z) = \langle A_i | (\mathcal{L}-z)^{-1} | A_j\rangle$$

backwards Liouville operator $\mathcal{L}$

↳ resolvent operator $R(z) = (\mathcal{L}-z)^{-1}$

$R(z)$ needed only in subspace $|A_i\rangle$, $i=1..n$

Def: Projection operator

$$P = |A_i\rangle (C^{-1}_{ij}) \langle A_j| \, , \quad i=1..n$$

with static overlaps $C_{ij} = \langle A_i | A_j \rangle$

$= C_{ij}(t=0)$

property of projection $P^2 = P$, $P^2|x\rangle = P|x\rangle$

idempotent

also $P^+ = P$, adjoint operator

orthogonal projection operator $Q = \mathbb{1} - P$

also $Q^2 = Q = Q^+$

$Q|x\rangle \perp P|x\rangle \Leftrightarrow \langle Qx | Px \rangle = \langle x | Q^+ P | x \rangle = 0$

def: reduced Liouville operator $\mathcal{L}_Q = Q\mathcal{L}Q$

goal: block representation of resolvent

$$R(z) = \begin{array}{c} \begin{pmatrix} R_{pp}(z) & R_{pq}(z) \\ R_{qp}(z) & R_{qq}(z) \end{pmatrix} \begin{array}{l} \}\, n \\ \}\, m \end{array} \\ \begin{array}{cc} \underbrace{\qquad\qquad}_{n} & \underbrace{\qquad\qquad}_{m} \end{array} \end{array}$$

respecting resolvent equation $\boxed{(\mathcal{L} - z) R(z) = \mathbb{1}}$

$$\begin{pmatrix} \mathcal{L}_{pp} - z\cdot\mathbb{1}_n & \mathcal{L}_{pq} \\ \mathcal{L}_{qp} & \mathcal{L}_{qq} - z\mathbb{1}_m \end{pmatrix} \begin{pmatrix} R_{pp} & R_{pq} \\ R_{qp} & R_{qq} \end{pmatrix} = \begin{pmatrix} \mathbb{1}_n & 0 \\ 0 & \mathbb{1}_m \end{pmatrix}$$

1st component $(\mathcal{L}_{pp} - z\mathbb{1}_n) R_{pp}(z) + \mathcal{L}_{pq} R_{qp}(z) = \mathbb{1}_n$

2nd component $\mathcal{L}_{qp} R_{pp}(z) + (\mathcal{L}_{qq} - z\mathbb{1}_m) R_{qp} = 0$

$\Rightarrow R_{QP}(z) = -(\mathcal{L}_{QQ} - z\mathbb{1}_m)^{-1} \mathcal{L}_{QP} R_{PP}(z)$

↳ into 1st component:

$$[\mathcal{L}_{PP} - z\mathbb{1}_n - \mathcal{L}_{PQ}(\mathcal{L}_{QQ} - z\mathbb{1}_m)^{-1}\mathcal{L}_{QP}] R_{PP}(z) = \mathbb{1}_n$$

$$\boxed{R_{PP}(z) = -[z\mathbb{1}_n - \mathcal{L}_{PP} + \mathcal{L}_{QP}(\mathcal{L}_{QQ} - z\mathbb{1}_m)^{-1}\mathcal{L}_{QP}]^{-1}}$$

strategy: choose n variables of interest, and hide difficult part in m variables, approximations guided by finding

for $\mathcal{L}_{QP}$ or $\mathcal{L}_{PQ} = 0 \Rightarrow R_{PP}(z) = (\mathcal{L}_{PP} - z\mathbb{1}_n)^{-1}$

R_{PP} acts only in $n \times n$ subspace

Mori-Zwanzig operator identity

$$\boxed{\begin{aligned} &(*)\quad (\mathcal{L} - z)^{-1} = (\mathcal{L}Q - z)^{-1} - (\mathcal{L}Q - z)^{-1}\mathcal{L}P(\mathcal{L} - z)^{-1} \\ &(**)\quad z(\mathcal{L} - z)^{-1} = z(\mathcal{L}Q - z)^{-1} \\ &\qquad\qquad - [\mathcal{L}Q(Q\mathcal{L}Q - z)^{-1}Q\mathcal{L} - \mathcal{L}]P(\mathcal{L} - z)^{-1} \end{aligned}}$$

proof: $(\mathcal{L}Q - z)\,(*)\,(\mathcal{L} - z)$

$\Rightarrow (\mathcal{L}Q - z) = (\mathcal{L} - z) - \mathcal{L}P \quad \| + \mathcal{L}P$

