particle current

$$\boxed{\vec{j}(\vec{r},t) = \sum_{i=1}^{N} \frac{1}{m} \vec{p}_i(t)\, \delta(\vec{r} - \vec{R}_i(t))}$$

local variable

spatial Fourier transform

$$\vec{j}_{\vec{q}}(t) = \int d^d\vec{r}\, e^{i\vec{q}\vec{r}}\, \vec{j}(\vec{r},t) = \sum_{i=1}^{N} \frac{1}{m} \vec{p}_i(t)\, e^{i\vec{q}\vec{R}_i(t)}$$

$$i\vec{q}\,\vec{j}_{\vec{q}}(t) = \sum_{i=1}^{N} i\vec{q}\,\dot{\vec{R}}_i(t)\, e^{i\vec{q}\vec{R}_i(t)} = \frac{d}{dt} \sum_{i=1}^{N} e^{i\vec{q}\vec{R}_i(t)}$$

$$\boxed{\partial_t\, \hat{\rho}_{\vec{q}}(t) = i\vec{q}\,\hat{\vec{j}}_{\vec{q}}(t)}$$

continuity equation for particle conservation

current correlation function

$$\boxed{C_{\alpha\beta}(\vec{q},t) = \frac{1}{N} \langle \hat{j}_{\alpha\vec{q}}(t)^{*}\, \hat{j}_{\beta\vec{q}}(0) \rangle \\ \alpha, \beta \text{ spatial components}}$$

Current correlation function

rotational symmetry

$$\boxed{C_{\alpha\beta}(\vec{q},t) = \hat{q}_\alpha \hat{q}_\beta C^L(q,t) + (\delta_{\alpha\beta} - \hat{q}_\alpha \hat{q}_\beta) C^T(q,t)}$$

$\hat{q}_\alpha = q_\alpha / |\vec{q}|$ L ongitudinal / T ransversal component

longitudinal current $\boxed{\hat{j}^L_{\vec{q}}(t) := \hat{\vec{q}} \cdot \vec{j}_{\vec{q}}(t)}$

$$C^L(q,t) = \hat{q}_\alpha \hat{q}_\beta C_{\alpha\beta}(q,t) = \frac{1}{N}\langle (\hat{\vec{q}} \cdot \vec{j}_{\vec{q}}(t))^* (\hat{\vec{q}} \cdot \vec{j}_{\vec{q}}) \rangle$$

(a) Longitudinal current and intermediate scattering function

$$\frac{d^2}{dt^2} S(q, t-t') = -\frac{d}{dt}\frac{d}{dt'} S(q, t-t') =$$

$$= -\frac{d}{dt}\frac{d}{dt'} \frac{1}{N} \langle \rho_{\vec{q}}(t)^* \rho_{\vec{q}}(t') \rangle =$$

$$= -\frac{1}{N} \langle \dot{\rho}_{\vec{q}}(t)^* \dot{\rho}_{\vec{q}}(t') \rangle =$$

$$= -\frac{1}{N} \langle \vec{q} \cdot \vec{j}_{\vec{q}}(t)^* \vec{q} \cdot \vec{j}(t') \rangle =$$

$$= -\frac{q^2}{N} \langle \hat{j}^L_{\vec{q}}(t)^* \hat{j}^L_{\vec{q}}(t')$$

hence $$\boxed{\frac{d^2}{dt^2} S(q,t) = -q^2 C^L(q,t)}$$

For $t=0$, $$\frac{d^2}{dt^2} S(q, t=0) = -q^2 \frac{1}{N} \langle |\hat{j}^L|^2 \rangle$$

