In the following, we will consider a vector $A(t) = \begin{pmatrix} \delta\rho_{\vec{k}} \\ j^L_{\vec{k}} \end{pmatrix}$ $= \sum_i e^{i\vec{k}\cdot\vec{r}_i(0)} - (2\pi)^3 \rho\, \delta(\vec{k})$ / $\langle\delta\rho\rangle$

$= \frac{1}{m}\sum_i \underbrace{\hat{k}}_{\text{unit vector}} \vec{p}_i(0)\, e^{i\vec{k}\cdot\vec{r}_i(0)}$

$$\Rightarrow C(t) = \begin{pmatrix} \langle \delta\rho_{\vec{k}}(t)\,\delta\rho_{\vec{k}}(0)\rangle & \langle \delta\rho(0)\, j(t)\rangle \\ \langle j(0)\,\delta\rho(t)\rangle & \langle j(0) j(t)\rangle \end{pmatrix}$$

18/07/2017

reminding our notations: $\begin{cases} PB = (A,B)\cdot(A,A)^{-1}A, \quad Q = 1-P \\ f = e^{iQ\mathcal{L}t}\, Q\dot{A} \\ K(t) = (f(0), f(t))\cdot(A,A^{-1}) \\ \quad = \langle f^*(0)\, e^{iQ\mathcal{L}t} f(t)\rangle\, \underline{(A,A^{-1})} \\ i\underline{\underline{\Omega}} = (\underline{A}, \dot{\underline{A}})(\underline{A},\underline{A})^{-1} \end{cases}$

⚠ $\begin{cases} A = A(0) \\ A(t) \text{ otherwise} \end{cases}$

$$(A,A) = \begin{pmatrix} \langle a_1^2\rangle & \langle a_1 a_2\rangle \\ \langle a_2 a_1\rangle & \langle a_2^2\rangle \end{pmatrix}$$

For our choice of A: $\underline{\underline{C}}(t) = \begin{pmatrix} \langle \delta\rho_{-\vec{k}}(0)\,\delta\rho_{\vec{k}}(t)\rangle & \langle \delta\rho_{\vec{k}}(0)\, j^L_{\vec{k}}(t)\rangle \\ \langle j^L_{-\vec{k}}(0)\,\delta\rho_{\vec{k}}(t)\rangle & \langle j^L_{-\vec{k}}(0)\, j^L_{\vec{k}}(t)\rangle \end{pmatrix} = \begin{pmatrix} F(k,t) & \propto \dot{F} \\ \propto \dot{F} & \end{pmatrix}$

intermediate scattering function F

$\dot{F}$

At initial time: $\underline{\underline{C}}(0) = \begin{pmatrix} N S(\vec{k}) & \cancelto{0}{\langle \delta\rho_{\vec{k}}(0)\, j^L_{\vec{k}}(0)\rangle} \\ \cancelto{0}{\langle j^L_{-k}(0)\,\delta\rho_k(0)\rangle} & \langle j^L_{-k}(0)\, j^L_k(0)\rangle \end{pmatrix} \Rightarrow (A,A)^{-1} = \begin{pmatrix} \frac{1}{NS(k)} & 0 \\ 0 & \frac{m}{NkT} \end{pmatrix}$

$$\langle v_i^x v_j^x\rangle = \delta_{ij}\frac{kT}{m} \quad \left\langle \left(\sum_i \hat{k}\, \dot{r}_i e^{-i\vec{k}\cdot\vec{r}_i}\right)\left(\sum_j \hat{k}\, \dot{r}_j e^{i\vec{k}\cdot\vec{r}_j}\right)\right\rangle = \frac{NkT}{m}$$

