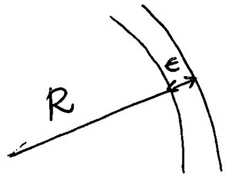
COMPUTATION OF THE PAIR CORRELATION FUNCTION

We wish to estimate $g^{(2)}(R) = V\langle \delta(R-(r_1-r_j))\rangle$

a) First, we use the fact that the result does not depend on i, j.

$$g^{(2)}(R) = \frac{2V}{N(N-1)} \sum_{i<j} \langle \delta(R - r_j + r_i)\rangle \qquad \left[\text{number of pairs: } \tfrac{1}{2}N(N-1)\right]$$

b)



We integrate over a shell of width ϵ

$$\int_{\text{shell}} d^3R \left[\sum_{i<j} \delta(R - r_1 - r_j)\right] =$$

$$= \left(\text{Number of pairs of particles such that } R < |r_1 - r_1| < R + \epsilon\right)$$

$$= N(R, \epsilon)$$

Therefore

$$\int_{\text{shell}} d^3R\, g^{(2)}(R) = \frac{2V}{N(N-1)} \langle N(R,\epsilon)\rangle$$

Now assume that ϵ is small so that we can assume $g^{(2)}(R)$ constant in the shell

$$\int_{\text{shell}} d^3R\, g^{(2)}(R) = g^{(2)}(R)\left(\begin{array}{c}\text{Volume}\\ \text{of the}\\ \text{shell}\end{array}\right) = g^{(2)}(R)\, V_\epsilon(R)$$

with $V_\epsilon(R) = \frac{4\pi}{3}(R+\epsilon)^3 - \frac{4\pi}{3}R^3$

It follows

$$g^{(2)}(R) = \frac{V}{V_\epsilon(R)} \cdot \frac{2}{N(N-1)} \langle N(R,\epsilon)\rangle$$

In practice:

a) choose ϵ (small)

b) compute a histogram for $N(R,\epsilon)$

If $M = \frac{L}{\epsilon}$ consider a vector $h(M)$ ($h=0$ at the beginning)

For $t = 1, \ldots$ N iterations

For $i = 1, \ldots, (N\text{particles} - 1)$

For $j = i+1, \ldots,$ Nparticles

compute $\hat{r}_{ij}$ (minimum image conv.)

n = integer part of $(\hat{r}_{ij}/\epsilon)$

$h(n)++$

End for

Endfor

End for

The loop over the iterations means that one should average over the results obtained at each different iteration IN EQUILIBRIUM. In the REAL CODE, the iteration loop will also include the update of the positions and the measurement of the other observables

c) for $n: 0, M-1$ $\quad h(n) = h(n)/$N iterations

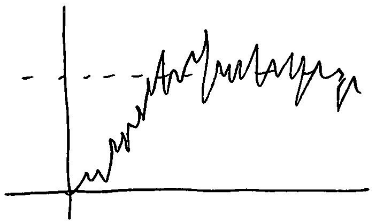
The vector $h(n)$ provides $\langle N(R,\epsilon)\rangle$

$$\langle N(n\epsilon,\epsilon)\rangle = h(n)$$

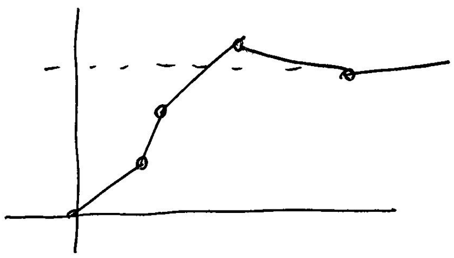
The practical problems

How to choose ϵ

1. start with ϵ small and look at the graph



If the result is this one, ϵ is **too small**
Repeat with a larger ϵ !

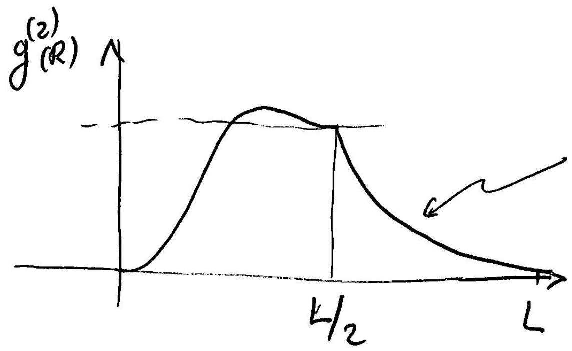


If the result is this one, ϵ is **too large**
Repeat with a smaller ϵ !

The aim is that ~~the~~ of obtaining a reasonably smooth curve with small fluctuations

Which is the range of acceptable values of R

The result of the procedure



Incorrect: for $R > \frac{L}{2}$ the minimum-image convention does not work: to get the correct $g^{(2)}$ IMAGES should be included.