

Segundos parciales de Física Teórica 3

Nota 1.

Estos parciales fueron hechos por un alumno mientras preparaba el parcial. Es por ello que es altamente probable que hayan errores. Úsense con responsabilidad. En caso de notar efectos adversos suspenda inmediatamente su uso y consulte a su profesor de cabecera.

Nota 2.

Todos los resultados que tienen un ✓ es porque fueron chequeados contra los “parciales resueltos oficiales” en páginas de la materia de cuatrimestres anteriores.



Encontrá más material de Alf en [este link](#).

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1. 23/11/2015

Consigna

Problema 1

Considere un sistema de bosones idénticos de masa m , espín 1 y momento magnético μ_m que no interactúan entre sí. Las partículas están confinadas en una trampa armónica tridimensional de frecuencia angular ω , y además están sometidas a un campo magnético uniforme de magnitud $B > 0$ en la dirección z . El hamiltoniano de una partícula es pues

$$\mathcal{H}(\mathbf{q}, \mathbf{p}, s) = \frac{|\mathbf{p}|^2}{2m} + \frac{1}{2}m\omega^2 |\mathbf{q}|^2 - \mu_m B s$$

donde s es la componente z del espín. El sistema está en equilibrio a una temperatura T y fugacidad z .

- Calcule el logaritmo de la función de partición grancanónica del sistema, Z_{GC} , y de ahí obtenga el valor medio del número de partículas, N . (Ayuda: le puede ser útil saber que el área de la esfera de radio 1 en un espacio de d dimensiones es $\frac{2\pi^{d/2}}{\Gamma(d/2)}$.)
- Obtenga los valores a los que tiende la temperatura crítica, T_C , del sistema en los límites $B \rightarrow 0$ y $B \rightarrow \infty$, como funciones de N y ω .
- Calcule la magnetización por partícula, M , del sistema como función de T , ω , B y N a temperaturas por debajo de la crítica.

Problema 2

El parámetro de orden asociado a la transición de fase líquido-superfluido es una función compleja, Ψ , que puede ser interpretada como el número de partículas en la fase superfluida multiplicado por su función de onda. La energía libre de Ginzburg-Landau correspondiente es

$$F(\Psi, T) = \int d^3r \left[\frac{\hbar^2}{2m} |\vec{\nabla}\Psi|^2 + \frac{a(T - T_C)}{2} |\Psi|^2 + \frac{b}{4} |\Psi|^4 \right]$$

donde T es la temperatura, T_C es la temperatura crítica y a , b y m son constantes positivas, la última de las cuales puede ser interpretada como la masa de las partículas que forman el superfluido.

- Obtenga la ecuación diferencial que debe satisfacer Ψ para ser un extremo de F .
- Suponiendo que $T < T_C$, obtenga una solución de esta ecuación que describa el superfluido con densidad uniforme no nula moviéndose a velocidad constante \mathbf{v} . ¿Cuál es el valor máximo que puede tomar $|\mathbf{v}|$ a una dada temperatura?
- Calcule el calor específico, c_V , del superfluido en la configuración del ítem anterior.

Problema 3

Considere una partícula browniana que se mueve en una dimensión en un medio con coeficiente de fricción γ bajo la influencia de un ruido blanco gaussiano de amplitud espectral g . Sea $P(x, t)$ la densidad de probabilidad de que la partícula se encuentre en la posición x en el instante t . En el límite de alta fricción, P obedece la ecuación de Fokker-Planck

$$\frac{\partial P}{\partial t} = \frac{g}{2\gamma^2} \frac{\partial^2 P}{\partial x^2}$$

- Encuentre la solución general de esta ecuación como una integral de la forma $P(x, t) = \int_{-\infty}^{\infty} dk P_k(t) e^{ikx}$.
- Obtenga explícitamente $P(x, t)$ para $t \geq 0$ suponiendo que, en el instante $t = 0$, la partícula se encuentra con certeza en la posición $x = 0$. (Ayuda: $\int_{-\infty}^{\infty} dk e^{-\alpha k^2 + ikx} = \sqrt{\pi/\alpha} e^{-x^2/4\alpha}$.)
- Calcule $\langle x(t) \rangle$, $\langle x^2(t) \rangle$ y la entropía de Shannon, $S(t) = -\int_{-\infty}^{\infty} dx P(x, t) \log P(x, t)$, para la densidad de probabilidad obtenida en el ítem anterior. Comente su resultado para $S(t)$.

Resolución

Nota. Para una resolución más refinada de este parcial, mirar en la página 41 donde lo volví a resolver luego de entender un poco mejor los temas. La resolución actual la hice ni bien empecé a preparar la materia, la otra la hice luego de una semana de práctica. Obviamente quedó mejor.

Problema 1

Ítem a (preguntar razonamiento inicial)

La función de partición del ensamble gran canónico es

$$Z = \sum_{\forall \text{ estados}} e^{-\beta(\epsilon_i - \mu N_i)}$$

Como los bosones son partículas indistinguibles y además no interactúan (consigna) entonces la función de partición del sistema se puede factorizar según (ver pag. 55)

$$Z = \prod_{\forall \text{ estados monoparticulares}} Z_{\text{monoparticular } i} \quad \text{con } Z_{\text{monoparticular } i} = \sum_{\forall n \text{ permitido}} e^{-\beta(\epsilon_i - \mu)n}$$

En consecuencia

$$\log Z = \sum_{\forall \text{ estados monoparticulares}} \log Z_{\text{monoparticular } i}$$

Debido a que los bosones no cumplen con el principio de exclusión de Pauli, entonces en un mismo estado pueden haber desde cero hasta infinitos. La función de partición monoparticular es entonces

$$\begin{aligned} Z_{\text{monoparticular } i} &= \sum_{n=0}^{\infty} e^{-\beta(\epsilon_i - \mu)n} \\ \text{Serie geométrica} \rightarrow &= \frac{1}{1 - e^{-\beta(\epsilon_i - \mu)}} \\ &= \frac{1}{1 - ze^{-\beta\epsilon_i}} \end{aligned}$$

donde $z \stackrel{\text{def}}{=} e^{\beta\mu}$ es la fugacidad y se asumió que, para que la serie converja, $e^{-\beta(\epsilon_i - \mu)} \in [0, 1)$.

Introducing the previous result into the expression for the partition function we get

$$\begin{aligned} \log Z &= \sum_{\forall \text{ estados monoparticulares}} \log Z_{\text{monoparticular } i} \\ &= - \sum_{\forall \text{ estados monoparticulares}} \log(1 - ze^{-\beta\epsilon_i}) \end{aligned}$$

Now the sum has to be done over each *estado monoparticular*. This is determined by the Hamiltonian of each particle. In this case the energy is going to be $\epsilon = \mathcal{H}(\mathbf{q}, \mathbf{p}, s)$ with no restrictions interconnecting \mathbf{q}, \mathbf{p} and s so

$$\begin{aligned} \log Z &= - \sum_{\text{allowed } \mathbf{q}, \mathbf{p} \text{ and } s} \log(1 - ze^{-\beta\mathcal{H}(\mathbf{q}, \mathbf{p}, s)}) \\ \mathbf{q}, \mathbf{p}, s \text{ are not connected} \rightarrow &= - \sum_{\forall \mathbf{q}} \sum_{\forall \mathbf{p}} \sum_{\forall s} \log(1 - ze^{-\beta\mathcal{H}(\mathbf{q}, \mathbf{p}, s)}) \\ \text{It is still exact} \rightarrow &= \sum_{\text{bad states } \ominus} \sum \sum \sum \log(1 - ze^{-\beta\mathcal{H}(\text{bad state}_i)}) - \sum_{\text{nice states } \oplus} \sum \sum \sum \log(1 - ze^{-\beta\mathcal{H}(\text{nice state}_i)}) \\ \text{Not exact anymore } \ominus \rightarrow &\approx - \sum_{\text{bad states } \ominus} \sum \sum \sum \log(1 - ze^{-\beta\mathcal{H}(\text{bad state}_i)}) - \int \int \sum_{\text{nice states } \oplus} \log(1 - ze^{-\beta\mathcal{H}(\text{nice state})}) \\ &= - \sum_{\text{bad states } \ominus} \sum \sum \sum \log(1 - ze^{-\beta\mathcal{H}(\text{bad state}_i)}) - \int \int \frac{d^3q d^3p}{h^3} \sum_{s \in \{-1, 0, 1\}} \log(1 - ze^{-\beta\mathcal{H}(\mathbf{q}, \mathbf{p}, s)}) \end{aligned}$$

The approximation to the continuous is good enough for the higher terms of the summation (which I have called *nice states*) while the lowest terms (which I have called *bad states*) can not be approximated. I can not find any justification right now

but it seems that, at least for this problem, the only bad state is the fundamental¹ so

$$\begin{aligned} \sum_{\text{bad states}} \log \left(1 - ze^{-\beta \mathcal{H}(\text{bad state}_i)} \right) &= \log \left(1 - ze^{-\beta \mathcal{H}(\mathbf{q}=\mathbf{0}, \mathbf{p}=\mathbf{0}, s=+1)} \right) \\ &= \log \left(1 - ze^{\beta \mu_m B} \right) \end{aligned}$$

and then

$$\log Z = -\log \left(1 - ze^{\beta \mu_m B} \right) - \int_{\forall \mathbf{q}} \int_{\forall \mathbf{p}} \frac{d^3 q d^3 p}{h^3} \sum_{s \in \{-1, 0, 1\}} \log \left(1 - ze^{-\beta \mathcal{H}(\mathbf{q}, \mathbf{p}, s)} \right)$$

Preguntar si la línea de razonamientos que me trajo hasta acá es la correcta o hay algo turbio...

From now on it is nothing more than to do the math. This is, calling $\boxed{A} \equiv \int_{\forall \mathbf{q}} \int_{\forall \mathbf{p}} \frac{d^3 q d^3 p}{h^3} \sum_{s \in \{-1, 1\}} \log \left(1 - ze^{-\beta \mathcal{H}(\mathbf{q}, \mathbf{p}, s)} \right)$,

$$\begin{aligned} \boxed{A} &= - \int_{\forall \mathbf{q}} \int_{\forall \mathbf{p}} \frac{d^3 q d^3 p}{h^3} \sum_{s \in \{-1, 0, 1\}} \log \left(1 - ze^{-\beta \mathcal{H}(\mathbf{q}, \mathbf{p}, s)} \right) \\ &= - \int_{\forall \mathbf{q}} \int_{\forall \mathbf{p}} \frac{d^3 q d^3 p}{h^3} \sum_{s \in \{-1, 0, 1\}} \log \left(1 - z \exp(\beta \mu_m B s) \exp \left(-\beta \frac{|\mathbf{p}|^2}{2m} \right) \exp \left(-\beta \frac{m\omega^2 |\mathbf{q}|^2}{2} \right) \right) \end{aligned}$$

Now we have to do a change of variables $\begin{cases} \mathbf{Q} \stackrel{\text{def}}{=} \sqrt{\frac{m\omega^2}{2}} \mathbf{q} \\ \mathbf{P} \stackrel{\text{def}}{=} \frac{\mathbf{p}}{\sqrt{2m}} \end{cases}$ and $z_s \stackrel{\text{def}}{=} ze^{\beta \mu_m B s}$ (this is just for less writing) so

$$\begin{aligned} \boxed{A} &= - \left(\frac{m\omega^2}{2} \right)^{-3/2} \left(\frac{1}{2m} \right)^{-3/2} \frac{1}{h^3} \int_{\forall \mathbf{Q}} \int_{\forall \mathbf{P}} d^3 Q d^3 P \sum_{s \in \{-1, 0, 1\}} \log \left(1 - z_s \exp \left(-\beta \left(|\mathbf{P}|^2 + |\mathbf{Q}|^2 \right) \right) \right) \\ &= - \left(\frac{2}{\omega h} \right)^3 \int_{\forall \mathbf{Q}} \int_{\forall \mathbf{P}} d^3 Q d^3 P \sum_{s \in \{-1, 0, 1\}} \log \left(1 - z_s \exp \left(-\beta \left(|\mathbf{P}|^2 + |\mathbf{Q}|^2 \right) \right) \right) \end{aligned}$$

Using another change of variables given by $\begin{cases} r \stackrel{\text{def}}{=} \sqrt{|\mathbf{P}|^2 + |\mathbf{Q}|^2} \\ \theta_5 \stackrel{\text{def}}{=} \text{the other stuff} \end{cases}$ and inspired by the fact that the integrand is of the form

$f(|\mathbf{p}|^2 + |\mathbf{q}|^2) \sim f(r^2)$ (i.e. passing to spherical coordinates) then

$$\boxed{A} = - \left(\frac{2}{\omega h} \right)^3 \int_{\Theta_5} d\theta_5 \sum_{s \in \{-1, 0, 1\}} \int_{r=0}^{\infty} dr r^5 \log \left(1 - z_s \exp \left(-\beta r^2 \right) \right)$$

(the factor r^5 is the Jacobian). Here, $\int_{\Theta_5} d\theta_5$ corresponds to the area of a sphere of radius 1 and dimension 6. So (using the help from the *consigna*)

$$\begin{aligned} \boxed{A} &= - \left(\frac{2}{\omega h} \right)^3 \frac{2\pi^3}{\Gamma(3)} \sum_{s \in \{-1, 0, 1\}} \int_{r=0}^{\infty} dr r^5 \log \left(1 - z_s \exp \left(-\beta r^2 \right) \right) \\ \Gamma(3) = 2 \rightarrow &= - \left(\frac{2\pi}{\omega h} \right)^3 \sum_{s \in \{-1, 0, 1\}} \int_{r=0}^{\infty} dr r^5 \log \left(1 - z_s \exp \left(-\beta r^2 \right) \right) \end{aligned}$$

¹i.e. the one with the lowest energy.

