

# Statistical physics solutions

Alessandro Pacco

December 26, 2019



# Chapter 6

## Exercise 6.3)

Remark: diffraction and diffusion.

Send a laser on a lens  $D1$ . We have  $A(x) = 0$  if the light doesn't pass, 1 otherwise. Introduce the angle  $\theta$ . Then  $r(x, z) \approx r_0(z) - x \sin(\theta)$ . This approximation is valid only if  $x \ll d$ . The spherical wave coming out of a hole is  $E(r) = \frac{E_0}{r} e^{i \frac{2\pi}{\lambda} (r-ct)}$ . Then

$$E_{tot}(z) = \int dx A(x) \frac{E_0}{r(x, z)} e^{i \frac{2\pi}{\lambda} r(x, z)} \underset{\substack{x \rightarrow x \\ \text{varie lentement}}}{\approx} \frac{E_0}{r_0(z)} e^{i \frac{2\pi}{\lambda} r_0(z)} \int dx A(x) e^{i 2\pi \frac{\sin \theta}{\lambda} x} = \frac{E_0}{r_0(z)} e^{i \frac{2\pi}{\lambda} r_0(z)} TF(A) \frac{\sin \theta}{\lambda}$$

if we measure the light on the screen, we get that

$$I(z) = |E_{tot}(z)|^2 \approx |TF(A)|^2 \approx |S|^2$$

.

1)

We have  $\rho^{(l)}(\vec{x}_1, \dots, \vec{x}_l) = \mathbb{P}(\text{particella 1 at } \vec{x}_1 \pm d^3 \vec{r} \cap \dots \cap \text{particella } l \text{ at } \vec{x}_l \pm d^3 \vec{r})$ . Moreover  $E_p = \sum_{i>j} U(\vec{r}_i - \vec{r}_j)$ .

2)

The kinetic energy is given by  $E_c = \sum_i \frac{p_i^2}{2m}$ .

3)

As always

$$Z = \frac{1}{h^{3N} \cdot N!} \int d\Gamma e^{-\beta(E_c + E_p)(\Gamma)} = \frac{1}{h^{3N} \cdot N!} \left( \sqrt{\frac{2\pi m}{\beta}} \right)^{3N} \int \prod d^3 \vec{r}_i e^{-\beta E_p(\Gamma)} = \frac{\lambda^{-3N}}{N!} Q$$

with  $\lambda = \sqrt{\frac{h^2 \beta}{2\pi m}}$

4)

In order to have a classical description we need to have that (average distance between particles)  $\gg \lambda$ . Hence since the average particle distance is  $(V/N)^{1/3}$  we get that we must have  $(V/N)^{1/3} = n^{-1/3} \gg \lambda$ .

5)

We proved that

$$\frac{1}{V} g(\vec{r}) d^3 \vec{r} = \mathbb{P}(\text{1 particle in } \vec{r} \pm d^3 \vec{r} | \text{1 part in } 0) \stackrel{GP}{=} \mathbb{P}(\text{1 part in } \vec{r} \pm d^3 \vec{r}) = \frac{d^3 \vec{r}}{V}$$

and so  $g_{GP}(\vec{r}) = 1$ .

6)

Benzene is non-polar, hence it is better than water for the diffraction. Difficulty to obtain some data for small  $\vec{r}$ ? If  $\vec{r}$  is too small with respect to the wavelength we don't get diffraction.

Estimation of the diameter:

7)

For diffraction we need that the  $\sigma$  is almost the same as the wavelenght of the incoming light. Hence We have resolution  $\sim \sigma \sim 500nm$  since we want  $\lambda \sim \sigma$ . Hence we need a laser of  $\lambda \sim 514nm$ .

8)

$$n = \frac{\text{number of particles}}{V} = \frac{\text{densite massique}}{\text{masse 1 particule}} = \frac{5 \cdot 39 \cdot 10^{-2}}{8 \cdot 10^{-15}} \approx 10^{19} m^{-3}$$

minimal volume  $\sim \sigma^3$ . We have that

$$n\sigma^3 = 10^{19}(5 \cdot 10^{-7})^3 = 125 \cdot 10^{19-21} \approx 1.25 \text{ particles/elementar volume}$$

Hence it is not at all dilute, but mainly dense.

9)

We work on the LHS:

$$\begin{aligned} \rho^{(2)} &= \sum_{i_1 \neq i_2} \langle \delta(\vec{r}_{i_1} - \vec{x}) \delta(\vec{r}_{i_2} - \vec{y}) \rangle = \frac{1}{Z} \int \prod_{i=1}^N \frac{d\vec{r}_i d\vec{p}_i}{h^3} e^{-\beta H(\dots)} \cdot \sum_{i_1 \neq i_2} \frac{1}{Q_3} \frac{1}{Q_N} \sum_{i_1 \neq i_2} \int \prod_{i=1}^N d^3 \vec{r}_i e^{-\beta E_p\{r_i\}} \delta(\vec{r}_{i_1} - \vec{x}) \delta(\vec{r}_{i_2} - \vec{y}) \\ &= \frac{1}{Q_N} N(N-1) \int \prod_{i=1}^N d^3 \vec{r}_i e^{-\beta \sum_{i < j} U(r_i - r_j)} \delta(\vec{r}_1 - \vec{x}) \delta(\vec{r}_2 - \vec{y}) \\ &= \frac{N(N-1)}{Q_N} \int \prod_{i=3}^N d^3 \vec{r}_i e^{-\beta [U(x-y) + \sum_{i=3}^N (U(x-r_i) + U(y-r_i)) + \sum_{i > j=3}^N U(r_i - r_j)]} \end{aligned}$$

