$$|A\rangle \qquad P = \frac{|A\rangle\langle A|}{\langle A|A\rangle} \qquad \langle A|B\rangle = \int d\Gamma\, A^*(\Gamma) B(\Gamma) \rho(\Gamma)$$

$$Q = 1 - P$$

$$C(\omega) = \langle A | i(\omega + L)^{-1} | A\rangle$$

$$= \int_0^\infty dt\, e^{i\omega t} \langle A | e^{iLt} | A\rangle = \ldots$$

$$\ldots = -\frac{\langle A|A\rangle}{i\omega + \Omega - M(\omega)} \quad \text{where}$$

$$\Omega = \frac{\langle A | iL | A\rangle}{\langle A|A\rangle}, \qquad M(\omega) = \frac{\langle R | i(\omega + LQ)^{-1} | R\rangle}{\langle A|A\rangle} \quad \text{memory function}$$

frequency

$$|R\rangle = Q iL |A\rangle \quad \text{"stochastic force"}$$

Study $\mu(\omega) = \langle R | i(\omega + \mathcal{L}Q)^{-1} | R \rangle$

vs. $\rho(\omega) = \langle R | i(\omega + \mathcal{L})^{-1} | R \rangle$

?

Special case: $i\mathcal{L}|A\rangle$ is already in the ~~past~~ space

$$Q\, i\mathcal{L}|A\rangle = i\mathcal{L}|A\rangle = |R\rangle$$

$$\langle A | i\mathcal{L} | A \rangle = 0 \Rightarrow \Omega = 0 \quad \text{last lect.}$$

$$(\omega+\mathcal{L})^{-1} = \underline{(\omega + \mathcal{L}Q)^{-1}} - (\omega + \mathcal{L}Q)^{-1}\mathcal{L}P(\omega+\mathcal{L})^{-1}$$

$$P = \frac{|A\rangle\langle A|}{\langle A|A\rangle}$$

$$\frac{1}{i}\rho(w) = \frac{1}{i}\mu(w) - \langle A | \mathcal{L}(w + \mathcal{L}Q)^{-1}\mathcal{L}P(w+\mathcal{L})^{-1}\mathcal{L}|A)$$

$$= \frac{1}{i}\mu(w) - \frac{1}{(A|A)}\langle A|\mathcal{L}(w+\mathcal{L}Q)^{-1}\mathcal{L}|A)\langle A|(w+\mathcal{L})^{-1}\mathcal{L}|A)$$

$$= \frac{1}{i}\mu(w) - \frac{1}{(A|A)}\frac{1}{i}\mu(w)\langle A|(w+\mathcal{L})^{-1}\mathcal{L}|A)$$

<u>Now</u>, $\langle A|(w+\mathcal{L})^{-1}\mathcal{L}|A) = \frac{1}{w}\langle A|\left(1+\frac{\mathcal{L}}{w}\right)^{-1}\mathcal{L}|A) =$

$$= \frac{1}{w}\langle A|\left(1-\frac{\mathcal{L}}{w}+\frac{\mathcal{L}^2}{w^2}-\frac{\mathcal{L}^3}{w^3}\cdots\right)\mathcal{L}|A) =$$

$$\underbrace{(A|\mathcal{L}|A)}_{=0}$$

$$= \left\langle A \,\middle|\, \overbrace{1 - \frac{\ell^2}{\omega^2}\left(1 + \frac{\ell}{\omega}\right)^{-1}} \,\middle|\, A \right\rangle =$$

$$= \left\langle R \,\middle|\, -\frac{1}{\omega^2}\left(1 + \frac{\ell}{\omega}\right)^{-1} \,\middle|\, R \right\rangle =$$

$$= -\frac{1}{\omega} \left\langle R \,\middle|\, (\omega + \ell)^{-1} \,\middle|\, R \right\rangle = -\frac{1}{i\omega}\,\rho(\omega)$$