We impose now another change of variable (the last one) given by $x \stackrel{\text{def}}{=} \beta r^2$ so $\begin{cases} r = \sqrt{x/\beta} \\ dr = \frac{dx}{2\sqrt{\beta x}} \end{cases}$ and

$$\begin{aligned} \boxed{A} &= -\left(\frac{2\pi}{\omega\hbar}\right)^3 \sum_{s \in \{-1,0,1\}} \int_{x=0}^{\infty} \frac{dx}{2\sqrt{\beta x}} \left(\frac{x}{\beta}\right)^{5/2} \log(1 - z_s e^{-x}) \\ &= -\frac{1}{2} \left(\frac{2\pi}{\omega\hbar\beta}\right)^3 \sum_{s \in \{-1,0,1\}} \int_{x=0}^{\infty} dx x^2 \log(1 - z_s e^{-x}) \\ \text{Intagracion by parts} \rightarrow &= -\frac{1}{2} \left(\frac{2\pi}{\omega\hbar\beta}\right)^3 \sum_{s \in \{-1,0,1\}} \left[\frac{x^3}{3} \log(1 - z_s e^{-x}) \Big|_{x=0}^{x \rightarrow \infty} - \int_{x=0}^{\infty} dx \frac{x^3}{3} \frac{z_s e^{-x}}{1 - z_s e^{-x}} \right] \\ &= \frac{1}{6} \left(\frac{2\pi}{\omega\hbar\beta}\right)^3 \sum_{s \in \{-1,0,1\}} \underbrace{\Gamma(4) \frac{1}{\Gamma(4)} \int_{x=0}^{\infty} dx \frac{x^{4-1}}{z_s^{-1} e^x - 1}}_{g_4(z_s)} \\ \Gamma(4) = (4-1)! = 6 \rightarrow &= \left(\frac{2\pi}{\omega\hbar\beta}\right)^3 \sum_{s \in \{-1,0,1\}} g_4(z_s) \\ z_s = z e^{\beta\mu_m B s} \rightarrow &= \left(\frac{2\pi}{\omega\hbar\beta}\right)^3 \sum_{s \in \{-1,0,1\}} g_4(z \exp(\beta\mu_m B s)) \end{aligned}$$

Finally, the partition function for this system is going to be

$$\log Z = -\log(1 - z e^{\beta\mu_m B}) + \left(\frac{2\pi}{\omega\hbar\beta}\right)^3 \sum_{s \in \{-1,0,1\}} g_4(z \exp(\beta\mu_m B s)) \checkmark$$

The mean value of the number of particles is, for the grand canonical ensemble,

$$\begin{aligned} \langle N \rangle &= z \frac{\partial}{\partial z} \log Z_{CG} \\ &= z \frac{\partial}{\partial z} \left[\left(\frac{2\pi}{\omega\hbar\beta}\right)^3 \sum_{s \in \{-1,0,1\}} g_4(z \exp(\beta\mu_m B s)) - \log(1 - z e^{\beta\mu_m B}) \right] \\ \frac{\partial g_\nu}{\partial z} = \frac{g_{\nu-1}}{z} \rightarrow &= z \left[\left(\frac{2\pi}{\omega\hbar\beta}\right)^3 \sum_{s \in \{-1,0,1\}} \frac{g_3(z e^{\beta\mu_m B s}) e^{\beta\mu_m B s}}{z e^{\beta\mu_m B s}} + \frac{e^{\beta\mu_m B}}{1 - z e^{\beta\mu_m B}} \right] \\ &= \left(\frac{2\pi}{\omega\hbar\beta}\right)^3 \sum_{s \in \{-1,0,1\}} g_3(z e^{\beta\mu_m B s}) + \frac{1}{z^{-1} e^{-\beta\mu_m B} - 1} \end{aligned}$$

or equivalently

$$\langle N \rangle = \left(\frac{k_B T}{\omega\hbar}\right)^3 \sum_{s \in \{-1,0,1\}} g_3(z e^{\beta\mu_m B s}) + \frac{1}{z^{-1} e^{-\beta\mu_m B} - 1} \checkmark$$

Item b

The critical temperature T_C is that temperature for which the number of particles in the fundamental level begins to increase². This is

$$\frac{\langle N_0 \rangle}{\langle N \rangle} = \begin{cases} \rightarrow 0 & T \geq T_C \\ > 0 & T < T_C \end{cases}$$

which means that above the critical temperature the fraction of particles that is at the fundamental level N_0 is vanishingly small, while below the critical temperature this fraction begins to be important.

²We are talking about a Bose-Einstein condensate. For other systems such as boiling water this is not the case for the critical temperature.

It can be shown³ that

$$\langle N \rangle = \sum_{\forall \text{monoparticular state}} \langle N_i \rangle \quad \text{with } \langle N_i \rangle = z \frac{\partial}{\partial z} \log Z_i$$

(where i stands for each monoparticular state) so

$$\langle N \rangle = \langle N_0 \rangle + \sum_{\text{all other states}} \langle N_i \rangle$$

and it must be true that

$$\langle N \rangle \Big|_{T \geq T_C} \approx \sum_{\text{all other states}} \langle N_i \rangle$$

Also, when the system is at the critical temperature, the fugacity z reaches its maximum⁴ value which is given by

$$z_{\max} = e^{-\beta_C \mu_m B} = e^{-\beta_C \epsilon_{\text{fundamental state}}}$$

This value is related with the fact that the partition function, which is $\log Z = \sum_{\forall \text{monoparticular state}} \log(1 - ze^{-\beta \epsilon_i})$, cannot diverge, so $z < e^{-\beta \epsilon_i} \forall i$, and this implies the value for z_{\max} .

Then, at the critical temperature, we have the conditions

$$T = T_C \quad \Rightarrow \quad \langle N \rangle \approx \sum_{\text{all states but } N_0} \langle N_i \rangle \quad \text{and } z = e^{-\beta_C \mu_m B}$$

so using the expression for $\langle N \rangle$ from the previous item

$$\begin{aligned} \langle N \rangle &= \left(\frac{k_B T_C}{\omega \hbar} \right)^3 \sum_{s \in \{-1, 0, 1\}} g_3(z_{\max} e^{\beta_C \mu_m B s}) + \frac{1}{\underbrace{z^{-1} e^{-\beta_C \mu_m B} - 1}_{\langle N_0 \rangle}} \\ &= \left(\frac{k_B T_C}{\omega \hbar} \right)^3 \sum_{s \in \{-1, 0, 1\}} g_3(e^{\beta_C \mu_m B (s-1)}) \\ &= \left(\frac{k_B T_C}{\omega \hbar} \right)^3 [g_3(e^{-2\beta_C \mu_m B}) + g_3(e^{-\beta_C \mu_m B}) + g_3(1)] \quad \checkmark \end{aligned}$$

When $B \rightarrow 0$ this becomes

$$\langle N \rangle \Big|_{B \rightarrow 0} = \left(\frac{k_B T_C}{\omega \hbar} \right)^3 3g_3(1)$$

so

$$T_C \xrightarrow{B \rightarrow 0} \frac{\omega \hbar}{k_B} \left(\frac{N}{3g_3(1)} \right)^{1/3} \quad \checkmark$$

and for $B \rightarrow \infty$

$$\langle N \rangle \Big|_{B \rightarrow \infty} = \left(\frac{k_B T_C}{\omega \hbar} \right)^3 [2g_3(0) + g_3(1)]$$

so

$$T_C \xrightarrow{B \rightarrow \infty} \frac{\omega \hbar}{k_B} \left(\frac{N}{g_3(1)} \right)^{1/3} \quad \checkmark$$

³ $\langle N \rangle = z \frac{\partial}{\partial z} \log Z_{CG} = z \frac{\partial}{\partial z} \left[\sum_{\forall \text{monoparticular state}} \log Z_i \right] = \sum_{\forall \text{monoparticular state}} z \frac{\partial}{\partial z} \log Z_i$ and $z \frac{\partial}{\partial z} \log Z_i = z \frac{\partial}{\partial z} \sum_{n=0}^{\infty} e^{-\beta(\epsilon_i - \mu)n} = z \frac{\partial}{\partial z} \sum_{n=0}^{\infty} z^n e^{-\beta \epsilon_i n} = z \sum_{n=0}^{\infty} n z^{n-1} e^{-\beta \epsilon_i n} = \sum_{n=0}^{\infty} n z^n e^{-\beta \epsilon_i n} = \sum_{n=0}^{\infty} n e^{-\beta(\epsilon_i - \mu)n} = \sum_{n=0}^{\infty} n \mathbb{P}(N_i = n)$ so $\langle N \rangle = \sum_{\forall \text{monoparticular state}} \langle N_i \rangle$ with $\langle N_i \rangle = z \frac{\partial}{\partial z} \log Z_i \checkmark$.

⁴The fugacity is of the form $z = \begin{cases} z(T) & T > T_C \\ z_{\max} & T \leq T_C \end{cases}$.

