$\mathbb{R}^3$: $\vec{r} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$ $\quad |r\rangle$

$\vec{r}^T = (x, y, z)$ $\quad \langle r|$

$\left.\begin{matrix} |r\rangle \\ \langle r| \end{matrix}\right\} \langle r_1 | r_2 \rangle = $

$= x_1 x_2 + y_1 y_2 + z_1 z_2$

$\vec{r}_1^T \vec{r}_2 = (x_1, y_1, z_1) \begin{pmatrix} x_2 \\ y_2 \\ z_2 \end{pmatrix}$

$= x_1 x_2 + y_1 y_2 + z_1 z_2$

$|e_x\rangle \hat{=} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$

$|e_y\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$

$|e_z\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

$|r\rangle = x|e_x\rangle + y|e_y\rangle + z|e_z\rangle$

$$\langle r_1 | r_2 \rangle = \left\{ x_1 \langle e_x | + y_1 \langle e_y | + z_1 \langle e_z | \right\}$$

$$\left\{ x_2 | e_x \rangle + y_2 | e_y \rangle + z_2 | e_z \rangle \right\} =$$

$$= x_1 x_2 \underbrace{\langle e_x | e_x \rangle}_{1} + y_1 y_2 \underbrace{\langle e_y | e_y \rangle}_{1} + z_1 z_2 \underbrace{\langle e_z | e_z \rangle}_{1}$$

$$+ x_1 y_2 \underbrace{\langle e_x | e_y \rangle}_{0} + \underbrace{\ldots}_{0} =$$

$$= x_1 x_2 + y_1 y_2 + z_1 z_2$$

$$|r_1\rangle\langle r_2|$$

$$\begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix} (x_2, y_2, z_2) = \begin{pmatrix} x_1 x_2 & x_1 y_2 & x_1 z_2 \\ y_1 x_2 & y_1 y_2 & y_1 z_2 \\ z_1 x_2 & z_1 y_2 & z_1 z_2 \end{pmatrix}$$

$$= x_1 x_2 \underbrace{\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}}_{|e_x\rangle\langle e_x|} + x_1 y_2 \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \ldots$$

$$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} (1, 0, 0) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

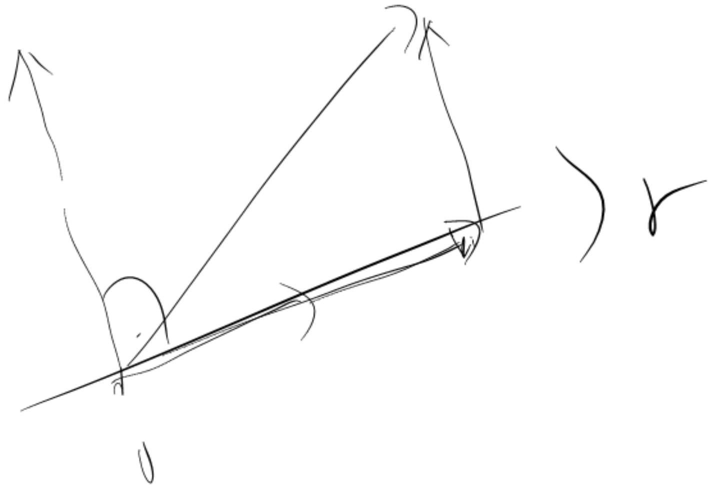
$$\hat{P} = \frac{|r\rangle\langle r|}{\langle r|r\rangle} = \text{projection operator}$$

$$\hat{P}|r\rangle = \frac{|r\rangle\langle r|r\rangle}{\langle r|r\rangle} = |r\rangle$$

λ scalar: $\quad \hat{P}\underline{\lambda|r\rangle} = \lambda\hat{P}|r\rangle = \underline{\lambda|r\rangle}$

u: $\quad |u\rangle \perp |r\rangle \quad ; \quad \langle u|r\rangle = 0$

$$\hat{P}|u\rangle = \frac{1}{\langle r|r\rangle}|r\rangle\underbrace{\langle r|u\rangle}_{=0} = 0$$



$/ \ \langle r|r\rangle$

$$P^2 = P: \quad \frac{|r\rangle\langle r|}{\langle r|r\rangle}\,\frac{|r\rangle\langle r|}{\langle r|r\rangle} =$$