$\underbrace{\mathcal{L}Q + \mathcal{L}P}_{\mathcal{L}\mathbb{1}} - z = \mathcal{L} - z)$

$\square$

$(**)\quad z(\mathcal{L}Q - z)^{-1} = (z - \mathcal{L}Q + \mathcal{L}Q)(\mathcal{L}Q - z)^{-1} =$

$= \mathbb{1} + \mathcal{L}Q(\mathcal{L}Q - z)^{-1}$

$z\cdot(*)$: $z(\mathcal{L}-z)^{-1} = z(\mathcal{L}Q-z)^{-1}$
$$-[\mathcal{L}Q(\underset{Q}{\uparrow}\mathcal{L}Q-z)^{-1}\underset{Q}{\uparrow}\mathcal{L}-\mathcal{L}]P(\mathcal{L}-z)^{-1}$$
insert

with $Q\underset{Q}{\uparrow}(\mathcal{L}Q-z)^{-1}\underset{Q}{\uparrow} = -\frac{1}{z}Q\underset{Q}{\uparrow} - \frac{1}{z^2}Q\underset{Q}{\uparrow}\mathcal{L}Q\underset{Q}{\uparrow}+\dots$;

Theorem: Zwanzig-Mori Representation

dynamic correlation functions

$$\boxed{\hat{C}_{ij}(z) = \langle A_i|(\mathcal{L}-z)^{-1}|A_j\rangle}$$

follow the equation of motion

$$\boxed{[z\delta_{ij} - \Omega_{ij} + \hat{M}_{ij}(z)]\hat{C}_{jk}(z) = -C_{ik}}$$

with frequency matrix

$$\boxed{\Omega_{ik} = \langle A_i|\mathcal{L}|A_j\rangle\,(C^{-1})_{jk}}$$

and memory kernel

$$\boxed{\hat{M}_{ik}(z) = \langle Q\mathcal{L}A_i|(Q\mathcal{L}Q-z)^{-1}|Q\mathcal{L}A_j\rangle(C^{-1})_{jk}}$$

proof: $\langle A_i|(*)|A_m\rangle = z\hat{C}_{im}(z) =$

$= z\langle A_i|(\mathcal{L}Q-z)^{-1}|A_m\rangle$

$+ \langle A_i|\mathcal{L}|A_j\rangle(C^{-1})_{jl}\langle A_l|(\mathcal{L}-z)^{-1}|A_m\rangle$

$- \langle A_i|\mathcal{L}Q(Q\mathcal{L}Q-z)^{-1}Q\mathcal{L}|A_j\rangle(C^{-1})_{jl}\langle A_l|(\mathcal{L}-z)^{-1}|A_m\rangle$

use Neumann series: $\langle A_i|(\mathcal{L}Q-z)^{-1}|A_m\rangle = -\frac{1}{z}C_{im}(z)$ □

notes

(1) static overlaps $C_{ij} = \langle A_i | A_j \rangle$ and characteristic frequencies Ω_{ij} known from series expansion → simple part

Ω_{ij} represents dynamics in n×n space

(2) memory kernel $\hat{M}_{ij}(z)$ represents

difficult part

(3) reduced Liouvillian operator $\mathcal{L}_Q$ defines reduced resolvent operator

$$R_Q(z) = (\mathcal{L}_Q - z)^{-1}$$

that is driving dynamics for correlation function $\hat{M}_{ij}(z)$

Corollary: Mori-Zwanzig Equations of Motion

$$\boxed{[z(C^{-1})_{ij} - w_{ij} + \hat{m}_{ij}(z)]\, \hat{C}_{jk}(z) = -\delta_{ik}}$$

with $w_{il} = (C^{-1})_{ij} \langle A_j | \mathcal{L} | A_k \rangle (C^{-1})_{kl} = w_{li}^*$

$$\hat{m}_{il}(z) = (C^{-1})_{ij} \langle Q\mathcal{L} A_j | R_Q(z) | Q\mathcal{L} A_k \rangle (C^{-1})_{kl}$$

and in the time domain

$$\boxed{\frac{d}{dt} C_{ik}(t) - i\, \Omega_{ij} C_{jk}(t) + \int_0^t dt'\, M_{ij}(t-t') C_{jk}(t') = 0}$$

II.1.F Liquid Dynamics

application of of projection-operator formalism with $A_1 = \rho_q$ and $A_2 = j^L_q$

particle density $\rho_q = \sum_{i=1}^{N} e^{i\vec{q}\vec{R}_i}$

longitudinal current density $j^L_q = \sum_{i=1}^{N} \frac{\vec{q}}{q} \frac{\vec{p}_i}{m} e^{i\vec{q}\vec{R}_i}$

