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

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

if we 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.

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 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

11.4

1)

Call q the number of defects in the chain. Then at each time we encounter a defect, we have to add a term -1, whereas inside the defect we only add $+1$ terms, because the particles have same spin. In simple words any meeting of two defect steals a spin link. Hence the hamiltonian will be given by

$$H = -J((N-q)-(q-1)) = -J(N-2q+1)$$

2)

The degeneracy of an energetic level is given by the number of possible configurations that lead to that energy. In particular since an energy is given by q, the number of possiblities that we can get that energy will be given by the number of possibilities to choose q defects. This is given by the number of possibilities to put $q-1$ sticks in $N-1$ holes, i.e. $\binom{N-1}{q-1}$, multiplied by 2, because for any defect configuration we can either start with up or with down. The canonical partition function will be given by

$$\begin{aligned}
Z &= \sum_{q=1}^{N} 2\binom{N-1}{q-1} e^{\beta J(N-2q+1)} = \sum_{q=0}^{N-1} 2\binom{N-1}{q} e^{\beta J(N-1-2q)} = 2e^{\beta J(N-1)} \sum_{q=0}^{N-1} \binom{N-1}{q} (e^{-2\beta J})^2 \\
&= 2e^{\beta J(N-1)}(1+e^{-2\beta J})^{N-1} = 2^N \cosh^{N-1}(\beta J)
\end{aligned}$$

3)

Let's fix the number of defects q. Then the energy is fixed at $H = -J(N-2q+1)$ and the associated partition function is given by

$$Z_q = 2\binom{N-1}{q-1} e^{\beta J(N-2q+1)}$$

The associated free energy is then given by

$$\begin{aligned}
F_q &= -k_B T \log(Z_q) = -k_B T \log\left(2\binom{N-1}{q-1} e^{\beta J(N-2q+1)}\right) = -k_B T\left(\log(2) + \log\left(\binom{N-1}{q-1}\right) + \beta J(N-2q+1)\right) \\
&\approx -k_B T\bigg(\log(2) + \beta J(N-2q+1) + (N-1)\log(N-1) - (q-1)\log(q-1) - (N-q)\log(N-q)\bigg)
\end{aligned}$$

4)

What the fucking hell do you want me to do?

5)

We have that

$$\begin{aligned}
\langle q \rangle &= \frac{\sum_{\{\sigma_i\}} q_{\{\sigma_i\}} e^{\beta J(N-2q+1)}}{Z} = \frac{e^{\beta J(N+1)}}{-2J} \frac{\partial_\beta \sum e^{-2\beta J q}}{Z} = -\frac{1}{2J}\frac{\partial}{\partial \beta} \log\left(\frac{Z}{e^{\beta J(N+1)}}\right) \\
&= -\frac{1}{2J}\frac{\partial}{\partial \beta}\bigg(\log(Z) - \beta J(N+1)\bigg) = \frac{N+1}{2} - \frac{1}{2J}\frac{\partial}{\partial \beta}\bigg(N\log(2) + (N-1)\log(\cosh\beta J)\bigg) \\
&= \frac{N+1}{2} - \frac{1}{2J}(N-1)\frac{\sinh(\beta J)J}{\cosh(\beta J)} = \frac{N+1}{2} - (N-1)\frac{\tanh(\beta J)}{2}
\end{aligned}$$

6)

We can define d as $d = \frac{N}{\langle q \rangle}$ so that

$$d = \frac{N}{\frac{N+1}{2} - (N-1)\frac{\tanh(\beta J)}{2}}$$

7)

The hamiltonian now is

$$H = -\sum_{i=1}^{N-1} J_i \sigma_i \sigma_{i+1}$$

We will suppose that any configuration of the type $\pm J_1 \pm J_2 \pm \cdots \pm J_{N-1}$ is unique and can be obtained with only one configuration of the σ_i. This way there is a bijection between the possible sums of the form above and the choice of the σ_i (up to changing the initial value of σ_i which automatically determines all the other values of the σ_i), therefore we will take the J_is with sign. Hence we get that

$$\begin{aligned} Z &= \sum_{J_i = \pm|J_i|} 2e^{-\beta H} = \sum_{J_i = \pm|J_i|} e^{\beta \sum_{i=1}^{N-1} J_i} = \sum_{J_1 = \pm|J_1|} e^{\beta J_1} \cdots \sum_{J_{N-1} = \pm|J_{N-1}|} e^{\beta J_{N-1}} \\ &= 2(2\cosh(\beta|J_1|)) \cdots (2\cosh(\beta|J_{N-1}|)) = 2^N \cosh(\beta|J_1|) \cdots \cosh(\beta|J_{N-1}|) \end{aligned}$$