Now we attack the gradient

$$\vec{\nabla}_{\vec{x}} \rho^{(2)}(x, y) = \frac{N(N-1)}{Q_N} \int \prod_{i=3}^N d^3 \vec{r}_i (-\beta \nabla U(x-y) - \beta \sum_{i=3}^N \nabla U(x-r_i)) \cdot e^{-\beta(\dots)} = \frac{N(N-1)}{Q_N} (-\beta \nabla U(x-y)) \int \prod_{i=3}^N d^3 \vec{r}_i e^{-\beta(\dots)}$$

Then we introduce  $\sum_{i=3}^N f(r_i) = \int dz f(z) \sum_{i=3}^N \delta(z - r_i)$ . With that decomposition we get

$$\nabla_{vecx} \rho^{(2)}(x, y) = -\beta (\nabla U(x-y)) \rho^{(2)}(x, y) - \beta \int dz \nabla U(x-z) \frac{N(N-1)}{Q_N \int \prod_{i=3}^N d\vec{r}_i e^{-\beta E_p(x, y, r_i > 3)}} \sum_{i=3}^N \delta(r_i - z)$$

where  $\langle \rangle$  is the canonical average.

### 0.0.1 10)

Born-Green is general.

$\nabla \rho^2 \approx f(\rho^2, \rho^3)$  and  $\nabla \rho^3 = f(\rho^3, \rho^4)$ , it doesn't stop.

$$\rho^{(l)}(\vec{x}_1, \vec{x}_2, \dots, \vec{x}_n) = \sum_{i_1 \neq \dots \neq i_l} \langle \delta(\vec{x}_{i_1} - vecx_1) \dots \delta(\vec{x}_{i_l} - \vec{x}_l) \rangle \approx_{dilue} \sum \langle \delta(\vec{x}_{i_1} - \vec{x}_{i_1}) \dots \delta(\dots) \rangle \approx n\sigma^3)^l$$

IN practice, if we suppose dilute then  $n\sigma^3 \ll 1$  implies that  $\rho^{(1)} \gg \rho^{(2)} \gg \dots$

In our case we have

*merdadafare*

By symmetry  $\rho^{(2)}(x, y) = \rho^{(2)}(x - y)$ . If we rewrite Born-Green at order 2 we get

$$\frac{d}{dr} \rho^{(2)} = -\beta \left( \frac{d}{dr} U(r) \right) \rho^{(2)}(r) \Rightarrow \rho^{(2)}(r) = A e^{-\beta U(r)}$$

We determine  $A$  with  $\rho^{(2)} \underset{r \rightarrow \infty}{=} n^{-2}$  and  $U(r) \underset{r \rightarrow \infty}{\rightarrow} 0$ , so that  $A = n^{-2}$ .

11)

on paper

12)

Computing the TF of  $g(\vec{r}) - 1$ . Hors  $g(\vec{r}) = g(r, \emptyset, \emptyset)$ .

$$TF(g-1)(\vec{q}) = \int d^3\vec{r} e^{i\vec{q}\cdot\vec{r}} (g(\vec{r})-1) = (\text{coordspherzalign}\vec{q}) = \int 4\pi r^2 dr \int_0^\pi d\theta \sin\theta e^{iqr \cos\theta} (g(r)-1) = 4\pi \int r^2 dr (g(r)-1) \int_{-1}^1 dx e^{iqr x}$$

with  $\int (merda - 11) = 2 \frac{\sin(qr)}{qr}$ .  
Hence

$$TF(g-1)(q) = \frac{8\pi}{q} \int dr \cdot r (g(r) - 1) \sin(qr) = \frac{4\pi}{q^3} \left( (e^{\beta\epsilon} - 1)(\sin \alpha\sigma q - \alpha q \cos \alpha\sigma q) + e^{\beta\epsilon}(\sigma q \cos(\sigma q) - \sin(\sigma q)) \right)$$

pseudoperiod  $\sim \frac{2\pi}{\sigma}, \frac{2\pi}{\alpha\sigma}$ .  $\rho^2 \sim$  period  $\sigma, \alpha\sigma$ . Then we get

$$S(q) = 1 + nTF(g-1)(q)$$

and so  $S(0) = 1 + n + 4\pi(-(e^{\beta\epsilon})(\alpha\sigma)^3 + e^{\beta\epsilon}\sigma^3)$  since  $\sin(x) - x \cos(x) = x - x^3/6 - x(1 - x^2/2) = x^3/3 + o(x^3)$  (S behaves well in 0).

14)

Fig. 6.3, we can read  $S(0)$  and know  $n, \beta$ : for  $\alpha$ , we take  $o(1)$ ,  $\alpha = 2$  for example. Then  $\beta\epsilon_{exp} \underset{\alpha^3 \gg 1}{\approx}$   $\frac{1-S(0)}{4\pi n\sigma^3/3} \alpha^{-3} \approx 10^{-2}$ ,  $\frac{\epsilon}{k_B} \sim 3K$  (on the paper 70K).  $\epsilon_{exp} \ll k_B T$  implies that the thermic agitation dominates.

15)

Experimentally, we have that  $S(q) \rightarrow_{TF^{-1}exact} g(r) \sim e^{-\beta U(r)}$  (approximation diluee). We can determine experimentally the approxiative interactions  $U(r)$

$$U_{exp}(r) = -k_B T \ln(g_{exp}(r))$$

FIg 6.3  $\Phi(r) = -\ln g_{exp}(r)$ .



# Chapter 11