Item c

The magnetization of the system is

$$\begin{aligned}
 M &= \frac{1}{N\beta} \frac{\partial}{\partial B} \log Z_{GC} \\
 &= \frac{1}{N\beta} \frac{\partial}{\partial B} \left[-\log(1 - ze^{\beta\mu_m B}) + \left(\frac{2\pi}{\omega\hbar\beta}\right)^3 \sum_{s \in \{-1,0,1\}} g_4(z \exp(\beta\mu_m Bs)) \right] \\
 &= \frac{1}{N} \left[-\frac{ze^{\beta\mu_m B} \mu_m}{1 - ze^{\beta\mu_m B}} + \left(\frac{2\pi}{\omega\hbar\beta}\right)^3 \sum_{s \in \{-1,0,1\}} \frac{g_3(ze^{\beta\mu_m Bs})}{ze^{\beta\mu_m Bs}} ze^{\beta\mu_m Bs} \mu_m s \right] \\
 &= \frac{\mu_m}{N} \left[\frac{1}{z^{-1}e^{-\beta\mu_m B} - 1} + \left(\frac{2\pi}{\omega\hbar\beta}\right)^3 \sum_{s \in \{-1,0,1\}} g_3(ze^{\beta\mu_m Bs}) s \right] \\
 &= \frac{\mu_m}{N} \left[\frac{1}{z^{-1}e^{-\beta\mu_m B} - 1} + \left(\frac{2\pi}{\omega\hbar\beta}\right)^3 (g_3(ze^{\beta\mu_m B}) - g_3(ze^{-\beta\mu_m B})) \right]
 \end{aligned}$$

Here we recognize the term $N_0 = \frac{1}{z^{-1}e^{-\beta\mu_m B} - 1}$ (see previous item) so

$$M = \mu_m \left[\frac{N_0}{N} + \frac{1}{N} \left(\frac{2\pi}{\omega\hbar\beta}\right)^3 (g_3(ze^{\beta\mu_m B}) - g_3(ze^{-\beta\mu_m B})) \right] \checkmark$$

If the system were at $T \geq T_C$ then $\frac{N_0}{N}$ would be very small, but we are asked for $T < T_C$ so it cannot be canceled \odot . Because $T < T_C$ then the fugacity is $z = z_{\max} = e^{-\beta\mu_m B}$ (see previous item) so

$$M = \mu_m \left[\frac{N_0}{N} + \frac{1}{N} \left(\frac{k_B T}{\omega\hbar}\right)^3 (g_3(1) - g_3(e^{-2\beta\mu_m B})) \right]$$

For the term $\frac{N_0}{N}$ we can calculate it as follows: we know that

$$N = \left(\frac{k_B T}{\omega\hbar}\right)^3 \sum_{s \in \{-1,0,1\}} g_3(ze^{\beta\mu_m Bs}) + \underbrace{\frac{1}{z^{-1}e^{-\beta\mu_m B} - 1}}_{N_0}$$

so

$$1 = \frac{N_0}{N} + \frac{1}{N} \left(\frac{k_B T}{\omega\hbar}\right)^3 \sum_{s \in \{-1,0,1\}} g_3(ze^{\beta\mu_m Bs})$$

and then

$$\frac{N_0}{N} = 1 - \frac{1}{N} \left(\frac{k_B T}{\omega\hbar}\right)^3 \sum_{s \in \{-1,0,1\}} g_3(ze^{\beta\mu_m Bs})$$

For $T < T_C$ the fugacity is $z = z_{\max} = e^{-\beta\mu_m B}$ so

$$\begin{aligned}
 \frac{N_0}{N} &= 1 - \frac{1}{N} \left(\frac{k_B T}{\omega\hbar}\right)^3 \sum_{s \in \{-1,0,1\}} g_3(e^{\beta\mu_m B(s-1)}) \\
 &= 1 - \frac{1}{N} \left(\frac{k_B T}{\omega\hbar}\right)^3 [g_3(e^{-2\beta\mu_m B}) + g_3(e^{-\beta\mu_m B}) + g_3(1)] \checkmark
 \end{aligned}$$

Replacing $\frac{N_0}{N}$ into the expression for M we get

$$\begin{aligned}
 M &= \mu_m \left[1 - \frac{1}{N} \left(\frac{k_B T}{\omega\hbar}\right)^3 [g_3(e^{-2\beta\mu_m B}) + g_3(e^{-\beta\mu_m B}) + g_3(1)] + \frac{1}{N} \left(\frac{k_B T}{\omega\hbar}\right)^3 (g_3(1) - g_3(e^{-2\beta\mu_m B})) \right] \\
 &= \mu_m \left[1 - \frac{1}{N} \left(\frac{k_B T_C}{\omega\hbar}\right)^3 (-2g_3(e^{-2\beta\mu_m B}) - g_3(e^{-\beta\mu_m B})) \right] \checkmark
 \end{aligned}$$

Problem 2

Item a (ask for $\nabla^2\Psi$)

If Ψ is an extreme of F then δF must vanish for $\delta\Psi$. δF is

$$\begin{aligned}\delta F &= \delta \left(\int d^3r \left[\frac{\hbar^2}{2m} |\vec{\nabla}\Psi|^2 + \frac{a(T-T_C)}{2} |\Psi|^2 + \frac{b}{4} |\Psi|^4 \right] \right) \\ &= \int d^3r \left[\frac{\hbar^2}{2m} \delta |\vec{\nabla}\Psi|^2 + \frac{a(T-T_C)}{2} \delta |\Psi|^2 + \frac{b}{4} \delta |\Psi|^4 \right]\end{aligned}$$

Now we use

$$\begin{cases} \delta |\vec{\nabla}\Psi|^2 = \vec{\nabla}\Psi^* \cdot \vec{\nabla}\delta\Psi + \vec{\nabla}\Psi \cdot \vec{\nabla}\delta\Psi^* \\ \delta |\Psi|^2 = \Psi^* \delta\Psi + \Psi \delta\Psi^* \\ \delta |\Psi|^4 = 2 |\Psi|^2 \delta |\Psi|^2 \end{cases}$$

so

$$\begin{aligned}\delta F &= \int d^3r \left[\frac{\hbar^2}{2m} (\vec{\nabla}\Psi^* \cdot \vec{\nabla}\delta\Psi + \vec{\nabla}\Psi \cdot \vec{\nabla}\delta\Psi^*) + \frac{a(T-T_C)}{2} (\Psi^* \delta\Psi + \Psi \delta\Psi^*) + \dots \right. \\ &\quad \left. \dots + \frac{b}{2} |\Psi|^2 (\Psi^* \delta\Psi + \Psi \delta\Psi^*) \right] \\ \vec{\nabla}\Psi^* \cdot \vec{\nabla}\delta\Psi \stackrel{?}{=} -\nabla^2\Psi^* \delta\Psi \rightarrow &= \int d^3r \left[-\frac{\hbar^2}{2m} \nabla^2\Psi^* + \frac{a(T-T_C)}{2} \Psi^* + \frac{b}{2} |\Psi|^2 \Psi^* \right] \delta\Psi + \dots \\ &\quad \dots + \left[-\frac{\hbar^2}{2m} \nabla^2\Psi + \frac{a(T-T_C)}{2} \Psi + \frac{b}{2} |\Psi|^2 \Psi \right] \delta\Psi^* \\ z + z^* = 2\text{Re}(z) \rightarrow &= \int d^3r \text{Re} \left(\left[-\frac{\hbar^2}{m} \nabla^2\Psi + a(T-T_C) \Psi + b |\Psi|^2 \Psi \right] \delta\Psi^* \right) \\ &= \text{Re} \left(\int d^3r \left[-\frac{\hbar^2}{m} \nabla^2\Psi + a(T-T_C) \Psi + b |\Psi|^2 \Psi \right] \delta\Psi^* \right)\end{aligned}$$

Now $\delta F = 0$ implies $[\dots] = 0$ so the differential equation for Ψ is

$$-\frac{\hbar^2}{m} \nabla^2\Psi + a(T-T_C) \Psi + b |\Psi|^2 \Psi = 0 \quad \checkmark$$

Item b (why?)

We know that $\int d^3r |\Psi|^2 = N_0$ where N_0 is the number of particles in the superfluid phase (this is because we are said to consider Ψ in this way). So $|\Psi| = \sqrt{n_0}$ with $n_0 = \frac{N_0}{V}$ is the density of particles in the superfluid phase. If the density is going to be uniform then n_0 is independent of \mathbf{r} .

I don't know exactly why but (why??)

$$\Psi = \sqrt{n_0} e^{i\mathbf{k}\cdot\mathbf{r}}$$

where $\mathbf{k} = \frac{m\mathbf{v}}{\hbar}$ because $\mathbf{p} = \hbar\mathbf{k} = m\mathbf{v}$. Then, introducing this into the equation for Ψ we obtain

$$\begin{aligned}\frac{\hbar^2}{m} \left(\frac{m\mathbf{v}}{\hbar} \right)^2 \sqrt{n_0} + a(T-T_C) \sqrt{n_0} + b n_0^{3/2} &= 0 \\ \sqrt{n_0} (m\mathbf{v}^2 + a(T-T_C) + b n_0) &= 0\end{aligned}$$

Because we are looking for nontrivial solutions with $n_0 \neq 0$ then

$$n_0 = \frac{a(T_C - T) - m\mathbf{v}^2}{b} \quad \checkmark$$

so the solution is

$$\Psi = \sqrt{\frac{a(T_C - T) - m\mathbf{v}^2}{b}} \exp\left(i \frac{m}{\hbar} \mathbf{v} \cdot \mathbf{r}\right) \quad \checkmark$$

The value of n_0 must be greater than zero so

$$\frac{a(T_C - T) - m\mathbf{v}^2}{b} > 0 \quad \Rightarrow \quad \mathbf{v}^2 < \frac{a(T_C - T)}{m} \quad \checkmark$$

Item c

We know the Helmholtz free energy $F(\Psi, T)$ because we know Ψ so the specific heat can be obtained as

$$\begin{aligned}
 C &= T \frac{\partial S}{\partial T} \\
 S = -\frac{\partial F}{\partial T} &\rightarrow = -T \frac{\partial^2 F}{\partial T^2} \\
 F = F(\Psi, T) \text{ from consigna} &\rightarrow = -T \frac{\partial^2}{\partial T^2} \int d^3r \left[\frac{\hbar^2}{2m} |\vec{\nabla}\Psi|^2 + \frac{a(T - T_C)}{2} |\Psi|^2 + \frac{b}{4} |\Psi|^4 \right] \\
 \Psi = \sqrt{n_0(T)} \exp\left(i\frac{m}{\hbar}\mathbf{v} \cdot \mathbf{r}\right) &\rightarrow = -T \frac{\partial^2}{\partial T^2} \underbrace{\int d^3r}_V \left[\frac{m\mathbf{v}^2}{2} n_0(T) + \frac{a(T - T_C)}{2} n_0(T) + \frac{b}{4} n_0^2(T) \right] \\
 n_0 = \frac{a(T_C - T) - m\mathbf{v}^2}{b} &\rightarrow = -TV \frac{\partial^2}{\partial T^2} \left[\frac{b}{2} n_0(T) \left(\overbrace{\frac{a(T - T_C) + m\mathbf{v}^2}{b}}^{-n_0} + \frac{1}{2} n_0(T) \right) \right] \\
 &= TV \frac{\partial^2}{\partial T^2} \left[\frac{b}{4} n_0^2(T) \right] \\
 n_0 = \frac{a(T_C - T) - m\mathbf{v}^2}{b} &\rightarrow = \frac{TV}{4b} \frac{\partial^2}{\partial T^2} [a(T - T_C) - m\mathbf{v}^2]^2 \\
 &= TV \frac{a^2}{2b} \checkmark
 \end{aligned}$$

Problem 3

Item a

The equation is a typical wave equation and the solution we are asked for is basically its Fourier transform along the space coordinate x . What can be done is introduce the solution into the equation and see what happens. Lets do it! Each derivative is

$$\begin{cases} \frac{\partial P}{\partial t} = \int_{\mathbb{R}} dk \frac{\partial P_k}{\partial t} e^{ikx} \\ \frac{\partial^2 P}{\partial x^2} = - \int_{\mathbb{R}} dk k^2 P_k e^{ikx} \end{cases}$$

so

$$\int_{\mathbb{R}} dk \frac{\partial P_k}{\partial t} e^{ikx} = -\frac{g}{2\gamma^2} \int_{\mathbb{R}} dk k^2 P_k e^{ikx}$$

or

$$\int_{\mathbb{R}} dk \left(\frac{\partial P_k}{\partial t} + \frac{g}{2\gamma^2} k^2 P_k \right) e^{ikx} = 0$$

which implies that⁵ $(\dots) = 0$ so

$$\frac{\partial P_k}{\partial t} = -\frac{gk^2}{2\gamma^2} P_k$$

and the solution is

$$P_k(t) = A_k \exp\left(-\frac{gk^2}{2\gamma^2} t\right) \checkmark$$

So in general the solution is given by

$$P(x, t) = \int_{\mathbb{R}} dk A_k \exp\left(-\frac{gk^2}{2\gamma^2} t + ikx\right)$$

⁵I don't know why it does not imply that $(\dots) = e^{ikx\alpha}$ with $\alpha \neq 1$, which is in fact the orthogonality of the Fourier basis if I do remember well...

