

Virial expansion for the partition function of hard disks

Settings

System:

N disks of radius σ in a square of side L and surface $V = L^2$.

Density:

$$\eta = \frac{\text{occupied surface}}{\text{total surface}} = \frac{N\pi\sigma^2}{L^2} \quad (1)$$

Probability distribution (not normalized) of the centers $(\mathbf{x}_0, \dots, \mathbf{x}_{N-1})$ of the disks:

$$\pi(\mathbf{x}_0, \dots, \mathbf{x}_{N-1}) = \begin{cases} 1 & \text{if there is no overlap between disks} \\ 0 & \text{otherwise} \end{cases} \quad (2)$$

Partition function at density η

$$Z(\eta) = \int d\mathbf{x}_0 \dots d\mathbf{x}_{N-1} \pi(\mathbf{x}_0, \dots, \mathbf{x}_{N-1}) \quad (3)$$

Expansion of the partition function

Rewriting of $Z(\eta)$ with the non-overlapping constraint made explicit:

$$Z(\eta) = \int d\mathbf{x}_0 \dots d\mathbf{x}_{N-1} \underbrace{[1 - \Upsilon(\mathbf{x}_0, \mathbf{x}_1)] [1 - \Upsilon(\mathbf{x}_0, \mathbf{x}_2)] \dots [1 - \Upsilon(\mathbf{x}_{N-2}, \mathbf{x}_{N-1})]}_{\frac{1}{2}N(N-1) \text{ factors}} \quad (4)$$

The integral runs over the $2N$ individual coordinates, each of them running on $[0, L]$.

Indicator function:

$$\Upsilon(\mathbf{x}_k, \mathbf{x}_l) = \begin{cases} 1 & \text{if } \text{dist}(\mathbf{x}_k, \mathbf{x}_l) < 2\sigma \\ 0 & \text{otherwise} \end{cases} \quad (5)$$

0th order term of the expansion of the product of $[\dots]$'s in (4):

$$\int d\mathbf{x}_0 \dots d\mathbf{x}_{N-1} = Z(0) = V^N \quad (6)$$

1st order terms of this expansion all include an integral of the form:

$$\int d\mathbf{x}_k d\mathbf{x}_l \Upsilon(\mathbf{x}_k, \mathbf{x}_l) = V \underbrace{\int d\mathbf{x}_k \Upsilon(\mathbf{x}_k, \mathbf{x}_l)}_{\text{volume of the excluded region for } \mathbf{x}_k} = V \cdot 4\pi\sigma^2 \quad (7)$$

Gathering the term of 0th order and those of 1st order [there are $\frac{1}{2}N(N-1)$ of those]:

$$Z(\eta) = V^N - \frac{1}{2}N(N-1) \cdot \overbrace{V \cdot 4\pi\sigma^2}^{(7)} \cdot \overbrace{V^{N-2}}^{\text{other integrals than the } \int d\mathbf{x}_k d\mathbf{x}_l \text{ of (7)}} \quad (8)$$

$$= V^N \left(1 - 4\pi\sigma^2 \frac{N(N-1)}{2V} + \dots \right) \quad (9)$$

$$\simeq \underbrace{V^N}_{Z(0)} \underbrace{\exp[-2(N-1)\eta]}_{p_{\text{accept}}(\eta)} \quad (10)$$

Taking the logarithm:

$$\log Z(\eta) = N \log V - 2(N-1)\eta + \dots \quad (11)$$

Differentiating with respect to the volume V :

$$\frac{\partial \log Z(\eta)}{\partial V} = \frac{N}{V} + 2N(N-1)\pi\sigma^2 \frac{1}{V^2} + \dots \quad (12)$$

Multiplying by V/N :

$$\frac{V}{N} \frac{\partial \log Z(\eta)}{\partial V} = 1 + 2(N-1)\pi\sigma^2 \frac{1}{V} + \dots \quad (13)$$

The expansion to higher order, corresponding to products of **two** Υ 's, **three** Υ 's, etc., when expanding the product of [...]'s in (4), takes the form:

$$\frac{V}{N} \frac{\partial \log Z(\eta)}{\partial V} = 1 + 2(N-1)\pi\sigma^2 \frac{1}{V} + (\dots) \frac{1}{V^2} + (\dots) \frac{1}{V^3} + \dots \quad (14)$$