$$= -q^2 v_{th}^2$$

with thermal velocity $v_{th}^2 = \frac{k_B T}{m}$

(b) com in frequency domain

$$\frac{d^2}{dt^2} S(q,t) = -q^2 C^L(q,t), \quad S(q,t=0) = S_q$$

$$\frac{d}{dt} S_q(t=0) = 0$$

$$-iz\,\hat{\dot{S}}(q,z) - i\underbrace{\dot{S}(q,t=0)}_{=0} =$$

$$= -iz\left[-iz\,\hat{S}(q,z) - iS_q\right] = -q^2 \hat{C}^L(q,z)$$

$$\boxed{z^2 \hat{S}(q,z) + z S_q = q^2 \hat{C}^L(q,z)}$$

(c) short-time expansion $S(q,t)$

$$S(q,t) = S_q t^0 + 0\,t^1 - q^2 v_{th}^2 \frac{t^2}{2} + \mathcal{O}(t^4)$$

↳ characteristic frequency $\boxed{\Omega_q^2 = \frac{q^2 v_{th}^2}{S_q}}$

↳ $\phi_q(t) = \frac{S(q,t)}{S_q} = 1 - \Omega_q^2 t^2/2 + \mathcal{O}(t^4)$

(d) short-time expansion $C^L(q,t)$

$$C^L(q,t) / \underbrace{C^L(q,t=0)}_{= v_{th}^2} = 1 - \omega_L^2(q) \frac{t^2}{2} + \mathcal{O}(t^4)$$

$$-\omega_L^2(q) = \frac{1}{v_{th}^2} \frac{d^2}{dt^2} C^L(q,t)\Big|_{t=0}$$

$$\boxed{\omega_L^2(q)\, v_{th}^2 = \frac{d^4}{dt^4} S(q,t)\Big|_{t=0} = \frac{1}{N}\langle |\ddot{\hat{\rho}}_{\vec{q}}|^2 \rangle}$$

chose wave vector in z-direction

$$\vec{q} = q\,\hat{e}_z \ , \quad \dot{p}_{iz} = -\partial_{z_i} \mathcal{U} \ , \ \text{interaction } \mathcal{U}$$

$$\ddot{\vec{\rho}}_{\vec{q}} = i q \frac{d}{dt} \vec{j}_{\vec{q}} = i q \frac{d}{dt} \sum_{i=1}^{N} \frac{p_{iz}}{m} \exp\{iqz_i\}$$

$$= -iq \sum_{i=1}^{N} \frac{1}{V} \partial_{z_i} \mathcal{U} e^{iqz_i} - q^2 \sum_{i=1}^{N} \left(\frac{p_{iz}}{m}\right)^2 e^{iqz_i}$$

$$\frac{1}{N}\langle |\ddot{\rho}_{\vec{q}}|^2\rangle = \frac{q^4}{N} \sum_{i,j=1}^{N} \left\langle \left(\frac{p_{iz}}{m}\right)^2 \left(\frac{p_{jz}}{m}\right)^2 e^{iq(z_i - z_j)} \right\rangle \quad (1)$$

$$+ \frac{q^2}{Nm^2} \sum_{i,j=1}^{N} \left\langle \partial_{z_i} \mathcal{U}\, \partial_{z_j} \mathcal{U}\, e^{iq(z_i - z_j)} \right\rangle \quad (2)$$

$$+ \frac{iq^3}{Nm} \sum_{i,j=1}^{N} \left\langle \left[\left(\frac{p_{iz}}{m}\right)^2 \partial_{z_j} \mathcal{U} - \left(\frac{p_{jz}}{m}\right)^2 \partial_{z_i} \mathcal{U} \right] e^{iq(z_i - z_j)} \right\rangle \quad (3)$$

(1) $$= \frac{q^4}{N} \sum_{i=1}^{N} \left\langle \left(\frac{p_{iz}}{m}\right)^4 \right\rangle + \frac{q^4}{N} \sum_{\substack{i,j=1 \\ i \neq j}} \left\langle \left(\frac{p_{iz}}{m}\right)^2 \left(\frac{p_{jz}}{m}\right)^2 e^{iq(z_i - z_j)} \right\rangle$$

p_{iz} is Gauß distributed

$$= 3\,(q v_{th})^4 + (q v_{th})^4 \underbrace{\frac{1}{N} \sum_{i \neq j} \left\langle e^{iq(z_i - z_j)} \right\rangle}_{S_q - 1} =$$

$$= (q v_{th})^4 \left[2 + S_q \right]$$

(2) identity $\langle V \partial_{z_i} \mathcal{U} \rangle = k_B T \langle \partial_{z_i} V \rangle$

proof: $\int d\Gamma\, V\, \partial_{z_i} \mathcal{U} \frac{1}{Z} e^{-\beta \mathcal{H}}$, $\mathcal{H} = \mathcal{U} + E_{kin}$

$$= \int d\Gamma \, V \left(-k_B T \, \partial_{z_i} \frac{1}{Z} e^{-\beta \mathcal{H}}\right) = \text{integration by parts}$$

$$= k_B T \int d\Gamma \, \partial_{z_i} V \, \frac{1}{Z} e^{-\beta \mathcal{H}} =$$