Item b

If at $t = 0$ the particle is at $x = 0$ this means that

$$P(x, t = 0) = \delta_D(x)$$

If we consider that the coefficients A_k are independent of k and the change of variable given by $\alpha = \frac{g}{2\gamma^2}t$, then the general solution from the previous item becomes

$$P(x, t) = A \int_{\mathbb{R}} dk e^{-\alpha k^2 + ikx}$$

Help from consigna \rightarrow $= A \sqrt{\frac{\pi}{\alpha}} e^{-\frac{x^2}{4\alpha}}$

The next step is considering the fact that⁶

$$\int_{\mathbb{R}} \sqrt{\frac{\pi}{\alpha}} e^{-\frac{x^2}{4\alpha}} dx = 2\pi$$

so

$$\lim_{\alpha \rightarrow 0} \sqrt{\frac{\pi}{\alpha}} e^{-\frac{x^2}{4\alpha}} = 2\pi \delta_D(x)$$

with implies that

$$\begin{aligned} \lim_{t \rightarrow 0} P(x, t) &= \lim_{\alpha \rightarrow 0} A \sqrt{\frac{\pi}{\alpha}} e^{-\frac{x^2}{4\alpha}} \\ &= 2\pi A \delta_D(x) \end{aligned}$$

so if we want $P(x, t = 0) = \delta_D(x)$ we need that $A = \frac{1}{2\pi}$ so the solution for this particular case is

$$P(x, t) = \sqrt{\frac{\gamma^2}{2\pi gt}} \exp\left(-\frac{x^2 \gamma^2}{2gt}\right) \checkmark$$

Item c (me dio distinto el resultado)

The mean value for x , intuitively, has to be zero. Lets check our intuition, come on!

$$\begin{aligned} \langle x \rangle (t) &\stackrel{\text{def}}{=} \int_{\mathbb{R}} x P(x, t) dx \\ &= \sqrt{\frac{\gamma^2}{2\pi gt}} \underbrace{\int_{\mathbb{R}} x \exp\left(-\frac{x^2 \gamma^2}{2gt}\right) dx}_0 \\ &= 0 \checkmark \end{aligned}$$

which is zero because it is the integral over \mathbb{R} of an odd function x times an even function e^{-x} , which results in an odd function.

The other quantity, $\langle x^2 \rangle$, coincides with the standard deviation σ_x^2 because $\sigma_x^2 \stackrel{\text{def}}{=} \langle x^2 \rangle - \langle x \rangle^2$. My intuition says that it must be linear with t . The math is

$$\begin{aligned} \langle x^2 \rangle (t) &\stackrel{\text{def}}{=} \int_{\mathbb{R}} x^2 P(x, t) dx \\ &= \sqrt{\frac{\gamma^2}{2\pi gt}} \underbrace{\int_{\mathbb{R}} x^2 \exp\left(-\frac{x^2 \gamma^2}{2gt}\right) dx}_{\sqrt{\frac{8\pi g^3 t^3}{\gamma^6}}} \\ &= \frac{2g}{\gamma^2} t \end{aligned}$$

⁶See https://en.wikipedia.org/wiki/Dirac_delta_function and plug this in Wolfram Alpha: `integral -infty ^+infty (pi/a)^0.5*e^(-x^2/(4a)) dx`

Yeah! It is linear in t as my intuition said ☺. (A Guillem le dio sin el 2)

The Shannon entropy is

$$\begin{aligned}
 S(t) &\stackrel{\text{def}}{=} - \int_{\mathbb{R}} dx P(x, t) \log P(x, t) \\
 &= - \int_{\mathbb{R}} dx \sqrt{\frac{\gamma^2}{2\pi gt}} \exp\left(-\frac{x^2 \gamma^2}{2gt}\right) \log\left(\sqrt{\frac{\gamma^2}{2\pi gt}} \exp\left(-\frac{x^2 \gamma^2}{2gt}\right)\right) \\
 \Psi &\stackrel{\text{def}}{=} \frac{\gamma^2}{2gt} \rightarrow = -\sqrt{\frac{\Psi}{\pi}} \int_{\mathbb{R}} dx e^{-x^2 \Psi} \log\left(\sqrt{\frac{\Psi}{\pi}} e^{-x^2 \Psi}\right) \\
 \mathcal{P} &\stackrel{\text{def}}{=} \log \sqrt{\frac{\Psi}{\pi}} \rightarrow = -\sqrt{\frac{\Psi}{\pi}} \int_{\mathbb{R}} dx e^{-x^2 \Psi} [\mathcal{P} - x^2 \Psi] \\
 &= -\sqrt{\frac{\Psi}{\pi}} \left[\mathcal{P} \int_{\mathbb{R}} dx e^{-x^2 \Psi} - \Psi \int_{\mathbb{R}} dx x^2 e^{-x^2 \Psi} \right] \\
 &= -\sqrt{\frac{\Psi}{\pi}} \left[\mathcal{P} \sqrt{\frac{\pi}{\Psi}} - \Psi \sqrt{\frac{\pi}{\Psi^3}} \right] \\
 &= -\mathcal{P} - \sqrt{\frac{\pi}{\Psi}} \\
 &= \log \sqrt{\frac{2\pi gt}{\gamma^2}} - \sqrt{\frac{2\pi gt}{\gamma^2}}
 \end{aligned}$$

This result is not in coincidence with the result obtained by the professor, which is $S(t) = \log \sqrt{\frac{2\pi gt}{\gamma^2}} - \frac{1}{2}$. I cannot find where I have mistaken.

We observe that $S(t)$ is increasing with time, which is consistent with the fact that the more time it passes the less we know about the position of the particle. This also indicates that the particle reaches an equilibrium⁷ (?).

⁷This is what the professor said... I don't know about which equilibrium are we talking about because at any instant the situation of the particle is the same: it is in a random place moving in a random way.

2. 29/06/2016

Consigna

Problema 1

Un gas de N fermiones libres e idénticos, de masa m y espín s , está contenido en una caja de volumen V . Una mitad de la caja está a potencial 0 y la otra a potencial Δ , con $0 < \Delta \ll \frac{\hbar^2}{2m} \left(\frac{N}{V}\right)^{2/3}$. El gas se encuentra en equilibrio a temperatura T .

- Calcule la energía de Fermi ϵ_F del sistema. (*Ayuda:* podría serle útil saber que $\Gamma(5/2) = \frac{3\sqrt{\pi}}{4}$).
- Encuentre la fracción de partículas en cada mitad de la caja en los casos $T \gg \frac{\epsilon_F}{k_B}$ y $T = 0$. Discuta sus resultados.
- Calcule la energía del sistema en los dos casos del ítem anterior.

Problema 2

Considere un sistema de partículas idénticas de espín 0 que no interactúan entre sí. Las partículas se mueven en un espacio de d dimensiones y están atrapadas en una trampa armónica de frecuencia angular ω , de manera que las energías monoparticulares son

$$\epsilon = \hbar\omega (n_1 + \dots + n_d)$$

donde n_1, \dots, n_d son números naturales y el origen de las energías se ha elegido convenientemente.

- Calcule la función de partición gran canónica del sistema, suponiendo que $\beta\hbar\omega \ll 1$. (*Ayuda:* puede serle útil saber que $\frac{(m+k)!}{m!} \approx m^k$ cuando $m \gg k$ o bien, según cómo afronte el problema, que el área de una esfera de radio 1 en un espacio de $2d$ dimensiones es $\frac{2\pi^d}{\Gamma(d)}$).
- ¿Qué condición debe satisfacer d para que haya condensación de Bose-Einstein?. Asumiendo que se satisface esa condición, calcule la temperatura crítica del sistema, T_C , en función del número de partículas (que como siempre asumimos arbitrariamente grande).
- Calcule y grafique la fracción de partículas en el estado fundamental, f , en función de la temperatura T y en términos de T_C .
- Calcule y grafique el calor específico, c_V , del sistema en función de T y en términos de T_C , en los casos $T \leq T_C$ y $T \gg T_C$. Discuta sus resultados.

Problema 3

Considere el modelo de Potts en una dimensión, cuyo hamiltoniano es

$$\mathcal{H}(s_1, \dots, s_N) = -J \sum_{i=1}^N \delta_{s_i s_{i+1}}$$

donde J es una constante positiva, δ_{kl} es la delta de Kronecker y, para cada $i = 1, \dots, N$, s_i puede tomar $q \geq 2$ valores distintos.

- Obtenga las ecuaciones del grupo de renormalización correspondientes a decimar el sistema sumando sobre todos los sitios pares. (*Ayuda:* tenga en cuenta que $e^{\alpha\delta_{kl}} = 1 + \delta_{kl}(e^\alpha - 1)$).
- Definiendo $x = e^{-K}$, donde $K = \beta J$, escriba la ecuación $x' = R(x)$ que describe cómo cambia x bajo el grupo de renormalización. Encuentre los puntos fijos y estudie su estabilidad. Discuta sus resultados.

Resolución

Problem 1

Item a (preguntar varias cosas)

According to what we were told in class, the Fermi energy can be defined as

$$\epsilon_F(V, N) \stackrel{\text{def}}{=} \lim_{T \rightarrow 0} \mu(T, V, N)$$

where μ is the chemical potential. Then, if we find $\mu(T, V, N)$ we should know ϵ_F . The way to do this is obtaining $N(T, V, \mu)$, I don't know if there is any better way. I will go that way.

The Hamiltonian for each of the particles of this gas is

$$\mathcal{H} = \frac{p^2}{2m} + a\Delta$$

where $a \in \{0, 1\}$ indicates the position of the particle inside the box.

Because particles do not interact with each other then the partition function is

$$Z_{GC} = \prod_{\forall \text{monoparticular states } i} Z_{\text{monoparticular } i}$$

with

$$Z_{\text{monoparticular } i} = \sum_{\forall \text{ allowed } n} e^{-\beta(\epsilon_i - \mu)n}$$

As the consigna says we are dealing with fermions. Thus the allowed values of n for each monoparticular state are $n \in \{0, 1\}$ so

$$\begin{aligned} Z_{\text{monoparticular } i} &= \sum_{n \in \{0, 1\}} e^{-\beta(\epsilon_i - \mu)n} \\ &= 1 + ze^{-\beta\epsilon_i} \end{aligned}$$

The partition function then is

$$Z_{GC} = \prod_{\forall i} 1 + ze^{-\beta\epsilon_i}$$

so its logarithm becomes

$$\log Z_{GC} = \sum_{\forall i} \log(1 + ze^{-\beta\epsilon_i})$$

The states i of each particle are all the values of position \mathbf{q} , momentum \mathbf{p} and potential a in which the particle can be, plus the degeneration $g(\mathbf{q}, \mathbf{p}, a)$ of each state⁸. Thus

$$\log Z_{GC} = \sum_{\forall \mathbf{q}, \mathbf{p}, a} \sum_{\forall g(\mathbf{q}, \mathbf{p}, a)} \log(1 + ze^{-\beta\mathcal{H}(\mathbf{q}, \mathbf{p}, a)})$$

In this case we assume only degeneration due to spin so $g(\mathbf{q}, \mathbf{p}, a) = g$ is constant and

$$\begin{aligned} \log Z_{GC} &= g \sum_{\forall \mathbf{q}, \mathbf{p}, a} \log(1 + ze^{-\beta\mathcal{H}(\mathbf{q}, \mathbf{p}, a)}) \\ \mathbf{q}, \mathbf{p}, s \text{ are independent} &\rightarrow = g \sum_{\forall \mathbf{q}} \sum_{\forall \mathbf{p}} \sum_{\forall s} \log(1 + ze^{-\beta\mathcal{H}(\mathbf{q}, \mathbf{p}, s)}) \\ \stackrel{\text{}}{\approx} &\rightarrow \approx g \int_{\mathbf{q} \in V} \int_{\mathbf{p} \in \mathbb{R}^3} \sum_{s \in \{0, 1\}} \frac{d^3r d^3p}{h^3} \log(1 + ze^{-\beta\mathcal{H}(\mathbf{q}, \mathbf{p}, s)}) \\ &= g \int_{\mathbf{q} \in V} \int_{\mathbf{p} \in \mathbb{R}^3} \sum_{s \in \{0, 1\}} \frac{d^3r d^3p}{h^3} \log\left(1 + ze^{-\beta\left(\frac{p^2}{2m} + s\Delta\right)}\right) \\ &= g \frac{V}{h^3} \int_{\mathbf{p} \in \mathbb{R}^3} d^3p \left[\log\left(1 + ze^{-\beta\frac{p^2}{2m}}\right) + \log\left(1 + ze^{-\beta\left(\frac{p^2}{2m} + \Delta\right)}\right) \right] \end{aligned}$$

⁸In principle nothing forbids for each state to have a different degree of degeneration, although we always consider, for simplicity, constant degeneration.

