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

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

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

$$S(\mathbf{k}) = \frac{< \tilde{\rho}(\mathbf{k})\tilde{\rho}(-\mathbf{k}) >}{N} \tag{2}$$

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

1. Express the structure factor $S(\mathbf{k})$ as a function in terms of $< e^{-i\mathbf{k}\mathbf{r}_{ij}} >$, where $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ with $i \neq j$.
2. Show that $S(\mathbf{k}) \to 1$ when $\mathbf{k} \to +\infty$.
3. 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 ?
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.

   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 ($N \to \infty$) show that the structure factor vanishes within the Brillouin zone ($-\frac{\pi}{a} < k < \frac{\pi}{a}$) (see Glossary).

   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

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

   and the structure factor becomes

$$S_d(\mathbf{k}) = \frac{< \tilde{\rho}_d(\mathbf{k})\tilde{\rho}_d(-\mathbf{k}) >}{2N}. \tag{9}$$

6. Show that $S_d(k) = 2 < \cos(ku)^2 > +2 < \cos(ku) >^2 (S(k) - 1)$.
7. Assuming that the moments $< u^2 >$ and $< u^4 >$ are finite, calculate the expansion of $S_d(k)$ to the order k^4. Configurations corresponding to the vanishing structure factor when $k \to 0$, are "super-uniform" (or hyperuniform). Justify this terminology. Hint : What is this limit for a uniform perfect gas.
8. Simulations have been performed for dense granular systems that unveils 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 ?

   For a liquid close the critical temperature of the liquid-gas transition. The spatial correlation function the 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 diverge at small wave vectors as k^{-A}, where A is an exponent to be determined

A Glossary

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

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

and the inverse transform is given by

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

For a Gaussian function

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

the Fourier transform is

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

Conversely, if

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

the inverse Fourier transform is

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

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

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