$$\Rightarrow \frac{1}{i}\,\rho(\omega) = \frac{1}{i}\,\mu(\omega) - \frac{1}{\langle A | A \rangle}\,\frac{1}{i}\,\mu(\omega)\left(-\frac{1}{i\omega}\,\rho(\omega)\right)$$

$$\Big| \cdot \frac{i}{\rho(\omega)\,\mu(\omega)}$$

$$\boxed{\frac{1}{\mu(\omega)} = \frac{1}{\rho(\omega)} + \frac{1}{i\omega\langle A|A\rangle}}$$

$$\frac{\rho(\omega)}{\mu(\omega)} = 1 + \frac{\rho(\omega)}{i\omega\langle A/A\rangle}$$

$$\frac{\mu(\omega)}{\rho(\omega)} = \frac{1}{1 + \frac{\rho(\omega)}{i\omega\langle A|A\rangle}} \overset{??}{\approx} 1$$

YES, for hydro-dynamic variables in the hydrodynamic limit hydrodynamics $\equiv$ conservation law

+ local dynamics

+ large length & time scales

$$\int d^3\vec{r}\ \phi(\vec{r},t) = \text{const.} \Rightarrow$$

$$\frac{\partial}{\partial t}\phi(\vec{r},t) + \vec{\nabla}\cdot\vec{j} = 0$$

$\vec{j}$ → some current

ϕ ↑ conserved field

$$\tilde{\phi}(\vec{k},t) := \int d^3\vec{r}\ \phi(\vec{r},t)\, e^{-i\vec{k}\cdot\vec{r}}$$

$$\tilde{\vec{j}}(\vec{k},t) := \int d^3\vec{r}\ \vec{j}(\vec{r},t)\, e^{-i\vec{k}\cdot\vec{r}}$$

$$\frac{\partial}{\partial t}\tilde{\Phi}(\vec{k},t) + \int d^3\vec{r}\, e^{-i\vec{k}\cdot\vec{r}}\, \vec{\nabla}\cdot\vec{j} = 0$$

$$\frac{\partial}{\partial t}\tilde{\Phi}(\vec{k},t) + i\vec{k}\cdot\vec{\tilde{j}}(\vec{k},t) = 0$$

$$\frac{\partial}{\partial t}\tilde{\Phi}(\vec{k},t) + i k_\alpha \underbrace{\tilde{j}_\alpha(\vec{k},t)}_{} = 0$$

$$= \tilde{j}^{(0)}_\alpha(t) + \tilde{j}^{(1)}_{\alpha\beta}(t)\, i k_\beta + O(k^2)$$

Set $|A) = \tilde{\Phi}(\vec{k}, t)$

$$iL|A) = \frac{d}{dt}|A) = \frac{\partial}{\partial t}\tilde{\Phi} = \underline{-ik_\alpha \tilde{j}_\alpha}$$

$$(A|iL|A) = -ik_\alpha \langle \tilde{\Phi}^*(\vec{k}, t=0)\, j_\alpha(\vec{k}, t=0) \rangle$$

$$= 0 \quad \text{rotational symmetry}$$

$\Omega = 0$, $|R) = -ik_\alpha \tilde{j}_\alpha$

<u>assume</u>: $\tilde{j}$ is <u>not</u> conserved

$$(R|i(\omega + L)^{-1}|R) \propto k^2$$

$$\langle R | (\omega + k Q)^{-1} | R \rangle \propto k^2 \quad \underline{\underline{\text{for all } \omega}}$$

$$\mu(\omega) \propto k^2 \qquad \frac{\mu(\omega)}{\rho(\omega)} = \frac{1}{1 + \frac{\rho(\omega)}{i\omega \langle A | A \rangle}}$$