$q = |\vec{q}|$ modulus of wave vector

assume isotropic system $\rho_{\vec{q}} = \rho_q$

equations of motion, conservation laws

$$\boxed{\frac{d}{dt}\rho_q(t) = i\mathcal{L}\rho_q(t) = iq\, j^L_q(t)}$$

particle conservation

$$\boxed{\frac{d}{dt} j^L_q(t) = i\mathcal{L} j^L_q(t) - iq\,\sigma^L_q(t)}$$

conservation of longitudinal momentum

σ^L_q : longitudinal stress tensor

MZ-step 1: static overlaps and projection operator

$\langle \rho_q | \rho_q \rangle = N S_q$

$\langle j^L_q | j^L_q \rangle = N v_{th}^2$

$\langle j^L_q | \rho_q \rangle = 0$, parity, $\frac{p_i}{m} = v_i$ odd variable

$\langle \rho_q | j^L_q \rangle = 0$, parity

$$C_{ij} = \begin{pmatrix} N S_q & 0 \\ 0 & N v_{th}^2 \end{pmatrix}, \quad (C^{-1})_{ij} = \begin{pmatrix} 1/NS_q & 0 \\ 0 & 1/Nv_{th}^2 \end{pmatrix}$$

↳ projection operator

$$\boxed{P = |\rho_q\rangle \frac{1}{NS_q} \langle \rho_q| + |j_q^L\rangle \frac{1}{Nv_{th}^2} \langle j_q^L|}$$

MZ-step 2: frequency matrix

$$\langle \rho_q |\mathcal{L}| \rho_q\rangle = \langle \rho_q | iq\, j_q^L\rangle = 0, \text{ parity}$$

$$\langle j_q^L |\mathcal{L}| j_q^L\rangle = 0 \quad , \text{parity}$$

$\Rightarrow$ diagonal elements of Ω_{ij} zero

$$\langle j_q^L |\mathcal{L}| \rho_q\rangle = q\langle j_q^L | j_q^L\rangle = Nq\, v_{th}^2$$

$$= \langle \rho_q |\mathcal{L}| j_q^L\rangle$$

$$\Rightarrow \omega = \begin{pmatrix} \frac{1}{NS_q} & 0 \\ 0 & \frac{1}{Nv_{th}^2} \end{pmatrix} \begin{pmatrix} 0 & Nq\, v_{th}^2 \\ Nq\, v_{th}^2 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{NS_q} & 0 \\ 0 & \frac{1}{Nv_{th}^2} \end{pmatrix}$$

$$\omega = \begin{pmatrix} 0 & q v_{th}^2 / S_q \\ q & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{NS_q} & 0 \\ 0 & \frac{1}{Nv_{th}^2} \end{pmatrix}$$

$$\boxed{\omega = \begin{pmatrix} 0 & q/NS_q \\ q/NS_q & 0 \end{pmatrix}}$$

MZ-step 3: memory kernel

by construction $Q\mathcal{L}\rho_q = q\, Q j_q^L = 0$

$$Q\mathcal{L} j_q^L = q\, Q\sigma_q^L \quad \text{, slow for } q\to 0$$

$$\hat{m}_q(z) = \begin{pmatrix} \frac{1}{\sqrt{N S_q}} & 0 \\ 0 & \frac{1}{\sqrt{N v_{th}^2}} \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & \tilde{m}_{j\rho}(q,z) \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{N S_q}} & 0 \\ 0 & \frac{1}{\sqrt{N v_{th}^2}} \end{pmatrix}$$

$$\tilde{m}_{j\rho}(q,z) = q^2 \langle Q\sigma_q^L | R_Q(z) | Q\sigma_q^L\rangle$$

generalized longitudinal viscosity

$$\boxed{\frac{\hat{\Gamma}(q,z)}{mn} = \frac{1}{N v_{th}^2} \langle Q\sigma_q^L | R_Q(z) | Q\sigma_q^L\rangle}$$

MZ-step 4: equation of motion

dynamic structure factor $\hat{S}(q,z)$

$$\boxed{\hat{S}(q,z) = \frac{-S_q}{z - \dfrac{q^2 v_{th}^2/S_q}{z + q^2\hat{\Gamma}(q,z)/nm}}}$$

eom in time domain

$$\boxed{\frac{d^2}{dt^2} S(q,t) + \Omega_q^2 S(q,t) + \frac{q^2}{mn}\int_0^t dt'\, \Gamma_q(t-t')\, \partial_{t'} S(q,t')} \quad *$$

generalized harmonic oscillator