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

$$Q = 1 - P$$

projection onto the orthogonal space

let $|u\rangle$ be an arbitrary vector

$$\langle r | \underbrace{Q|u\rangle}_{\text{image}} = \langle r|u\rangle - \langle r|P|u\rangle =$$

$$= \langle r|u\rangle - \langle r| \frac{|r\rangle\langle r|}{\langle r|r\rangle} |u\rangle = 0 \checkmark$$

$$Q^2 = (1-P)^2 = 1 - 2P + P^2 =$$

$$= 1 - 2P + P = 1 - P = Q$$

$$\langle A | B \rangle = \int d\Gamma \, A^*(\Gamma) \, B(\Gamma) \, \rho(\Gamma)$$

$$\frac{d}{dt} | A \rangle = i \underbrace{\mathcal{L}}_{\text{Liouville}} | A \rangle$$

$$(A | B) = \int d\Gamma \, A^*(\Gamma) \, B(\Gamma)$$

$\mathcal{L}$ is self-adjoint wrt. $(\, | \,)$ <u>and</u> $\langle \, | \, \rangle$

$$| A(t) \rangle = e^{i\mathcal{L}t} | A(0) \rangle$$

$$\langle B^*(0)\, A(t) \rangle_{th} = \langle B | A(t) \rangle =$$

$$= \langle B | e^{iLt} | A \rangle$$

$|A\rangle$: supposed to be "slow"

orthogonal space "fast"

$$iL|A\rangle = \frac{d}{dt}|A\rangle \quad \underline{\text{small}}$$

$|B\rangle$ in the orth. sp.: $\frac{d}{dt}|B\rangle = iL|B\rangle$ <u>large</u>

$|B\rangle$ general:

$$|B\rangle = P|B\rangle + Q|B\rangle$$

$$P = \frac{|A\rangle\langle A|}{\langle A|A\rangle}$$ projector onto the slow space

$$Q = 1 - P$$ " " " fast "

$$\frac{d}{dA}|B\rangle = i\mathcal{L}|B\rangle = \overbrace{i\mathcal{L}\underbrace{P|B\rangle}_{\substack{\propto |A\rangle \\ \text{slow}}}}^{\text{small}} + \overbrace{i\mathcal{L}\underbrace{Q|B\rangle}_{\substack{\perp |A\rangle \\ \text{fast}}}}^{\text{large}}$$

$\Rightarrow \underline{\underline{iL \simeq iLQ}} +$ corrections from slow variables

<u>interested in</u>

$$C(t) = \langle A^*(t=0)\, A(t) \rangle = \underbrace{\langle A | e^{iLt} | A \rangle}$$

$$C(\omega) := \int_0^{+\infty} dt\, e^{i\omega t}\, C(t) =$$

$$= \langle A | \int_0^{\infty} dt\, \exp[i(\omega + L)t] \,| A \rangle$$

$$C(t \to \infty) \to 0 \qquad = \underbrace{\langle A | i(\omega + L)^{-1} | A \rangle}$$

$$\int_0^\infty dt\, e^{i\varphi t} = \frac{e^{i\varphi t}}{i\varphi}\Bigg|_{t=0}^{t=\infty} = -\frac{1}{i\varphi} = +\frac{i}{\varphi}$$

$$(\omega + \mathcal{L})^{-1} = (\omega + \mathcal{L}Q)^{-1} + S \quad \leftarrow =?$$

↳ contribution from the slow stuff

$$S = (\omega + \mathcal{L})^{-1} - (\omega + \mathcal{L}Q)^{-1} \quad \Big|\, (\omega + \mathcal{L})$$

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

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

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

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

$$= \langle A | i\underset{\sim\sim\sim\sim}{(\omega + \mathcal{L}Q)}^{-1} | A \rangle$$

$$- \langle A | i(\omega + \mathcal{L}Q)^{-1}\mathcal{L}P(\omega + \mathcal{L})^{-1} | A \rangle$$

$$\hookrightarrow \frac{|A\rangle\langle A|}{\langle A|A\rangle}$$

$$(\omega + \ell Q)^{-1}|A\rangle = \frac{1}{\omega}\left(1+\frac{\ell Q}{\omega}\right)^{-1}|A\rangle =$$

$$\frac{1}{\omega}\left(1-\frac{\ell Q}{\omega}+\frac{\ell Q}{\omega}\frac{\ell Q}{\omega}-\frac{\ell Q}{\omega}\frac{\ell Q}{\omega}\frac{\ell Q}{\omega}+\dots\right)|A\rangle =$$

$$\underset{Q|A\rangle = 0}{=} \frac{1}{\omega}|A\rangle$$

$$C(\omega) = \frac{1}{\omega}\langle A|A\rangle - \frac{1}{\langle A|A\rangle}\langle A|(\omega+\ell Q)^{-1}\underbrace{\ell|A\rangle}_{\text{slow}}\; C(\omega)$$

$\omega \to \infty \Rightarrow$?