8)

We have that

$$\begin{aligned} \langle \sigma_i \sigma_{i+1} \rangle &= \frac{\sum_{\{J_k\}} \sigma_i \sigma_{i+1} 2e^{\beta \sum_{k=1}^{N-1} J_k}}{Z} = 2\frac{\sum_{J_1 = \pm|J_1|} e^{\beta J_1} \cdots \sum_{J_i = \pm|J_i|} \operatorname{sgn}(J_i) e^{\beta J_i} \cdots \sum_{J_{N-1} = \pm|J_{N-1}|} e^{\beta J_{N-1}}}{Z} \\ &= \frac{2(2\cosh(\beta|J_1|) \cdots (2\sinh(\beta|J_i|)) \cdots (2\cosh(\beta|J_{N-1}|)}{Z} = \tanh(\beta|J_i|) \end{aligned}$$

More easily we could have seen that $\langle \sigma_i \sigma_{i+1} \rangle = \frac{1}{Z\beta} \frac{\partial Z}{\partial J_i}$ (with the old notation in which we keep J_i with its original sign and we multiply it by $\sigma_i \sigma_{i+1}$).

9)

Let's get back to the original notation since here we saw it becomes easier. We have:

$$\begin{aligned} \langle \sigma_i \sigma_{i+2} \rangle &= \langle \sigma_i \sigma_{i+1} \sigma_{i+1} \sigma_{i+2} \rangle = \frac{\sum_{\{\sigma_i\}} (\sigma_i \sigma_{i+1})(\sigma_{i+1} \sigma_{i+2}) 2e^{\beta \sum_{k=1}^{N-1} \sigma_k \sigma_{k+1} J_k}}{Z} = \frac{1}{Z\beta^2} \frac{\partial^2 Z}{\partial J_i \partial J_{i+1}} \\ &= \tanh(\beta J_i) \tanh(\beta J_{i+1}) \end{aligned}$$

Then for $J_i = J$ we get

$$\langle \sigma_i \sigma_{i+1} \rangle = \tanh^2(\beta J)$$

10)

We have that

$$\langle \sigma_i \sigma_{i+r} \rangle = \langle \sigma_i \sigma_{i+1} \ldots \sigma_{i+r-1} \sigma_{i+r} \rangle = \frac{1}{Z\beta^r} \frac{\partial^r Z}{\partial J_i \ldots \partial J_{i+r}} = \tanh(\beta J_i) \ldots \tanh(\beta J_{i+r})$$

and by using $J_i = J$ we finally get $\langle \sigma_i \sigma_{i+r} \rangle = (\tanh(\beta J))^r$.

Per trovare $g(r)$ manca $\langle \sigma \rangle^2$ (WTF??)

11)

By using $g(r) = (\tanh \beta J)^r$ (which I am not sure being true wtf lepre mela puttana) then we get that

$$g(r) = e^{-r/\xi} \Leftrightarrow \xi = -\frac{1}{\ln(\tanh \beta J)}$$

For N big we have that

$$d \approx \frac{2}{1 - \tanh(\beta J)}$$

and for $\beta J >> 1$ we have

$$\xi \approx -\frac{1}{\tanh \beta J - 1} = \frac{1}{1 - \tanh \beta J}$$

hence we can directly see the direct proportionality between d and ξ.

12)

The proportionality factor is 2.

13)

Suppose that we have a finite temperature T with interactions at short distance. Then if there was a ferromagnetic phase, then there wouldn't be lost of information through the chain, i.e. the first spin would be influencing all the others (which is what would happen at zero temperature), however we see that the cprrelation function goes to zero as r goes to infinity, which means that the at high distance two spins are completely unrelated.