$$= k_B T \langle \partial_{z_i} V \rangle \quad \square$$

$$① = \frac{q^2}{N m^2} \sum_{i,j} k_B T \langle \partial_{z_i} [\partial_{z_j} U \, e^{iq(z_i - z_j)}] \rangle$$

$$= \frac{q^2}{N m^2} k_B T \sum_{i,j} \langle \partial_{z_i} \partial_{z_j} U \, e^{iq(z_i - z_j)} \rangle$$

$$+ \frac{i q^3}{N m^3} k_B T \underbrace{\sum_{i \neq j} \langle \partial_{z_j} U \, e^{iq(z_i - z_j)} \rangle}_{k_B T (-iq) \sum_{i \neq j} \langle e^{iq(z_i - z_j)} \rangle}$$

$$① = (q v_{th})^2 \sum_{i,j} \partial_{z_i} \partial_{z_j} U e^{iq(z_i - z_j)}$$

$$+ (q v_{th})^4 [S_q - 1]$$

$$③ = i q^3 v_{th}^2 \frac{1}{N m} \sum_{i,j} \langle [\partial_{z_i} U - \partial_{z_j} U] e^{iq(z_i - z_j)} \rangle$$

$$= i q^3 v_{th}^4 \frac{1}{N} \sum_{i \neq j} \langle (\partial_{z_i} - \partial_{z_j}) e^{iq(z_i - z_j)} \rangle =$$

$$= -2 (q v_{th})^4 [S_q - 1]$$

together

$$\boxed{\omega_L^2(q) \, \Omega^2(q) = 3 (q v_{th})^4 + (q v_{th})^2 \frac{1}{N m} \left\langle \sum_{i,j} \partial_{z_i} \partial_{z_j} U e^{iq(z_i - z_j)} \right\rangle}$$

assume pairwise interactions

$$\mathcal{U} = \sum_{i<j} \mathcal{U}_{ij} = \sum_{i<j} \mathcal{U}(|\mathbf{R}_i - \mathbf{R}_j|)$$

$$\frac{1}{N} \sum_{ij} \langle \partial_{z_i} \partial_{z_j} e^{iq(z_i - z_j)} \rangle = (N-1) \langle \partial^2_{z_1} \mathcal{U}_{12} \rangle$$

$$+ (N-1) \langle \partial_{z_1} \partial_{z_2} \mathcal{U}_{12} \, e^{iq(z_1 - z_2)} \rangle$$

only averages of pairs $\Rightarrow$ only pair correlations

$$\omega_L^2(q)\, \Omega^2(q) = 3 (q v_{th})^4 + (q v_{th})^2 \frac{n}{m} \int d^3r\, g(r) \times$$

$$\times [1 - \cos(qz)]\, \partial_z^2 \mathcal{U}(r)$$

with $\Omega^2(q) = (q v_{th})^2$

$$\boxed{\omega_L^2(q) = 2\, \Omega^2(q) + \frac{n}{m} \int d^3r\, g(r) [1 - \cos qz]\, \partial_z^2 \mathcal{U}(r)}$$

hence, the expansion of intermediate scattering function

$$S(q,t) = S_q \left[1 - \Omega^2(q) \frac{t^2}{2} + \Omega^2(q)\, \omega_L^2(q) \frac{t^4}{4!} + \mathcal{O}(t^6) \right]$$

$$\hat{S}(q,z) = S_q \left[-\frac{1}{z} - \Omega^2(q) \frac{1}{z^3} - \Omega^2(q)\, \omega_L^2(q) \frac{1}{z^5} + \mathcal{O}(z^{-7}) \right]$$

representation possible as a double fraction

$$\boxed{\hat{S}(q,z) = \frac{-S_q}{z - \dfrac{\Omega^2(q)}{z + \hat{M}(q,z)}}}$$

yields in $\frac{1}{z}$ expansion

$$\hat{S}(q,z) = S_q \left\{ -\frac{1}{z} - \Omega^2(q) \frac{1}{z^3} - \Omega^4(q) \frac{1}{z^5} + \Omega^2(q)\, \hat{M}(q,z) \frac{1}{z^4} + \mathcal{O}(z^{-3}) \right\}$$

$$\Rightarrow \boxed{\hat{M}(q,z) = -\frac{1}{z}\left[\omega_L^2(q) - \Omega^2(q)\right] + \mathcal{O}(z^{-3})}$$

further extension of short-time expansion possible but tedious