In the step marked with the symbol \simeq , if the particles were bosons we should have take into account the fact that they can be all in one state, thus making some of the terms in the previous summations very important as to approximate with an integral. **Because we are dealing with fermions, we can approximate with no much care (?)**.

The first of the integrals is

$$\int d^3p \log \left(1 + ze^{-\beta \frac{p^2}{2m}} \right) = \frac{2\pi^{\frac{3}{2}}}{\Gamma\left(\frac{3}{2}\right)} \int_0^\infty dr r^2 \log \left(1 + ze^{-\beta \frac{r^2}{2m}} \right) \leftarrow d^d p = \frac{2\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}\right)} r^{d-1} dr$$

$$x \stackrel{\text{def}}{=} \beta \frac{r^2}{2m} \Rightarrow \begin{cases} dx = \frac{\beta}{m} r dr \\ r = \sqrt{\frac{2mx}{\beta}} \end{cases} \rightarrow = 4\pi \int_0^\infty \overbrace{\frac{dr}{\beta} r}^{\frac{dx}{m}} \overbrace{\sqrt{\frac{2mx}{\beta}}}^r \log(1 + ze^{-x})$$

$$= 4\pi\sqrt{2} \left(\frac{m}{\beta}\right)^{3/2} \int_0^\infty dx \sqrt{x} \log(1 + ze^{-x})$$

Parts $\int uv' = uv - \int u'v \rightarrow$

$$= 4\pi\sqrt{2} \left(\frac{m}{\beta}\right)^{3/2} \left[\frac{x^{3/2}}{3/2} \log(1 + ze^{-x}) \right]_0^\infty - \int_0^\infty dx \frac{x^{3/2}}{3/2} \frac{-ze^{-x}}{1 + ze^{-x}}$$

$$= 4\pi\sqrt{2} \frac{2}{3} \left(\frac{m}{\beta}\right)^{3/2} \underbrace{\int_0^\infty dx \frac{x^{\frac{5}{2}-1}}{z^{-1}e^x + 1}}_{f_{5/2}(z)}$$

$$= \frac{8\sqrt{2}}{3} \pi \left(\frac{m}{\beta}\right)^{3/2} f_{5/2}(z)$$

and the second, considering the change of variable $\alpha = ze^{-\beta\Delta}$, is exactly the same. So the partition function is

$$\log Z_{GC} = g \frac{V}{h^3} \frac{8\sqrt{2}}{3} \pi \left(\frac{m}{\beta}\right)^{3/2} [f_{5/2}(z) + f_{5/2}(ze^{-\beta\Delta})] \rightarrow \text{Is this wrong?}$$

Here I find a difference between this result and the one I think it should be, which is

$$\log Z_{GC} = g \frac{V}{2\lambda^3} [f_{5/2}(z) + f_{5/2}(ze^{-\beta\Delta})]$$

with $\lambda = \sqrt{\frac{2\pi\hbar^2}{mk_B T}}$ being the thermal wavelength. In my result there is a difference for a constant factor involving π and $\sqrt{2}$. From now on I will consider that $\log Z_{GC}$ is as the second expression.

The number of particles in the system must satisfy

$$N(T, V, z(T, \mu)) = z \frac{\partial}{\partial z} \log Z_{GC}$$

$$= \frac{gV}{2\lambda^3} [f_{3/2}(z) + f_{3/2}(ze^{-\beta\Delta})] \checkmark$$

Now we take the low temperature limit in which $z = e^{\beta\mu} \gg 1$ so we can apply Sommerfeld's approximation (see *Resumen de fórmulas y cosas* in page 54. **What I don't know is why we use it at order zero, i.e. $(\log z)^0$, but this is what the professor did so I will to.** This is

$$\text{Sommerfeld} \rightarrow \begin{cases} f_{3/2}(z) \approx \frac{(\log z)^{3/2}}{\Gamma(5/2)} = \frac{(\beta\mu)^{3/2}}{\Gamma(5/2)} \\ f_{3/2}(ze^{-\beta\Delta}) \approx \frac{(\log z - \beta\Delta)^{3/2}}{\Gamma(5/2)} = \frac{(\beta\mu - \beta\Delta)^{3/2}}{\Gamma(5/2)} \end{cases}$$

so

$$N \approx \frac{gV}{2\Gamma(5/2)} \left(\frac{m}{2\pi\hbar^2\beta}\right)^{3/2} [(\beta\mu)^{3/2} + (\beta\mu - \beta\Delta)^{3/2}] \rightarrow \text{For } T \rightarrow 0$$

Now we use the definition of the Fermi energy, $\epsilon_F \stackrel{\text{def}}{=} \mu(T \rightarrow 0)$, so

$$N = \frac{gV}{2\Gamma(5/2)} \left(\frac{m}{2\pi\hbar^2}\right)^{3/2} [\epsilon_F^{3/2} + (\epsilon_F - \Delta)^{3/2}] \checkmark$$

The next is to solve for ϵ_F . This seems to be impossible, but we can make an approximation as follows: first we solve for $[\dots] = \dots$ in the next way

$$\epsilon_F^{3/2} + (\epsilon_F - \Delta)^{3/2} = \frac{2N\Gamma(5/2)}{gV} \left(\frac{2\pi\hbar^2}{m} \right)^{3/2}$$

so, if $\Delta = 0$ then

$$\epsilon_F|_{\Delta=0} \stackrel{\text{def}}{=} \epsilon_{F0} = \left(\frac{N\Gamma(5/2)}{gV} \right)^{2/3} \frac{2\pi\hbar^2}{m} \checkmark$$

and we can write

$$\epsilon_F^{3/2} + (\epsilon_F - \Delta)^{3/2} = 2\epsilon_{F0}^{3/2}$$

Now we consider the data from the *consigna* that says that $0 < \Delta \ll \frac{\hbar^2}{2m} \left(\frac{N}{V} \right)^{2/3}$ which implies

$$0 < \Delta \ll \frac{\hbar^2}{2m} \left(\frac{N}{V} \right)^{2/3} \sim \frac{\hbar^2}{2m} \left(\frac{N}{V} \right)^{2/3} 4\pi \left(\frac{\Gamma(5/2)}{g} \right)^{2/3} = \epsilon_{F0} \odot$$

so at the end we are told that $0 < \Delta \ll \epsilon_{F0}$. I don't understand what the professor did next, he made some magical approximations and finally got

$$\epsilon_F = \epsilon_{F0} + \frac{\Delta}{2}$$

but if $\Delta \ll \epsilon_{F0}$ this is like saying $\epsilon_F = \epsilon_{F0} \dots$ Isn't?

Item b

We know that

$$\begin{aligned} N &= \sum_{\text{monoparticular states}} N_i \\ &= N_0 + N_\Delta \end{aligned}$$

where N_0 contains all the monoparticular states that are in the half side with zero potential energy and N_Δ those at the Δ side. We know from the previous item that $N = \frac{gV}{2\lambda^3} [f_{3/2}(z) + f_{3/2}(ze^{-\beta\Delta})]$ so

$$\begin{cases} N_0 = \frac{gV}{2\lambda^3} f_{3/2}(z) \\ N_\Delta = \frac{gV}{2\lambda^3} f_{3/2}(ze^{-\beta\Delta}) \end{cases}$$

High temperatures In the case of high temperatures we got $z \gg 1$ so we can approximate

$$\begin{cases} f_{3/2}(z) \approx z \\ f_{3/2}(ze^{-\beta\Delta}) = f_{3/2}(e^{\beta(\mu-\Delta)}) \approx ze^{-\beta\Delta} \end{cases}$$

where I have assumed $\mu > \Delta$. Then

$$\text{High temperature} \rightarrow \begin{cases} N_0 = \frac{gV}{2\lambda^3} z \\ N_\Delta = \frac{gV}{2\lambda^3} ze^{-\beta\Delta} \\ N = \frac{gV}{2\lambda^3} z (1 + e^{-\beta\Delta}) \end{cases}$$

so

$$\frac{N_0}{N} = \frac{1}{1 + e^{-\beta\Delta}} \checkmark \qquad \frac{N_\Delta}{N} = \frac{1}{e^{\beta\Delta} + 1} \checkmark$$

If $T \rightarrow \infty$ then $\beta \rightarrow 0$ and $\frac{N_0}{N}, \frac{N_\Delta}{N} \rightarrow \frac{1}{2}$ which means that the particles begin to distribute uniformly and independently of the difference of potential of each side of the box. This makes sense \odot .

Low temperatures For low temperatures Sommerfeld's approximation must be used. In this case (see *item a*)

$$\text{Low temperature} \rightarrow \begin{cases} N_0 = \frac{gV}{2\Gamma(5/2)\lambda^3} \beta^{3/2} \epsilon_F^{3/2} \\ N_\Delta = \frac{gV}{2\Gamma(5/2)\lambda^3} \beta^{3/2} (\epsilon_F - \Delta)^{3/2} \\ N = \frac{gV}{2\Gamma(5/2)\lambda^3} \beta^{3/2} [\epsilon_F^{3/2} + (\epsilon_F - \Delta)^{3/2}] \end{cases}$$

and the fractions are

$$\frac{N_0}{N} = \frac{\epsilon_F^{3/2}}{\epsilon_F^{3/2} + (\epsilon_F - \Delta)^{3/2}} \quad \frac{N_\Delta}{N} = \frac{(\epsilon_F - \Delta)^{3/2}}{\epsilon_F^{3/2} + (\epsilon_F - \Delta)^{3/2}}$$

We observe the fact that $\frac{N_0}{N} \neq 0$ and $\frac{N_\Delta}{N} \neq 0$. If Boltzmann's statistics (i.e. classical mechanics) were valid, then we would get that $\frac{N_\Delta}{N} = 0$ for low temperatures because all particles would prefer to be in the N_0 side. The exclusion principle forbids this and $\frac{N_\Delta}{N} \neq 0$ even for low temperatures \checkmark .

Item c

The energy for the grand canonical ensemble is to be calculated as

$$U = - \left. \frac{\partial}{\partial \beta} \right|_{z,N} \ln Z_{GC}$$

It seems that, as happened with N , it is valid that

$$\begin{aligned} U &= \sum_{\forall \text{monoparticle state}} U_i \\ &= U_0 + U_\Delta \end{aligned}$$

with

$$U_i = - \left. \frac{\partial}{\partial \beta} \right|_{z,N} \ln Z_i$$

so the task should not be very complicated.