$$\rho(\omega) \propto k^2$$

$$\underset{k \to 0}{\simeq} 1 \qquad \underline{\text{first}} \quad k \to 0$$

$$\underline{\text{then}} \quad \omega \to 0$$

Example 1: Brownian motion

one particle, coord. $\vec{R}$, mom. $\vec{P}$, mass m

$$\underbrace{|A) = \exp(i\vec{k}\cdot\vec{R})}_{= \int d^3\vec{r}\, e^{i\vec{k}\vec{r}}\, \delta(\vec{r}-\vec{R}(t))} \underset{\vec{k}=k\hat{e}_x}{=} \exp(ikR_x)$$

$$\int d^3\vec{r}\, \underbrace{\delta(\vec{r}-\vec{R}(t))}_{\phi(\vec{r},t)} = 1$$

$$i\mathcal{L}\,|A) = \frac{d}{dt}|A) = \frac{d}{dt}\exp(i\vec{k}\cdot\vec{R}) =$$

$$= \exp(i\vec{k}\cdot\vec{R})\, i\vec{k}\cdot\frac{\vec{P}}{m} = \exp(ikR_x)\, ik\frac{P_x}{m}$$

$$(A|i\mathcal{L}|A) = \frac{ik}{m}\left\langle e^{-ikR_x} P_x\, e^{ikR_x}\right\rangle =$$

$$= \frac{ik}{m}\langle P_x\rangle = 0 \qquad \Omega = 0$$

$$|R) = ik\frac{P_x}{m}\exp(ikR_x) \qquad (A|A) = 1$$

Memory function:

$$M(\omega) = \underbrace{\frac{1}{(A|A)}}_{=1} \left(R \middle| i(\omega + L Q)^{-1} \middle| R \right) =$$

hydrodyn. limit

$$= \left(R \middle| i(\omega + L)^{-1} \middle| R \right) =$$

$$= \int_0^\infty dt\, e^{i\omega t} \langle R^*(0)\, R(t) \rangle =$$

$$= \frac{k^2}{m^2} \int_0^\infty dt\, e^{i\omega t} \langle P_x(0) \underbrace{e^{-ikR_x(0)}}_{\to 1} P_x(t) \underbrace{e^{+ikR_x(t)}}_{\to 1} \rangle$$

$$\underset{k \to 0}{\simeq} \frac{k^2}{m^2} \int_0^\infty dt\, e^{i\omega t} \langle P_x(0)\, P_x(t) \rangle =$$

$$= k^2 \int_0^\infty dt\, e^{i\omega t} \langle v_x(0)\, v_x(t) \rangle$$

velocity autocorrelation function

$\omega \to 0$ limit

$$\underline{M(\omega = 0)} = k^2 \int_0^\infty dt \langle v_x(0)\, v_x(t) \rangle = D k^2$$

diffusion constant

approximated memory eq.:

$$C(\omega) = -\frac{1}{i\omega + 0 - Dk^2} = \underline{\underline{\frac{1}{Dk^2 - i\omega}}}$$

random walk model: $R_x(t)$ Gaussian random variable

$$\langle [R_x(t) - R_x(0)]^2 \rangle = 2Dt$$

$$\Rightarrow C(t) = \langle A^*(0)\, A(t) \rangle =$$

$$= \langle \exp(-ik R_x(0)) \exp(+ik R_x(t)) \rangle =$$

$$= \langle \exp(ik \underbrace{(R_x(t) - R_x(0))}_{\text{Gaussian}}) \rangle$$

$$= \exp\left(-\frac{k^2}{2} \langle (R_x(t) - R_x(0))^2 \rangle\right) =$$

$$= \exp\left(-\frac{k^2}{2}\, 2Dt\right) = \exp(-Dk^2 t)$$

diffusive decay

$$\Rightarrow C(\omega) = \int_0^\infty dt\, e^{i\omega t} \exp(-Dk^2 t) =$$

$$= -\frac{1}{i\omega - Dk^2} = \underline{\underline{\frac{1}{Dk^2 - i\omega}}}$$

