

2D Structure factor

#structurefactor

#2D

#randinit

#liquids

Like in the 1D case ([1D Structure factor](#)) I define:

I **define** the (2D) structure factor

$$S(q_x, q_y) \equiv \langle |\int e^{-i\mathbf{q}\cdot\mathbf{x}} u(\mathbf{x}) dxdy|^2 \rangle$$

where:

- $|\dots|^2 = (\dots)^*(\dots)$ is the norm.
- $\langle \dots \rangle$ is an average over multiple simulations, all starting from a **random initial condition** (different each time).

There is a problem - Need a function of ONE variable!

In 2D the structure factor is a function of two variables: q_x, q_y . While in all the articles it is presented a function of only one variable! So how do we compute this quantity $\hat{S}(q)$ from $S(q_x, q_y)$?

My idea

As there are **no preferential directions**, I expect that the structure factor is a function only of $q = |\mathbf{q}|$ and not of the direction. As a consequence, it is possible to choose a direction in q -space (passing through the origin) and evaluate $S(\mathbf{q})$ along that direction.

So the most simple way of estimating $\hat{S}(q)$ is to evaluate $S(q_x, q_y)$ along the direction $q_x = 0$ and along $q_y = 0$ and then take the average.

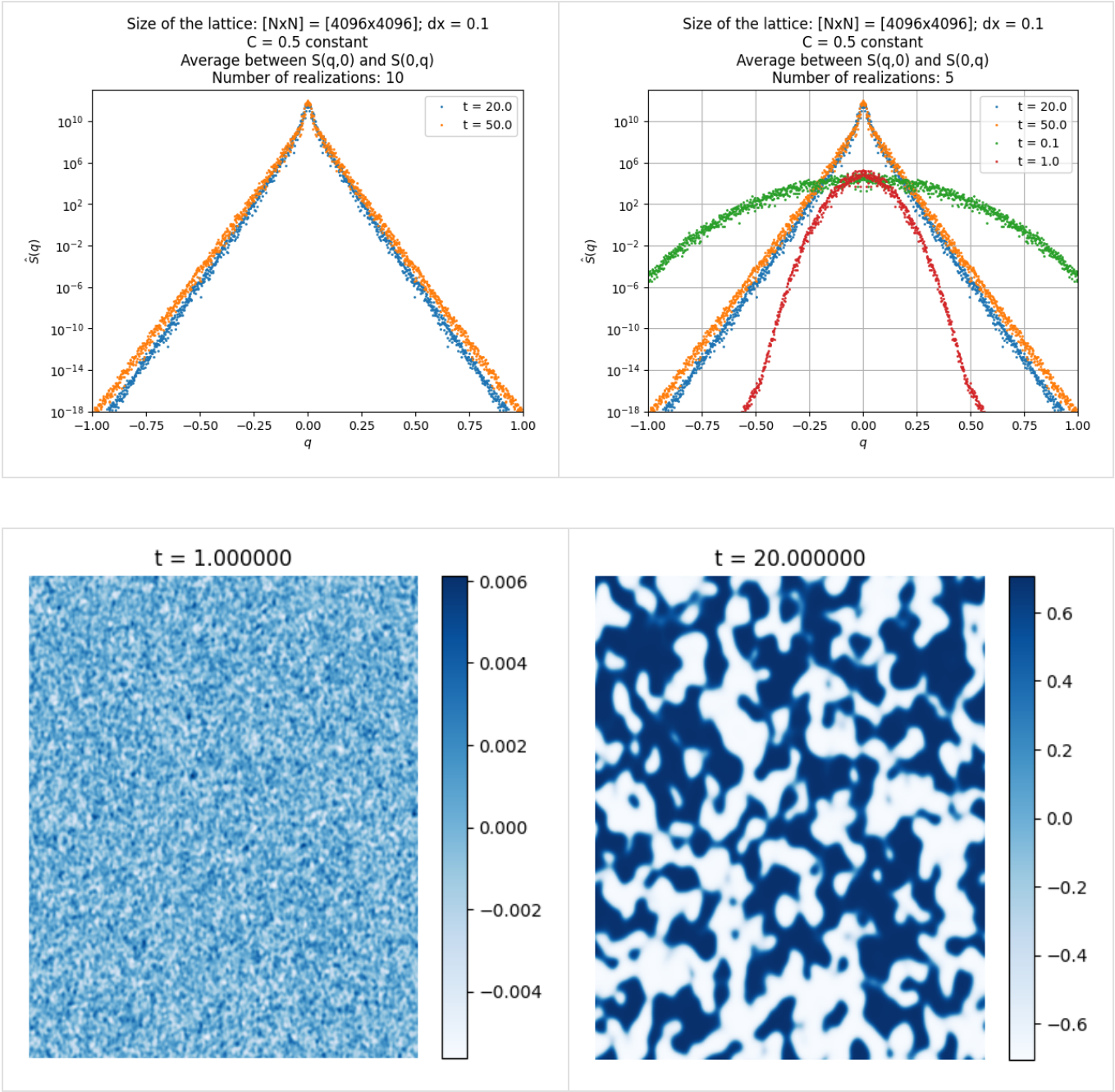
$$\hat{S}(q) = \frac{1}{2}[S(q, 0) + S(0, q)]$$

(considering other directions is not an available option, as in the other directions the points of the lattice are separated by a different distance, so we cannot compare the functions associated to those lines with the horizontal and vertical lines).

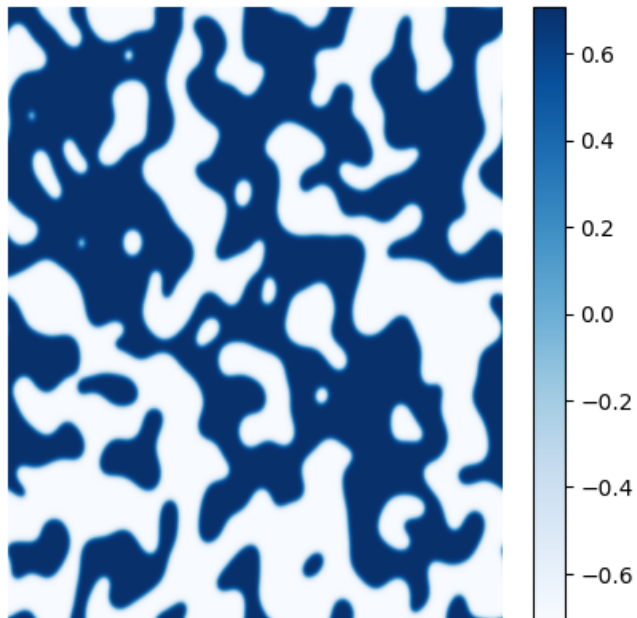
This approach of evaluating $S(\mathbf{q})$ along one direction is **motivated** by what happens experimentally with 3D liquids, **where to sample one point of the spectrum $\hat{S}(q)$ the structure factor is sampled at only one vector \mathbf{q} with that norm.** So they do not measure multiple vectors to take then an average, as they fix the angle φ of the detector's position.

See [Structure factor in liquids](#) for a **motivation** of the present approach.

Here $C = 0.5$ constant.



$t = 50.100000$



$t = 500.200000$