From item a we have $\log Z_{GC} = g \frac{V}{2\lambda^3} [f_{5/2}(z) + f_{5/2}(ze^{-\beta\Delta})]$ so (replacing $\lambda = \sqrt{\frac{2\pi\hbar^2\beta}{m}}$)

$$\begin{cases} \log Z_0 = \frac{gV}{2} \left(\frac{m}{2\pi\hbar^2\beta} \right)^{3/2} f_{5/2}(z) \\ \log Z_\Delta = \frac{gV}{2} \left(\frac{m}{2\pi\hbar^2\beta} \right)^{3/2} f_{5/2}(ze^{-\beta\Delta}) \end{cases}$$

Then

$$\begin{aligned} U_0 &= - \left. \frac{\partial}{\partial \beta} \right|_{z,N} \log Z_0 \\ &= \frac{3gV}{4} \left(\frac{m}{2\pi\hbar^2} \right)^{3/2} f_{5/2}(z) \beta^{-5/2} \checkmark \end{aligned}$$

and

$$\begin{aligned} U_\Delta &= - \left. \frac{\partial}{\partial \beta} \right|_{z,N} \log Z_\Delta \\ &= - \frac{gV}{2} \left(\frac{m}{2\pi\hbar^2} \right)^{3/2} \left. \frac{\partial}{\partial \beta} \right|_{z,N} \left[\beta^{-3/2} f_{5/2}(ze^{-\beta\Delta}) \right] \\ &= - \frac{gV}{2} \left(\frac{m}{2\pi\hbar^2} \right)^{3/2} \left[-\frac{3}{2} \beta^{-5/2} f_{5/2}(ze^{-\beta\Delta}) + \beta^{-3/2} \frac{f_{3/2}(ze^{-\beta\Delta})}{ze^{-\beta\Delta}} ze^{-\beta\Delta} (-\Delta) \right] \\ &= \frac{3}{2} \frac{gV}{2\lambda^3 \beta} f_{5/2}(ze^{-\beta\Delta}) + \underbrace{\frac{gV}{2\lambda^3} f_{3/2}(ze^{-\beta\Delta}) \Delta}_{N_\Delta} \\ &= \frac{3}{2} \frac{gV}{2\lambda^3 \beta} f_{5/2}(ze^{-\beta\Delta}) + \Delta N_\Delta \checkmark \end{aligned}$$

The energies are

$$\begin{cases} U_0 = \frac{3}{2} \frac{gV}{2\lambda^3\beta} f_{5/2}(z) \checkmark \\ U_\Delta = \frac{3}{2} \frac{gV}{2\lambda^3\beta} f_{5/2}(ze^{-\beta\Delta}) + \Delta N_\Delta \checkmark \end{cases}$$

so

$$\begin{aligned} U &= U_0 + U_\Delta \\ &= \frac{3}{2} \frac{gV}{2\lambda^3\beta} [f_{5/2}(z) + f_{5/2}(ze^{-\beta\Delta})] + \Delta N_\Delta \end{aligned}$$

High temperatures In this case $f_\nu \approx z$ and we can apply the results from item b that $N = \frac{gV}{2\lambda^3} z (1 + e^{-\beta\Delta})$ and $N_\Delta = \frac{N}{e^{\beta\Delta} + 1}$ to get

$$U = \frac{3}{2} k_B T N + N \frac{\Delta}{e^{\beta\Delta} + 1}$$

If $T \rightarrow \infty$ then we recover the ideal classical gas.

Low temperatures For low temperatures Sommerfeld comes to the rescue. The energies are going to be

$$\begin{cases} U_0 = \frac{3}{2} \frac{gV}{2\lambda^3\beta} \frac{(\log z)^{5/2}}{\Gamma(7/2)} = \frac{3}{2} \frac{gV}{2\lambda^3\beta} \frac{\beta^{5/2}}{\Gamma(7/2)} \epsilon_F^{5/2} \\ U_\Delta = \frac{3}{2} \frac{gV}{2\lambda^3\beta} \frac{(\log(ze^{-\beta\Delta}))^{5/2}}{\Gamma(7/2)} + \Delta N_\Delta = \frac{3}{2} \frac{gV}{2\lambda^3\beta} \frac{\beta^{5/2}}{\Gamma(7/2)} (\epsilon_F - \Delta)^{5/2} + \Delta N_\Delta \end{cases}$$

The total energy is thus

$$\begin{aligned} U &= U_0 + U_\Delta \\ &= \frac{3}{2} \frac{gV}{2\lambda^3\beta} \frac{\beta^{5/2}}{\Gamma(7/2)} [\epsilon_F^{5/2} + (\epsilon_F - \Delta)^{5/2}] + N_\Delta \frac{(\epsilon_F - \Delta)^{3/2}}{\epsilon_F^{3/2} + (\epsilon_F - \Delta)^{3/2}} \end{aligned}$$

where I have used $N_\Delta = N \frac{(\epsilon_F - \Delta)^{3/2}}{\epsilon_F^{3/2} + (\epsilon_F - \Delta)^{3/2}}$ from item b.

Problem 2

Item a

Because the particles do not interact and are identical, then we can apply the *theorem of indistinguishable and non interacting particles* (see page 55). Thus the partition function is

$$Z_{GC} = \prod_{\forall \text{monoparticular state}} Z_i \quad \text{with } Z_i = \sum_{\forall \text{allowed } n} e^{-\beta(\epsilon_i - \mu)n}$$

We are told that the particles have spin 0 so they must be bosons. This implies that the allowed values of n for each energy is from 0 to ∞ . Then

$$\begin{aligned} Z_i &= \sum_{n=0}^{\infty} (ze^{-\beta\epsilon_i})^n \\ \text{Geometric series } \rightarrow &= \frac{1}{1 - ze^{-\beta\epsilon_i}} \end{aligned}$$

Thus

$$\log Z_{GC} = - \sum_{\forall \text{monoparticular state}} \log(1 - ze^{-\beta\epsilon_i})$$

The monoparticular states are given by the fact that each particle is a harmonic oscillator of d dimensions. Then it has d independent quantum numbers as the *consigna* says. Then we have

$$\begin{aligned} \log Z_{GC} &= - \sum_{\forall \{n_1, \dots, n_d\}} \log(1 - ze^{-\beta\epsilon(n_1, \dots, n_d)}) \\ &= - \sum_{\forall n_1} \dots \sum_{\forall n_d} \log(1 - ze^{-\beta\epsilon(n_1, \dots, n_d)}) \end{aligned}$$

This separation from one summation over all allowed combinations of $\{n_1, \dots, n_d\}$ into many individual summations for each n_i can be done because there is no restriction connecting one n_i with any other, i.e. they are all independent from one another.

Replacing the energy $\epsilon = \hbar\omega (n_1 + \dots + n_d)$ we get

$$\begin{aligned} \log Z_{GC} &= - \sum_{\forall n_1} \dots \sum_{\forall n_d} \log \left(1 - ze^{-\beta\epsilon(n_1+\dots+n_d)} \right) \\ n \stackrel{\text{def}}{=} n_1 + \dots + n_d \rightarrow &= - \sum_{n=0}^{\infty} g(n, d) \log \left(1 - ze^{-\beta\hbar\omega n} \right) \end{aligned}$$

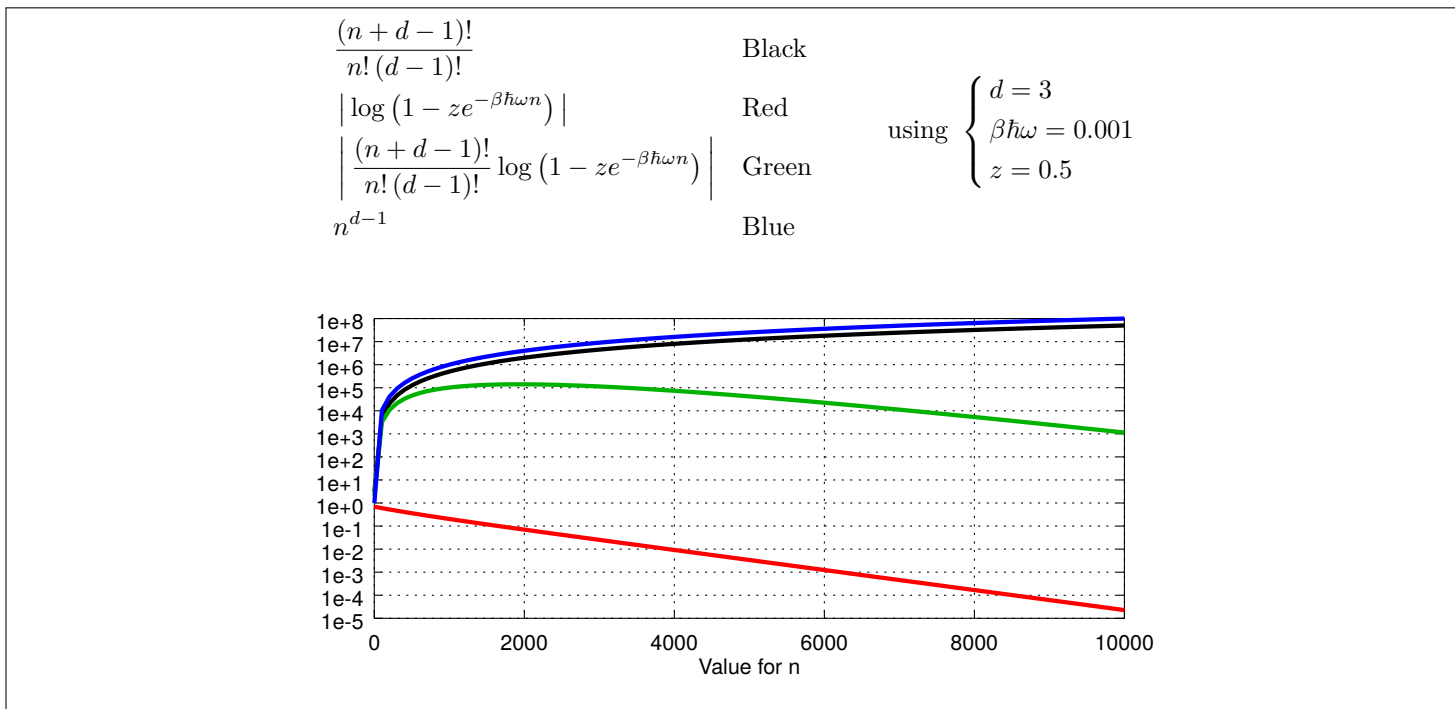
being $g(n, d)$ the degeneration for each value of n . This is the hard part in which we have to count. $g(n, d)$ can be thought off as being the number of ways that n indistinguishable books can be stored into d indistinguishable boxes. Then

$$g(n, d) = \binom{n+d-1}{n}$$

so

$$\begin{aligned} \log Z_{GC} &= - \sum_{n=0}^{\infty} \binom{n+d-1}{n} \log \left(1 - ze^{-\beta\hbar\omega n} \right) \\ &= - \sum_{n=0}^{\infty} \frac{(n+d-1)!}{n!(d-1)!} \log \left(1 - ze^{-\beta\hbar\omega n} \right) \end{aligned}$$

Now we can consider the help from the *consigna* because the term $\frac{(n+d-1)!}{n!(d-1)!}$ grows with n very much faster than the logarithm decreases as the next plot shows



So it is evident (after doing the plot) that the sum is dominated by the terms with n big so we can approximate as

$$\log Z_{GC} \approx \frac{-1}{(d-1)!} \sum_{n=0}^{\infty} n^{d-1} \log \left(1 - ze^{-\beta\hbar\omega n} \right)$$

As $\beta\hbar\omega \rightarrow 0$ the summation converges more slowly and we are told that $\beta\hbar\omega \ll 1$ so we can approximate the summation

with an integral

$$\begin{aligned}
 \log Z_{GC} &\approx \frac{-1}{(d-1)!} \int_0^\infty dn n^{d-1} \log(1 - ze^{-\beta\hbar\omega n}) \\
 \text{Parts} \rightarrow &= \frac{-1}{(d-1)!} \left[\frac{n^d}{d} \log(1 - ze^{-\beta\hbar\omega n}) \right]_0^\infty - \int_0^\infty dn \frac{n^d}{d} \frac{-ze^{-\beta\hbar\omega n} (-\beta\hbar\omega)}{1 - ze^{-\beta\hbar\omega n}} \\
 &= \frac{1}{d!} \int_0^\infty dn \frac{\beta\hbar\omega n^d}{z^{-1}e^{\beta\hbar\omega n} - 1} \\
 x \stackrel{\text{def}}{=} \beta\hbar\omega n \rightarrow &= \frac{1}{(\beta\hbar\omega)^d} \underbrace{\frac{1}{d!} \int_0^\infty dx \frac{x^d}{z^{-1}e^x - 1}}_{g_{d+1}(z)} \leftarrow d! = \Gamma(d+1) \\
 &= \frac{g_{d+1}(z)}{(\beta\hbar\omega)^d} \checkmark
 \end{aligned}$$

Item b

Let me call N_0 the number of particles in the fundamental state and N_ϵ the number of particles in levels that are not the fundamental. Then

$$N = N_0 + N_\epsilon$$

If the system is going to have a BEC state then⁹

$$\boxed{\text{BEC}} \iff N_0 = \begin{cases} 0 & T \geq T_C \\ N_0(T) & T < T_C \end{cases} \leftarrow \text{This is the BEC state} \iff N_\epsilon = \begin{cases} 1 & T \geq T_C \\ 1 - N_0(T) & T < T_C \end{cases}$$

with

$$N_0(T) = \begin{cases} 0 & T \rightarrow T_C \\ N & T \rightarrow 0 \end{cases} \quad \text{and} \quad z = \begin{cases} z(T) & T > T_C \\ z_{\max} = \exp\left(\frac{\epsilon_{\text{fundamental}}}{k_B T_C}\right) & T \leq T_C \end{cases}$$

For this system in particular it is $z_{\max} = 1$ because $\epsilon_{\text{fundamental}} = 0$.