<u>we get:</u> – random walk model

– Green-Kubo for D

Example 2

$$\vec{k} = k\, e_x$$

$$|A) = \exp(i\vec{k}\cdot\vec{P}) = \int d^3\vec{p}\, e^{i\vec{k}\cdot\vec{p}}\, \delta(\vec{p} - \vec{P}(t))$$

$$\int d^3\vec{p}\, \delta(\vec{p} - \vec{P}(t)) = 1$$

force

$$iL|A) = \frac{d}{dt}|A) = \frac{d}{dt}\exp(i\vec{k}\cdot\vec{P}) = ik F_x\, e^{i\vec{k}\cdot\vec{P}}$$

$$(A|iL|A) = ik\left(e^{-i\vec{k}\cdot\vec{P}} F_x\, e^{+i\vec{k}\vec{P}}\right) \propto (F_x) = 0$$

$$\Omega = 0 \qquad |R) = iL|A) = ikF_x\, e^{i\vec{k}\cdot\vec{P}}$$

$$(A|A) = (1) = 1$$

changing symbols from Ex 1 $\quad k \to 0$

$$\to \quad M(\omega) \simeq k^2 \int_0^\infty dt \, e^{i\omega t} \langle F_x(0) \, F_x(t) \rangle$$

$\omega \to 0$

$$M(\omega = 0) = k^2 \underbrace{\int_0^\infty dt \, \langle F_x(0) \, F_x(t) \rangle}_{\Gamma}$$

some transport coefficient

analogous to Ex. 1:

$$C(\omega) = \frac{1}{\Gamma k^2 - i\omega}$$

$$= \int_0^\infty dt\, e^{i\omega t} \left\langle \exp\left(i k \left[P_x(t) - P_x(0) \right] \right) \right\rangle$$

this describes a <u>random walk</u> process in P with

$$\boxed{\left\langle \left(P_x(t) - P_x(0) \right)^2 \right\rangle = 2 \Gamma t}$$

phenomenological model for momentum relaxation

$$\frac{d}{dt} p_x = -\frac{\xi}{m} p_x + \text{"noise"}$$

friction, ξ friction coefficient

$$\frac{d}{dt} \langle p_x(0)\, p_x(t) \rangle = -\frac{\xi}{m} \langle p_x(0)\, p_x(t) \rangle + 0$$

$$\langle p_x(0)\, p_x(t) \rangle = \langle p_x^2 \rangle \exp\left(-\frac{\xi}{m} t\right) = mT \exp\left(-\frac{\xi}{m} t\right)$$

$$\langle p_x^2 \rangle = 2m \left\langle \frac{p_x^2}{2m} \right\rangle = 2m \frac{T}{2} = mT$$

$$\langle v_x(0)\, v_x(t) \rangle = \frac{T}{m} \exp\left(-\frac{\xi}{m} t\right)$$

$$\underbrace{\int_0^\infty dt \, \langle v_x(0)\, v_x(t) \rangle}_{D} = \frac{T}{m} \frac{m}{\xi} = \frac{T}{\xi}$$

Einstein relation

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

$$= 2mT - 2mT \exp\left(-\frac{\xi}{m} t\right) =$$

$$= 2mT \left\{ 1 - \exp\left(-\frac{\xi}{m} t\right) \right\}$$

Study this for short times:

$$\langle (P_x(t) - P_x(0))^2 \rangle \simeq 2mT \frac{\xi}{m} t = 2\xi T t$$

Mori-Zwanzig:

$$\langle (P_x(t) - P_x(0))^2 \rangle = 2\Gamma t$$

$=$

$$\Gamma = \int_0^\infty dt \, \langle F_x(0) F_x(t) \rangle$$

$$\boxed{\xi = \frac{1}{T} \int_0^\infty dt \, \langle F_x(0) F_x(t) \rangle}$$

Green-Kubo for ξ