

Structure factor in different situations

In order to characterize the spatial correlations between particles, knowledge of the structure factor is essential. One proposes to show that the structure factor is suitable for exhibiting the specific features of particle correlations in different situations.

Consider N particles inside a box of volume V . The microscopic density is given as

$$\rho(\mathbf{r}) = \sum_{i=1}^N \delta(\mathbf{r} - \mathbf{r}_i) \quad (1)$$

where \mathbf{r}_i denotes the position of particle i . One defined the structure factor as

$$S(\mathbf{k}) = \frac{\langle \tilde{\rho}(\mathbf{k})\tilde{\rho}(-\mathbf{k}) \rangle}{N} \quad (2)$$

where $\tilde{\rho}(\mathbf{k})$ is the Fourier transform of the microscopic density and the brackets $\langle \dots \rangle$ denote the average over the available configurations of the system.

- Express the structure factor $S(\mathbf{k})$ as a function in terms of $\langle e^{-i\mathbf{k}\mathbf{r}_{ij}} \rangle$, where $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ with $i \neq j$.

Solution: The fourier transform of the microscopic density is given by

$$\tilde{\rho}(\mathbf{k}) = \sum_{i=1}^N e^{-i\mathbf{k}\mathbf{r}_i} \quad (3)$$

By splitting the self and distinct terms of the double summation, one obtains

$$S(\mathbf{k}) = 1 + \frac{1}{N} \sum_{i \neq j}^N \langle e^{-i\mathbf{k}\mathbf{r}_{ij}} \rangle \quad (4)$$

- Show that $S(\mathbf{k}) \rightarrow 1$ when $\mathbf{k} \rightarrow +\infty$.

Solution: When $(\mathbf{k}) \rightarrow \infty$, each term $\langle e^{-i\mathbf{k}\mathbf{r}_{ij}} \rangle$ goes to zero, and the structure factor goes to one.

- One considers a cubic simulation box with a linear dimension L and we are using periodic boundary conditions. What is the smallest wave vectors \mathbf{k} accessible in simulation ?

Solution: For each direction of the lattice, one has $k_i L = 2\pi$, where k_i is a coordinate of the wave vector. By taking the positive and negative wave coordinates, one has $|k_i|L = \pi$

4. Consider a lattice gas with a lattice step a . Particles occupy lattice sites, show that it exists a ultraviolet cutoff of accessible wave vectors. By using periodic boundary conditions, compute the number of wave vectors available in simulation.

Solution: The ultraviolet cutoff is given by $k = \frac{\pi}{a}$. The total number of wavevectors is given by

$$\sum_i \sum_j \sum_k = N^3$$

One now considers a finite one-dimensional lattice with a step a (with periodic boundary conditions, i.e. a ring). Each site is occupied by a particle.

5. Calculate $\tilde{\rho}(k)$ and infer the structure factor associated with this configuration. Taking the thermodynamic limit ($N \rightarrow \infty$) show that the structure factor vanishes within the Brillouin zone ($-\frac{\pi}{a} < k < \frac{\pi}{a}$) (see Glossary).

Solution:

$$\tilde{\rho}(\mathbf{k}) = \sum_{j=1}^N e^{-ika_j} = e^{-ika} \frac{1 - e^{-ikaN}}{1 - e^{-ika}} \quad (5)$$

$$S(k) = \frac{1}{N} \rho(\tilde{k}) \rho(\tilde{-k}) \quad (6)$$

$$= \frac{1}{N} \frac{\sin(kaN/2)^2}{\sin(ka/2)^2} \quad (7)$$

In the thermodynamic limit, one has that

$$\frac{1}{N} \frac{\sin(kaN/2)^2}{\sin(ka/2)^2} \rightarrow \sum_m \delta(k_m - \frac{m\pi}{L})$$

Therefore, $S(k) = 0$ within the Brillouin zone except $k = 0$.

Each particle is split into two particles which are identical and shifted symmetrically from the lattice node to a distance u . The distance is chosen randomly from the probability distribution $p(u)$. The microscopic density is given by

$$\rho_d(\mathbf{r}) = \sum_{i=1}^N (\delta(\mathbf{r} - \mathbf{r}_i - u_i) + \delta(\mathbf{r} - \mathbf{r}_i + u_i)) \quad (8)$$

and the structure factor becomes

$$S_d(\mathbf{k}) = \frac{\langle \tilde{\rho}_d(\mathbf{k}) \tilde{\rho}_d(-\mathbf{k}) \rangle}{2N}. \quad (9)$$