If we consider to be in the limit $T \rightarrow T_C^+$ then we must have

$$T \rightarrow T_C^+ \Rightarrow \begin{cases} N_0 = 0 \\ N_\epsilon = N \\ z = z_{\max} \end{cases}$$

with

$$\begin{aligned}
 N_\epsilon = N &= z \frac{\partial}{\partial z} \log Z \\
 &= \frac{g_d(z)}{(\beta\hbar\omega)^d} \checkmark
 \end{aligned}$$

This must not be infinite, otherwise the entire universe will be *chupated* by our system. Thus

$$d > 1 \checkmark$$

is the condition for $g_d(z=1) < \infty$.

For the critical temperature we know that, again for the case $T \rightarrow T_C^+$, we have the conditions previously listed. Thus

$$N(T = T_C, z = 1) = g_d(1) \left(\frac{k_B T_C}{\hbar\omega}\right)^d$$

so, using $g_d(1) = \zeta(d)$ (for $d > 1$) the critical temperature is

$$T_C = \left(\frac{N}{\zeta(d)}\right)^{\frac{1}{d}} \frac{\hbar\omega}{k_B} \checkmark$$

⁹This conditions are imposed by hand. If you do the math $N_0 = z \frac{\partial}{\partial z} \log Z_0 = \dots = \frac{z}{1-z}$ then clearly $N_0 \rightarrow \infty$ as $z \rightarrow z_{\max} = 1$ which is not one of this conditions. I call this a magical step.

Item c

According to my professor¹⁰ the number of particles of the system is

$$N(T, z) = \begin{cases} N_\epsilon(T, z) & T \geq T_C \\ N_0(T, z_{\max}) + N_\epsilon(T, z_{\max}) & T < T_C \end{cases} \quad N_\epsilon(T, z) = z \frac{\partial}{\partial z} \log Z_\epsilon \leftarrow \forall T, \forall z \quad (1)$$

with, for this system in particular, $N_\epsilon = \frac{g_d(z)}{(\beta\hbar\omega)^d}$ as obtained in a previous item.

For $T \geq T_C$ we have, by “definition of N_0 ”, that $\left. \frac{N_0}{N} \right|_{T \geq T_C} = 0$.

For the other situation, $T < T_C$, we have that $N = N_0 + N_\epsilon$ so

$$\begin{aligned} \left. \frac{N_0}{N} \right|_{T < T_C} &= 1 - \frac{N_\epsilon(T, z_{\max})}{N} \\ &= 1 - \frac{g_d(z_{\max})}{N(\beta\hbar\omega)^d} \end{aligned}$$

If N is to be constant then we can find it evaluating $N(T_C, z_{\max}) = N_\epsilon(T_C, z_{\max}) = \left(\frac{k_B T_C}{\hbar\omega}\right)^d g_d(z_{\max})$ so

$$\left. \frac{N_0}{N} \right|_{T < T_C} = 1 - \left(\frac{T}{T_C}\right)^d \quad \checkmark$$

Finally we can write

$$\frac{N_0}{N} = \begin{cases} 0 & T \geq T_C \\ \left[1 - \left(\frac{T}{T_C}\right)^d\right] & T < T_C \end{cases}$$

Item d

The energy is

$$\begin{aligned} U &= - \left. \frac{\partial}{\partial \beta} \right|_{V, z} \log Z_{GC} \\ &= - \left. \frac{\partial}{\partial \beta} \right|_{V, z} \left[\frac{g_{d+1}(z)}{(\beta\hbar\omega)^d} \right] \\ &= d\hbar\omega \frac{g_{d+1}(z)}{(\beta\hbar\omega)^{d+1}} \quad \checkmark \end{aligned}$$

so the specific heat is

$$\begin{aligned} C_V &= \left. \frac{\partial U}{\partial T} \right|_{V, N} \\ &= \left. \frac{\partial}{\partial T} \right|_{V, N} \left[d \frac{(k_B T)^{d+1}}{(\hbar\omega)^d} g_{d+1}(z) \right] \end{aligned}$$

Because we don't know how to calculate $\left. \frac{\partial}{\partial T} \right|_{V, N} g_{d+1}(z)$ is that we take the limits of temperature at this stage. Thus

$$C_V = \left. \frac{\partial}{\partial T} \right|_{V, N} \begin{cases} d \frac{(k_B T)^{d+1}}{(\hbar\omega)^d} z & T \gg T_C \\ d \frac{(k_B T)^{d+1}}{(\hbar\omega)^d} \zeta(d+1) & T < T_C \end{cases}$$

Now we need some expression for z that allows us to calculate $\left. \frac{\partial z}{\partial T} \right|_{V, N}$ for the case $T \gg T_C$. Luckily we have expression (1) from where we can obtain $z = z(T, V, N)$ for $T \gg T_C$. This is

$$\begin{aligned} N &= \frac{g_d(z)}{(\beta\hbar\omega)^d} \leftarrow T \geq T_C \\ T \gg T_C \Rightarrow g_d(z) \ll 1 &\iff z \ll 1 \Rightarrow g_d(z) \approx z \rightarrow \approx \frac{z}{(\beta\hbar\omega)^d} \end{aligned}$$

¹⁰He is a high crak, 3 consult classes. He deserves a monument.

or

$$z = N (\beta \hbar \omega)^d \leftarrow T \gg T_C$$

so, introducing this into the expression for C_V ,

$$\begin{aligned} C_V &= \left. \frac{\partial}{\partial T} \right|_{V,N} \begin{cases} d \frac{(k_B T)^{d+1}}{(\hbar \omega)^d} N \left(\frac{\hbar \omega}{k_B T} \right)^d & T \gg T_C \\ d \frac{(k_B T)^{d+1}}{(\hbar \omega)^d} \zeta(d+1) & T < T_C \end{cases} \\ &= \begin{cases} d N k_B & T \gg T_C \\ d(d+1) k_B \frac{\zeta(d+1)}{(\beta \hbar \omega)^d} & T < T_C \end{cases} \\ &= \begin{cases} d N k_B & T \gg T_C \\ d(d+1) k_B \frac{\zeta(d)}{(\beta \hbar \omega)^d} \frac{\zeta(d+1)}{\zeta(d)} & T < T_C \end{cases} \\ N_\epsilon = \frac{g d (z_{\max})}{(\beta \hbar \omega)^d} \text{ for } T < T_C \rightarrow &= \begin{cases} d N k_B & T \gg T_C \\ d(d+1) k_B N_\epsilon \frac{\zeta(d+1)}{\zeta(d)} & T < T_C \end{cases} \\ N_\epsilon = \left(\frac{T}{T_C} \right)^d \text{ for } T < T_C \rightarrow &= \begin{cases} d N k_B & T \gg T_C \\ d(d+1) k_B \frac{\zeta(d+1)}{\zeta(d)} \left(\frac{T}{T_C} \right)^d & T < T_C \quad \checkmark \end{cases} \end{aligned}$$

In particular, for $T \gg T_C$, the fact that $c_V = d k_B$ is the result we obtain from classical equipartition theorem.

Problem 3

Item a (impossible)

The Hamiltonian for the system is

$$\begin{aligned} \mathcal{H}_{\text{completo y posta}} &= -J \sum_{i=1}^N \delta_{s_i s_{i+1}} \\ k \stackrel{\text{def}}{=} \frac{i}{2} \rightarrow &= -J \sum_{k=1}^{N/2} (\delta_{s_{2k-1} s_{2k}} + \delta_{s_{2k} s_{2k+1}}) \quad \checkmark \end{aligned}$$

$$\begin{aligned} \mathbb{P}(s_{1:N}) &= \frac{1}{Q} \exp \left(\sum_{i=1}^N K \delta_{s_i s_{i+1}} \right) \\ &= \frac{1}{Q} \prod_{i=1}^N e^{K \delta_{s_i s_{i+1}}} \end{aligned}$$

$$\mathcal{H}_{\text{sólo pares}} = -J' \sum_{k=1}^{N/2} \delta_{s_k s_{k+1}}$$

$$\begin{array}{cccccccccccc} i= & \underline{1} & \underline{2} & \underline{3} & \underline{4} & \underline{5} & \underline{6} & \underline{7} & \underline{8} & \dots & \underline{N} \\ & \color{red}{\dot{1}} & \color{red}{\dot{2}} & \color{red}{\dot{3}} & \color{red}{\dot{2}} & \color{red}{\dot{3}} & \color{red}{\dot{4}} & \color{red}{\dot{3}} & \color{red}{\dot{4}} & \dots & \color{red}{\dot{N/2}} \end{array}$$

$$\begin{aligned} \mathbb{P}(s_1, s_3, \dots) &= \frac{1}{Q} \sum_{\{s_{\text{pares}}\}} \exp \left(K \sum_{k=1}^{N/2} (\delta_{s_{2k-1} s_{2k}} + \delta_{s_{2k} s_{2k+1}}) \right) \\ a = s_{\text{pares}} \rightarrow &= \frac{1}{Q} \prod_{k=1}^{N/2} \sum_{\forall a} \exp \left(K \sum_{k=1}^{N/2} (\delta_{s_{2k-1} a} + \delta_{a s_{2k+1}}) \right) \end{aligned}$$

Yo quiero que

$$\mathcal{H}_{\text{completo y posta}} = \mathcal{H}_{\text{sólo pares}}$$

The change of index $2k = i$ is nothing more than the decimation we are looking for. It consist in taking the summation over the even indexes as the next illustration tries to illustrate:

$$\begin{array}{ccccccccccc} i= & \underline{1} & \underline{2} & \underline{3} & \underline{4} & \underline{5} & \underline{6} & \underline{7} & \underline{8} & \dots & \underline{N} \\ & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ k= & \underline{1} & \underline{2} & & \underline{2} & & \underline{3} & & \underline{4} & & \underline{N/2} \end{array}$$