$$i\Omega = (\underline{A}, \dot{\underline{A}}) \cdot \begin{pmatrix} 1/NS(k) & 0 \\ 0 & m/NkT \end{pmatrix} = \begin{pmatrix} \overset{0}{\langle \delta\rho_{-k}\,\dot{\delta\rho}_k\rangle} & \overset{iN|k|k_BT/m}{\left\langle \delta\rho_{-k}\frac{d j^L_k}{dt}\right\rangle} \\ \underset{iN|k|k_BT/m}{\langle j^L_{-k}\,\dot{\delta\rho}_k\rangle} & \underset{0}{\left\langle \frac{dj^L_k}{dt}\,\delta\rho_k\right\rangle} \end{pmatrix}\begin{pmatrix} & \\ & \end{pmatrix}$$

$$= \begin{pmatrix} 0 & i|k| \\ \frac{i|k|k_BT}{mS(k)} & 0 \end{pmatrix}$$

fluctuating force

$$f(0) = Q\dot{A}(0) = \dot{\underline{A}} - i\underline{\underline{\Omega}}\,\underline{A} = \begin{bmatrix} \dot{\delta\rho}_k \\ \frac{dj^L_k}{dt} \end{bmatrix} - \begin{pmatrix} 0 & i|k| \\ \frac{i|k|k_BT}{mS(k)} & 0 \end{pmatrix}\begin{pmatrix} \delta\rho_k \\ j^L_k \end{pmatrix} = \begin{bmatrix} 0 \\ R_{\vec{k}} \end{bmatrix}$$

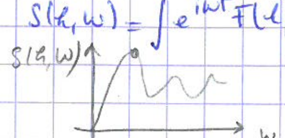
$$\boxed{R_{\vec{k}} = \frac{dj^L_k}{dt} - \frac{i|\vec{k}|k_BT}{mS(\vec{k})}\,\delta\rho_{\vec{k}}}$$

$$\underline{\underline{K}}(t) = \begin{bmatrix} 0 & 0 \\ 0 & \frac{m}{Nk_BT}\langle R_{-\vec{k}}\, e^{iQ\mathcal{L}t} R_{\vec{k}}\rangle \end{bmatrix} = (f(0), e^{i\mathcal{L}t} f(0))(A,A)^{-1}$$

21 element of **:

$$\boxed{\frac{d^2F(k,t)}{dt^2} + \frac{k^2k_BT}{mS(k)}F(k,t) + \frac{m}{Nk_BT}\int_0^t d\tau \langle R_{-\vec{k}}(0)\, e^{iQ\mathcal{L}t} R_{\vec{k}}(0)\rangle \cdot \frac{dF}{dt}(k, t-\tau) = 0}$$

$S(k,\omega) = \int e^{i\omega t} F(k,t)\, dt$ dynamic structure factor.



force term moving slowly & term fluctuating fast

$$\frac{d\vec{p_i}}{dt} = -\nabla \sum_{i\neq j} \phi(|\vec{r_i}-\vec{r_j}|) = \sum_{\vec{k}} i\vec{k}\, \underset{\downarrow \text{F.T.}}{\phi_{\vec{k}}}\, \delta\rho_{-k}\, \delta\rho_{k}\,.$$

↳ density modes propagating in opposite directions

$$e^{iQ\mathcal{L}t} \underset{\text{MCA}}{\simeq} P_2\, e^{i\mathcal{L}t}\, P_2$$ with P_2 projecting onto $\delta\rho\,\delta\rho$, $P_2 B = \sum_{\vec{k}_1 \dots \vec{k}_4} \delta\rho_{\vec{k}_1}\delta\rho_{\vec{k}_2} \langle \delta\rho_{\vec{k}_3}\delta\rho_{-\vec{k}_4} \cdot B\rangle \cdot \langle \delta\rho_{-\vec{k}_1}\delta\rho_{-\vec{k}_2}\delta\rho_{\vec{k}_3}\delta\rho_{\vec{k}_4}\rangle$

$$\Rightarrow \langle R_{-\vec{k}}\, e^{iQ\mathcal{L}t} R_{\vec{k}}\rangle \simeq \langle (P_2 R_{-\vec{k}}) e^{i\mathcal{L}t} (P_2 R_{\vec{k}})\rangle$$