6. Show that $S_d(k) = 2 \langle \cos(ku)^2 \rangle + 2 \langle \cos(ku) \rangle^2 (S(k) - 1)$.

Solution:

$$\tilde{\rho}_d(\mathbf{k}) = 2 \sum_{i=1}^N e^{ikr_i} \cos(ku_i)$$

Taking the average, one has

$$\langle |\tilde{\rho}_d(\mathbf{k})|^2 \rangle = 4N \sum_i \langle \cos(ku)^2 \rangle + 4N \langle \cos(ku) \rangle^2 \sum_{i=1 \neq j} e^{-ikr_{ij}}$$

The factor 2 comes from the particle splitting. Finally, one has

$$S_d(k) = 2(\langle \cos(ku)^2 \rangle + 2\langle \cos(ku) \rangle^2 [S(k) - 1])$$

7. Assuming that the moments $\langle u^2 \rangle$ and $\langle u^4 \rangle$ are finite, calculate the expansion of $S_d(k)$ to the order k^4 . Configurations corresponding to the vanishing structure factor when $k \rightarrow 0$, are “super-uniform” (or hyperuniform). Justify this terminology. Hint : What is this limit for a uniform perfect gas.

Solution: Performing the series expansion in k and using that $S(k) = 0$ (by using the above questions), one obtains

$$S_d(k) \frac{2}{3} (\langle u^4 \rangle - \langle u^2 \rangle^2) k^4 + \dots \quad (10)$$

For a perfect gas $S(k) = 1$, characterizing the absence of correlations at all length scales.

In real space, the limit of $S(k)$ when $k \rightarrow 0$ is proportional to the compressibility. This means that in a finite volume the variance of the particle number goes as the mean number.

$$\langle N^2 \rangle - \langle N \rangle^2 \simeq \langle N \rangle$$

Therefore if $S(k) \rightarrow 0$ when $k \rightarrow 0$, this means that

$$\langle N^2 \rangle - \langle N \rangle^2 \ll \langle N \rangle$$

and the state of the system is called hyperuniform.

8. Simulations have been performed for dense granular systems that reveals that the structure factor goes to zero as k when k goes to zero. Why does the simulation require a large number of particles (10^6 particles) in order to show this result?

Solution: The finite volume of the simulation box gives a infrared cutoff $k = \pi/L \sim \pi/N^{1/3}$. In order to investigate the low- k behavior, one must increase the box size.

For a liquid close the critical temperature of the liquid-gas transition. The spatial correlation function behaves as $h(r) \sim r^{-(d-2+\eta)}$ pour $r > r_c$, where η is the anomalous exponent.

9. By using the relationship between the correlation function and the structure factor, show that the structure factor diverges at small wave vectors as k^{-A} , where A is an exponent to be determined

Solution: By using the expression of $S(k)$, one has

$$S(k) = 1 + 4\pi\rho \int_0^\infty r^2 g(r) \frac{\sin(kr)}{kr} dr$$

If $g(r) \sim r^{1+\eta}$ when $r > r_c$, one has a singular part

$$S(k) \simeq 4\pi\rho \int_0^\infty r^{1-\eta} \frac{\sin(kr)}{kr} dr$$

By using a change of variable $u = r/r_c$, one obtains that

$$S(k) \sim k^{-2+\eta}$$

$A = 2 - \eta$. The structure factor diverges at small k . This is associated with the critical opalescence.

A Glossary

The three dimensional Fourier transform of a function f is defined as

$$\hat{f}(\mathbf{k}) = \int d^3\mathbf{r} f(\mathbf{r}) e^{-i\mathbf{k}\mathbf{r}} \quad (11)$$

and the inverse transform is given by

$$f(\mathbf{r}) = \frac{1}{(2\pi)^3} \int d^3\mathbf{k} \hat{f}(\mathbf{k}) e^{i\mathbf{k}\mathbf{r}} \quad (12)$$

For a Gaussian function

$$f(\mathbf{r}) = e^{-a\mathbf{r}^2/2} \quad (13)$$

the Fourier transform is

$$\hat{f}(\mathbf{k}) = \left(\frac{2\pi}{a}\right)^{3/2} e^{-\mathbf{k}^2/(2a)} \quad (14)$$

Conversely, if

$$\hat{f}(\mathbf{k}) = e^{-b\mathbf{k}^2/2} \quad (15)$$

the inverse Fourier transform is

$$f(\mathbf{r}) = \left(\frac{1}{2\pi b}\right)^{3/2} e^{-\mathbf{r}^2/(2b)} \quad (16)$$

Some identities for $\delta(\mathbf{r})$

$$\delta(\mathbf{r}) = \frac{1}{(2\pi)^3} \int d^3\mathbf{k} e^{i\mathbf{k}\mathbf{r}}, 1 = \int d^3\mathbf{r} e^{i\mathbf{k}\mathbf{r}} \delta(\mathbf{r}) \quad (17)$$