$$C(\omega) \simeq \frac{i}{\omega}(A|A) + \frac{1}{(A|A)}\frac{i}{\omega}\langle A|iL|A\rangle C(\omega)$$

$$\boxed{\frac{\langle A|iL|A\rangle}{(A|A)} =: \underline{\underline{\Omega}}}$$

unit: frequency or decay rate

$$C(\omega) = \frac{i}{\omega}(A|A) + i\frac{L}{\omega}C(\omega)$$

$$- \frac{1}{(A|A)}\langle A|\left(\omega + LQ\right)^{-1}L - \frac{L}{\omega}\,|A)\,C(\omega)$$

$$\left(\omega + LQ\right)^{-1}L - \frac{1}{\omega}L = \frac{1}{\omega}\left(1 + \frac{LQ}{\omega}\right)^{-1}L - \frac{1}{\omega}L =$$

$$= \frac{1}{\omega}\left\{1 - \frac{LQ}{\omega} + \frac{LQ}{\omega}\frac{LQ}{\omega} - \ldots\right\}L - \frac{1}{\omega}L =$$

$$= -\frac{LQ}{\omega}\underbrace{\left\{1 - \frac{LQ}{\omega} + \left(\frac{LQ}{\omega}\right)^2 + \ldots\right\}}_{\left(1+\frac{LQ}{\omega}\right)^{-1}}L = -LQ\left(\omega + LQ\right)^{-1}QL$$

<u>Define:</u> $Q i \mathcal{L} |A) =: |R)$

$|R)$ lives in the FAST space

call $|R)$ "noise" or "stochastic force"

$$(R| = -i (A| \mathcal{L} Q$$

$$C(\omega) = \frac{i}{\omega}(A|A) + i\frac{\Omega}{\omega} C(\omega)$$

$$- \frac{i}{\omega} \frac{(R| i(\omega + \mathcal{L}Q)^{-1} |R)}{(A|A)} C(\omega)$$

define: $M(\omega) := \dfrac{\langle R | i(\omega + \mathcal{L} Q)^{-1} | R \rangle}{\langle A | A \rangle}$

"memory function"

$$\Rightarrow C(\omega) = \frac{i}{\omega} \langle A | A \rangle + i \frac{\Omega}{\omega} C(\omega) - \frac{i}{\omega} M(\omega) C(\omega) \qquad | \cdot i\omega$$

$$i\omega C(\omega) = - \langle A | A \rangle - \Omega C(\omega) + M(\omega) C(\omega)$$

$$\boxed{C(\omega) = - \frac{\langle A | A \rangle}{i\omega + \Omega - M(\omega)}}$$

memory equation

memory equation in the time domain:

$$\boxed{\frac{d}{dt} C(t) = \underline{\Omega}\, C(t) - \int_0^t d\tau\, M(t-\tau)\, C(\tau)}$$

where $C(\omega) = \int_0^\infty dt\, e^{i\omega t} C(t)$

$$M(\omega) = \int_0^\infty dt\, e^{i\omega t} M(t)$$

<u>proof</u>: apply $\int_0^\infty dt\, e^{i\omega t}$ on both sides

lhs:

$$\int_0^\infty dt\, e^{i\omega t} \frac{d}{dt} C(t) =$$

$$= e^{i\omega t} C(t) \Big|_0^\infty - \int_0^\infty dt\, i\omega\, e^{i\omega t} C(t) =$$

$$= -\underbrace{C(t=0)}_{\langle A|A\rangle} - i\omega\, C(\omega) = -\langle A|A\rangle - i\omega\, C(\omega)$$

rhs: $\Omega\, C(\omega) - \int_0^\infty dt\, e^{i\omega t} \int_0^t d\tau\, M(t-\tau)\, C(\tau) =$

[define: $M(\tau) = 0$ for $\tau < 0$

$C(\tau) = 0$ " $\tau < 0$]

$$= \Omega\, C(\omega) - \int_0^\infty dt\, e^{i\omega t} \int_{-\infty}^\infty d\tau\, M(t-\tau)\, C(\tau) =$$

$$= \Omega\, C(\omega) - \int_{-\infty}^\infty d\tau \int_\tau^\infty dt\, M(t-\tau)\, C(\tau)\, e^{i\omega(t-\tau)} e^{i\omega\tau}$$

$$= \Omega\, C(\omega) - \int_{-\infty}^\infty d\tau\, C(\tau) e^{i\omega\tau} \int_0^\infty dt\, M(t) e^{i\omega t} = \Omega\, C(\omega) - C(\omega) \times M(\omega)$$

$$\Rightarrow -\langle A|A\rangle - i\omega\, C(\omega) = \Omega\, C(\omega) - M(\omega)\, C(\omega) \Rightarrow$$

$$\boxed{C(\omega) = -\frac{\langle A|A\rangle}{i\omega + \Omega - M(\omega)}}$$

Markov approximation

$M(t)$ decays quickly

$\Rightarrow \quad M(t) \longrightarrow \mu\, \delta(t)$

with $\mu = \int_0^\infty dt\, M(t)$ Green-Kubo integral

transport coefficient

approximate memory eq.:

$$\boxed{\frac{d}{dt} C(t) = \Omega\, C(t) - \mu\, C(t)}$$