Statistical physics solutions

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Chapter 6

Exercise 6.3)

Remark: diffraction and diffusion.

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

$$E_{tot}(z) = \int dx A(x) \frac{E_0}{r(x,z)} e^{i\frac{2\pi}{\lambda} r(x,z)} \underset{\substack{x \to x \\ \text{varie lentement}}}{\approx} \frac{E_0}{r_0(z)} e^{i\frac{2\pi}{\lambda} r_0(z)} \int dx A(x) e^{i2\pi\frac{\sin\theta}{\lambda}x} = \frac{E_0}{r_0(z)} e^{i\frac{2\pi}{\lambda} r_0(z)} TF(A) \frac{\sin\theta}{\lambda}$$

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

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

.

1)

We have $\rho^{(l)}(\vec{x}_1, \cdots, \vec{x}_l) = \mathbb{P}(\text{particella 1 at } \vec{x}_1 \pm d^3\vec{r} \cap \cdots \cap \text{particella } l \text{ at } \vec{x}_l \pm d^3\vec{r})$. 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)$>> \lambda$. Hence since the average particle distance is $(V/N)^{1/3}$ we get that we must have$(V/N)^{1/3} = n^{-1/3} >> \lambda$.

5)

We proved that

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

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

6)

Benzene is non-polar, hence it is better than water for the diffraction. Difficulty to obtein 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 diamater:

7)

For diffraction we need that the σ 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:

$$\rho^{(2)} = \sum_{i_1 \neq i_2} < \delta(\vec{r}_{i_1} - \vec{x})\delta(\vec{r}_{i_2} - \vec{y}) > = \frac{1}{Z} \int \prod_{i=1}^{n} \frac{d\vec{r}_i d\vec{p}_i}{h^3} e^{-\beta H(..)} \cdot \sum_{i_1 \neq i_2} \underset{Q3}{=} \frac{1}{Q_N} \sum_{i_1 \neq i_2} \int \prod_{i=1}^{N} d^3\vec{r}_i e^{-\beta E_p\{r_i\}} \delta(\vec{r}_{i_1} - \vec{x})\delta(\vec{r}_{i_2} - \vec{y})$$

$$= \frac{1}{Q_N} N(N-1) \int \prod_{i=1}^{N} d^3\vec{r}_i e^{-\beta \sum_{i<j} U(r_i - r_j)} \delta(\vec{r}_1 - \vec{x})\delta(\vec{r}_2 - \vec{y})$$

$$= \frac{N(N-1)}{Q_N} \int \prod_{i=3}^{N} d^3\vec{r}_i e^{-\beta\left[U(x-y) + \sum_{i=3}^{N}(U(x-r_i) + U(y-r_i)) + \sum_{i>j=3}^{N} U(r_i - r_j)\right]}$$

Now we attack the gradient

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

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

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

where <> is the canonical average.

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Born-Green is general.

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

$$\rho^{(l)}(\vec{x}_1, \vec{x}_2, .., \vec{x}_n) = \sum_{i_1 \neq .. \neq i_l} < \delta(\vec{x}_{i_1} - vecx_1)..\delta(\vec{x}_{i_l} - \vec{x}_l) > \underset{dilue}{\approx} \sum < \delta(\vec{x}_{i_1} - \vec{x}_{i_1})..\delta(..) > \approx n\sigma^3)^l$$

IN practice, if we suppose dilute then $n\sigma^3 << 1$ implies that $\rho^{(1)} >> \rho^{(2)} >> ....$

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

$$\frac{d}{dr}\rho^{(2)} = -\beta(\frac{d}{dr}U(r))\rho^{(2)}(r) \Rightarrow \rho^{(2)}(r) = Ae^{-\beta U(r)}$$

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

11)

on paper

12)

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

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

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

Hence

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

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, β: for α, we take $o(1)$, $\alpha = 2$ for example. THen $\beta\epsilon_{exp} \underset{\alpha^3>>1}{\approx} \frac{1-S(0)}{4\pi n\sigma^3/3}\alpha^{-3} \approx 10^{-2}$, $\frac{\epsilon}{k_B} \sim 3K$ (on the paper 70K). $\epsilon_{exp} << k_B T$ implies that the thermic agitation dominates.

15)

Experimentally, we have that $S(q) \to_{\mathrm{TF}^{-1} exact} g(r) \sim e^{-\beta U(r)}(approximationdiluee)$. 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