Hyperuniformity

A system, whose state is described by a scalar order parameter $u(\mathbf{x})$ is said to be **hyperhuniform** if the structure factor $S(q)$, defined as the **spherical average** of the Fourier transform of the pair correlation function, **vanishes** as $q \to 0$.
In particular, it can be shown that the spherical averaging leads to this expansion for small values of k ($k \to 0$):

$$S(q,t) = S_0(t) + S_2(t)q^2 + S_4(t)q^4 + \dots$$

And **hyperhuniformity** means not necessarily that S_0 vanishes as time passes, but at least that the higher order term (at least one) grows in time much faster than $S_0(t)$.

Physically, the coefficients S_i are the **multipole moments** of \g$(\mathbf{x})$. S_2 is the moment of order 2, but it can be shown to be proportional to the **dipole moment of** ρ as

$$S_i \propto \int \mathbf{x}^i g(\mathbf{x}) d\mathbf{x} = \frac{1}{V} \int d\mathbf{x} \int d\mathbf{y} \mathbf{x}^i \rho(\mathbf{y})\rho(\mathbf{x}+\mathbf{y})$$

Considering $i = 2$ and by making a substitution $\mathbf{x} \to \mathbf{x}+\mathbf{y} = \mathbf{z}$ we find

$$\int d\mathbf{z} \int d\mathbf{y} (\mathbf{z}-\mathbf{y})^2 \rho(\mathbf{y})\rho(\mathbf{z}) = \int d\mathbf{z} \int d\mathbf{y} (\mathbf{z}^2 + \mathbf{y}^2 + 2(\mathbf{z}\cdot\mathbf{y}))\rho(\mathbf{z})\rho(\mathbf{y})$$

And using that $\bar{\rho} = 0$

$$\int d\mathbf{z} z^2 \rho(\mathbf{z}) \int d\mathbf{y} \rho(\mathbf{y}) = 0$$

So we find that

$$S_2 \propto \int d\mathbf{z} \int d\mathbf{y} (\mathbf{z}\cdot\mathbf{y})\rho(\mathbf{z})\rho(\mathbf{y}) = (\int d\mathbf{z} \rho(\mathbf{z})\mathbf{z}) \cdot (\int d\mathbf{y} \rho(\mathbf{y})\mathbf{y})$$

So, if we define the **dipole moment** $\mathbf{p}$ or **center-of-mass vector** $\mathbf{R}$

$$\mathbf{p} = \mathbf{R} = \frac{1}{V} \int \mathbf{x}^2 \rho(\mathbf{x}) d\mathbf{x}$$

$$S_2 \propto |\mathbf{p}|^2 = |\mathbf{R}|^2$$

And including the prefactor:

$$S_2 \propto V|\mathbf{p}|^2$$

Definitions

- Spherical averaged structure factor

$$S(q) = \frac{1}{4\pi}\int d\Omega S(\mathbf{q}) = \frac{1}{4\pi}\int d\mathbf{x}\int_0^{2\pi} d\varphi_q \int_0^{\pi} d\theta_q \sin(\theta_q) e^{-i\mathbf{q}\cdot\mathbf{x}} g(\mathbf{x}) d\mathbf{x}$$

and aligning $\hat{z} \parallel \mathbf{q}$, then $\mathbf{k}\cdot\mathbf{x} = |\mathbf{k}||\mathbf{x}|\cos(\theta_q)$

$$S(q) = \int d\mathbf{x}\frac{\sin(kx)}{kx} g(\mathbf{x})$$

where $x = |\mathbf{x}|$ and $k = |\mathbf{k}|$.

- Structure factor

$$S(\mathbf{q}) = \int d\mathbf{x} e^{-i\mathbf{q}\cdot\mathbf{x}} g(\mathbf{x})$$

- Pair correlation function

$$g(\mathbf{x}) = \int d\mathbf{x_1}\rho(\mathbf{x_1})\rho(\mathbf{x}+\mathbf{x_1})$$

- Charge density (translated order parameter with zero average)

$$\rho(\mathbf{x}) = u(\mathbf{x}) - \bar{u}$$

$$\bar{u} = \int d\mathbf{x} u(\mathbf{x})$$

Small k expansion of S(q)

Expanding the sine for $k \to 0$

$$S(q) = \int d\mathbf{x}\frac{\sin(kx)}{kx} g(\mathbf{x}) = S_0 + S_2 k^2 + S_4 k^4 + \dots$$

where

$$S_{2n} = \frac{1}{(2n+1)!}\int d\mathbf{x} g(\mathbf{x})|\mathbf{x}|^{2n}$$

So

$$S_0 = \int d\mathbf{x} g(\mathbf{x}) = \frac{1}{V}\int d\mathbf{x}\int d\mathbf{y}\rho(\mathbf{y})\rho(\mathbf{x}+\mathbf{y})$$

that, by changing the variable $\mathbf{x} \to \mathbf{x}+\mathbf{y}$ is

$$S_0 = \frac{1}{V}\left(\int d\mathbf{x}\rho(\mathbf{x})\right)^2$$

and this term is **always zero, because $\bar{\rho} = 0$ by definition!**
But this would mean that **any** system is hyperhuniform!

To see

- Why the active current term breaks TRS and why TRS and detailed balance are the same thing?
- What is $\hat{J}$ and why if it is zero the mobility is not state dependent (constant)
- Only the velocity of changes in S2 is calculated and shown to decay with V. But we should compare this with the velocity of decay of higher order terms (e.g. S4) to state that S2 is negligible respect to S4
- Rescaled structure factor (coarsening)