$$\hookrightarrow P_2 R_{\vec{q}} = \sum_{\vec{k}_1 \vec{k}_2} \delta\rho_{\vec{k}_1}\delta\rho_{\vec{k}_2} \underbrace{\langle \delta\rho_{-\vec{k}_3}\delta\rho_{\vec{k}_4} R_{\vec{q}}\rangle \cdot \langle \delta\rho_{-\vec{k}_1}\delta\rho_{-\vec{k}_2}\delta\rho_{\vec{k}_3}\delta\rho_{\vec{k}_4}\rangle^{-1}}_{V_q(k_3,k_4)\ \text{vertex (static)}}$$

with $\vec{k} = \vec{k}_1 - \vec{k}_2$, $V_{\vec{q}}(\vec{k}_1,\vec{k}_2) = V_{\vec{k},\vec{q}-\vec{k}}$

$$= \frac{i\rho k_B T}{2mN}\left((\hat{q}\cdot\vec{k})\, C(k) + \hat{q}\cdot(\vec{q}-\vec{k})\, C(|\vec{k}-\vec{q}|)\right)$$

$$C(k) \equiv \frac{1}{\rho}\left(1 - \frac{1}{S(k)}\right)$$

so that $\langle R_{-k}(0)\, e^{iQ\mathcal{L}t} R_k(0)\rangle \simeq \sum |V|^2 \langle \rho_{k_1}\rho_{k_2}\rho_{k_3}(t)\rho_{k_4}(t)\rangle \simeq \sum |V|^2 \left(\delta_{-k_1 k_3} + \delta_{-k_2 k_4}\right) F(k_1,t)F(k_2,t)$

Missing a few steps, but the final equation reads:

$$\frac{d^2F(q,t)}{dt^2} + \frac{q^2 k_B T}{m S(q)} F(q,t) + \int_0^t d\tau\, K(q,t-\tau)\frac{\partial F}{\partial \tau}(q,\tau) = 0$$

$$K_{MCT}(q,t) = \frac{\rho k_B T}{16\pi^3 m}\int d\vec{k}\, |V_{\vec{q}-\vec{k},\vec{k}}|^2 F(|\vec{q}-\vec{k}|,t)\, F(k,t)$$

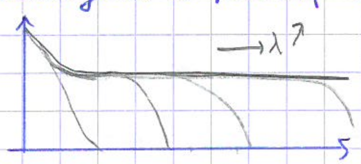
→ Closed equations on $F(q,t)$

→ Theory for liquid state that from T, ρ and $S(k)$ derives the dynamic! ↳ static!

→ connections with exact dynamics of MF p-spins!

Looking at the consequences:

Approximating in a first step $S(q) \simeq A\,\delta(q-q^*)$ peak → $\ddot{\phi} + \Omega^2\phi(t) + \lambda \int d\tau\, \phi^2(t-\tau)\,\dot{\phi}(\tau) = 0$ ($\phi = F(q^*,t)$)



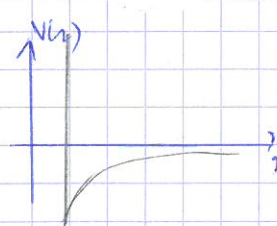
$\lambda_c = 4$ → freezing of the correlations + relaxation time divergence

$\tau \sim (\lambda-\lambda_c)^{-\gamma}$

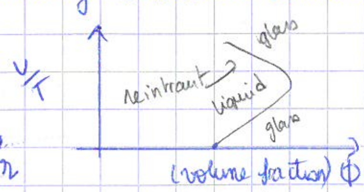
$\gamma = \frac{1}{2a} + \frac{1}{2b}$

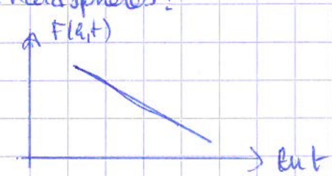
Leutheusser 1984.

Using the theory to describe short range attractions between hard spheres:



small range ~ $\frac{6}{10}$





↳ speed up relaxation by adding attraction

⇒ PREDICTED BY MCT BEFORE ANY EXPERIMENT.