The (canonical) partition function will thus be

$$\begin{aligned} Z &= \sum_{\forall \text{states}} e^{-\beta \epsilon_i} \\ &= \sum_{\forall \{s_1, \dots, s_N\}} e^{-\beta \epsilon(s_1, \dots, s_N)} \\ &= \sum_{\forall s_1} \sum_{\forall s_2} \dots \sum_{\forall s_N} e^{-\beta \epsilon(s_1, \dots, s_N)} \end{aligned}$$

where the last equality holds because all the s_i can take values independently of the states of the others. The following calculation is magical for me, I don't understand what we are doing but it is like this:

$$\begin{aligned} Z &= \overbrace{\sum \dots \sum}_{\forall \{s_1, s_3, \dots\}} \overbrace{\sum \dots \sum}_{\forall \{s_2, s_4, \dots\}} \exp(-\beta \epsilon(s_1, s_2, \dots, s_N)) \\ K \stackrel{\text{def}}{=} \beta J \rightarrow &= \sum_{\forall \{s_1, s_3, \dots\}} \sum_{\forall \{s_2, s_4, \dots\}} \exp \left(K \sum_{k=1}^{N/2} (\delta_{s_{2k-1} s_{2k}} + \delta_{s_{2k} s_{2k+1}}) \right) \\ &= \sum_{\forall \{s_1, s_3, \dots\}} \sum_{\forall \{s_2, s_4, \dots\}} \prod_{k=1}^{N/2} \exp(K (\delta_{s_{2k-1} s_{2k}} + \delta_{s_{2k} s_{2k+1}})) \\ &\stackrel{?}{=} \sum_{\forall \{s_1, s_3, \dots\}} \prod_{k=1}^{N/2} \sum_{\forall s} \exp(K (\delta_{s_{2k-1} s} + \delta_{s s_{2k+1}})) \\ &= \sum_{\forall \{s_1, s_3, \dots\}} \prod_{k=1}^{N/2} \sum_{\forall s} e^{K \delta_{s_{2k-1} s}} e^{K \delta_{s s_{2k+1}}} \\ \text{Help from consigna} \rightarrow &= \sum_{\forall \{s_1, s_3, \dots\}} \prod_{k=1}^{N/2} \sum_{\forall s} [1 + \delta_{s_{2k-1} s} (e^K - 1)] [1 + \delta_{s s_{2k+1}} (e^K - 1)] \\ &= \sum_{\forall \{s_1, s_3, \dots\}} \prod_{k=1}^{N/2} \sum_{\forall s} [1 + \delta_{s_{2k-1} s} (e^K - 1) + \delta_{s s_{2k+1}} (e^K - 1) + \delta_{s_{2k-1} s} \delta_{s s_{2k+1}} (e^K - 1)^2] \\ &= \sum_{\forall \{s_1, s_3, \dots\}} \prod_{k=1}^{N/2} [q + 2 (e^K - 1) + \delta_{s_{2k-1} s_{2k+1}} (e^K - 1)^2] \\ &\stackrel{?}{=} \sum_{\forall \{s_1, s_3, \dots\}} \exp \left(\sum_{k=1}^{N/2} (K'_0 + K' \delta_{s_{2k-1} s_{2k+1}}) \right) \\ \left\{ \begin{array}{l} s_{2k-1} = s'_k \\ s_{2k+1} = s'_{k+1} \end{array} \right. \rightarrow &= \sum_{\forall \{s'_k\}} \exp \left(\sum_{k=1}^{N/2} (K'_0 + K' \delta_{s'_k s'_{k+1}}) \right) \end{aligned}$$

3. 01/07/2015

Consigna

Problema 1

Considere un gas de electrones confinado a moverse en un plano de área A . Se aplica un campo magnético de módulo B en la dirección normal al plano. Sabemos que, clásicamente, las trayectorias de los electrones son círculos, por lo que cada una de las dos coordenadas cartesianas en el plano se comporta como un oscilador armónico. Como resultado, e ignorando la interacción entre el espín de los electrones y el campo magnético, se obtiene que los niveles de energía de una partícula son

$$\epsilon = 2\mu_B B \left(n + \frac{1}{2} \right) \quad n = 0, 1, \dots$$

donde $\mu_B = \frac{\hbar|q_e|}{2mc}$ es el magnetón de Bohr. Cada nivel de energía tiene una degeneración $g = \frac{2A|q_e|B}{hc}$.

- (a) A partir de la fórmula general para la función de partición gran canónica de un sistema de fermiones idénticos que no interactúan entre sí, pruebe que en este caso

$$\log Z(T, A, B, z) = 2A \frac{|q_e|B}{hc} \sum_{n=0}^{\infty} \log \left(1 + z \exp \left(-\beta 2\mu_B B \left(n + \frac{1}{2} \right) \right) \right)$$

donde z es la fugacidad y $\beta = \frac{1}{k_B T}$.

- (b) Calcule el número de partículas en función de T, A, B y z .
- (c) Aproxime los resultados de los dos ítems anteriores al orden más bajo en el límite de baja fugacidad ($z \ll 1$).
- (d) A partir de los resultados del ítem anterior calcule la magnetización

$$M = \frac{k_B T}{A} \left. \frac{\partial}{\partial B} \right|_{T, A, z} \log Z$$

en función de T, A, B y N al orden más bajo en el límite $z \ll 1$ y $\beta\mu_B B \ll 1$. Luego calcule la susceptibilidad magnética. El resultado ¿corresponde a un sistema para, ferro o diamagnético? *Ayuda:* $\frac{1}{\sinh x} \approx \frac{1}{x} - \frac{x}{6}$ para $x \ll 1$.

Problema 2

Ignorando los problemas asociados al estado fundamental, la función de partición gran canónica de un gas ideal de bosones de masa m y espín 0 está dada por la ecuación

$$\log Z(T, V, z) = \frac{V}{\lambda^3} g_{5/2}(z)$$

donde $\lambda = \frac{h}{\sqrt{2\pi m k_B T}}$ es la longitud de onda térmica y $g_\nu(z) = \frac{1}{\Gamma(\nu)} \int_0^\infty \frac{x^{\nu-1}}{z^{-1}e^x - 1}$ es una integral de Bose.

- (a) A partir de la ecuación anterior, obtenga la presión p y el número de partículas N como funciones de T, V y z .
- (b) Identifique el valor crítico x_c del parámetro $\frac{V}{N\lambda^3}$ por debajo del cual el número de partículas en el estado fundamental se vuelve macroscópico.
- (c) Obtenga la presión como función de T, V y N en los casos $\frac{V}{N\lambda^3} \gg x_c$ y $\frac{V}{N\lambda^3} < x_c$.
- (d) Calcule el valor al que tiende $\left. \frac{\partial p}{\partial V} \right|_{T, N}$ en el límite $\frac{V}{N\lambda^3} \rightarrow x_c^+$ (*ayuda:* recuerde que $g_{1/2}(z)$ diverge en el límite $z \rightarrow 1^-$).
- (e) A partir de los resultados obtenidos en los dos ítems anteriores, grafique p como función de V para T y N constantes. Interprete el gráfico.

Problema 3

Considere el modelo de Ising con hamiltoniano

$$\mathcal{H}(s_1, \dots, s_N) = -J \sum_{\langle ij \rangle} s_i s_j - \mu B \sum_{i=1}^N s_i$$

para una red bidimensional triangular (ver figura). Dividamos la red en celdas de tres espines como la que se muestra en la figura 2. Describiendo la interacción de cada celda con su entorno mediante la aproximación de campo medio, y tratando exactamente la interacción entre los espines de la celda, pruebe que la temperatura crítica del sistema T_C satisface la ecuación

$$x = \frac{1}{2} \frac{e^x + 3e^{-x}}{3e^x + e^{-x}} \quad x = \frac{2J}{k_B T_C}$$

Resolviendo esta ecuación numéricamente se obtiene $T_C \approx 5,64 \frac{J}{k_B}$. Este resultado ¿es mayor o menor que el que se obtiene mediante la aproximación de campo medio usual?



Resolución

Problem 1

Item a

Assuming the electrons don't interact with one another then

$$Z_{GC} = \prod_{\forall \text{monoparticular states}} Z_{\text{monoparticular } i} \quad \text{con } Z_{\text{monoparticular } i} = \sum_{\forall \text{ allowed } n} e^{-\beta(\epsilon_i - \mu)n}$$

Because the particles are electrons, they are fermions, so the allowed values for n are 0 and 1 so

$$\begin{aligned} Z_{\text{monoparticular } i} &= 1 + e^{-\beta(\epsilon_i - \mu)} \\ &= 1 + ze^{-\beta\epsilon_i} \end{aligned}$$

so the partition function becomes

$$\begin{aligned} \log Z_{GC} &= \sum_{\forall \text{monoparticular states}} \log(1 + ze^{-\beta\epsilon_i}) \\ &= \sum_{i=0}^{\infty} g(i) \log(1 + ze^{-\beta\epsilon_i}) \\ \epsilon_i = 2\mu_B B \left(i + \frac{1}{2}\right) \rightarrow &= \sum_{i=0}^{\infty} g(i) \log\left(1 + ze^{-2\beta\mu_B B(i + \frac{1}{2})}\right) \end{aligned}$$

where $g(i)$ is the degeneration for the level with energy ϵ_i . According to the *consigna* this degeneration is constant $g(i) = \frac{2A|q_e|B}{hc}$. Then

$$\log Z_{GC} = \frac{2A|q_e|B}{hc} \sum_{i=0}^{\infty} \log\left(1 + ze^{-2\beta\mu_B B(i + \frac{1}{2})}\right) \checkmark$$

Item b

The number of particles is going to be

$$\begin{aligned} N &= z \frac{\partial}{\partial z} \log Z_{GC} \\ &= \frac{2A|q_e|B}{hc} z \sum_{i=0}^{\infty} \frac{e^{-2\beta\mu_B B(i + \frac{1}{2})}}{1 + ze^{-2\beta\mu_B B(i + \frac{1}{2})}} \\ &= \frac{2A|q_e|B}{hc} \sum_{i=0}^{\infty} \frac{1}{z^{-1}e^{2\beta\mu_B B(i + \frac{1}{2})} + 1} \checkmark \end{aligned}$$

Item c

For $z \ll 1$ we have

$$\log(1 + ze^{-|\text{something}|}) \approx ze^{-|\text{something}|}$$

independently of the value of $|\text{something}|$. Then the partition function

$$\begin{aligned} \log Z_{GC} &\approx \frac{2A|q_e|B}{hc} ze^{-\beta\mu_B B} \sum_{i=0}^{\infty} (e^{-2\beta\mu_B B})^i \\ \text{Geometric series } \rightarrow &= \frac{2A|q_e|B}{hc} ze^{-\beta\mu_B B} \frac{1}{1 - e^{-2\beta\mu_B B}} \\ &= \frac{A|q_e|B}{hc} z \frac{2}{e^{\beta\mu_B B} - e^{-\beta\mu_B B}} \\ &= \frac{A|q_e|B}{hc} \frac{z}{\sinh(\beta\mu_B B)} \checkmark \end{aligned}$$

For the number of particles this is

$$\begin{aligned} N &= z \frac{\partial}{\partial z} \log Z_{GC} \\ z \ll 1 \rightarrow &\approx z \frac{\partial}{\partial z} \left[\frac{A |q_e| B}{hc} \frac{z}{\sinh(\beta \mu_B B)} \right] \\ &= \frac{A |q_e| B}{hc} \frac{z}{\sinh(\beta \mu_B B)} \checkmark \end{aligned}$$

Item d

The magnetization is going to be

$$\begin{aligned} M &= \frac{k_B T}{A} \left. \frac{\partial}{\partial B} \right|_{T,A,z} \left[\frac{A |q_e| B}{hc} \frac{z}{\sinh(\beta \mu_B B)} \right] \leftarrow z \ll 1 \\ &= \frac{1}{\beta A} \left[\frac{A |q_e|}{hc} \frac{z}{\sinh(\beta \mu_B B)} + \frac{A |q_e| B}{hc} \frac{z(-1)}{\sinh^2(\beta \mu_B B)} \cosh(\beta \mu_B B) \beta \mu_B \right] \\ &= \frac{1}{\beta A} \left[\frac{A |q_e|}{hc} \frac{z}{\sinh(\beta \mu_B B)} - \frac{A |q_e|}{hc} \frac{z}{\sinh(\beta \mu_B B)} \beta \mu_B B \frac{\cosh(\beta \mu_B B)}{\sinh(\beta \mu_B B)} \right] \\ &= \frac{|q_e|}{\beta hc} \frac{z}{\sinh(\beta \mu_B B)} [1 - \beta \mu_B B \coth(\beta \mu_B B)] \\ \beta \mu_B B \ll 1 \Rightarrow \begin{cases} \sinh x \approx x \\ \coth x \approx \frac{1}{x} + \frac{x}{3} \end{cases} \rightarrow &\approx \frac{|q_e|}{\beta hc} \frac{z}{\beta \mu_B B} \left[-\frac{(\beta \mu_B B)^2}{3} \right] \\ &= -\frac{|q_e| z \mu_B B}{3hc} \checkmark \end{aligned}$$

Next we replace $z = z(N)$ so as to obtain $M = M(T, A, B, N)$. This can be done easily for $\beta \mu_B B \ll 1$ considering the formula of the previous item $N = \frac{A |q_e| B}{hc} \frac{z}{\sinh(\beta \mu_B B)} \approx \frac{A |q_e| B}{hc} \frac{z}{\beta \mu_B B}$ so

$$z = \frac{N hc \beta \mu_B}{A |q_e|}$$

and finally

$$M = -N \frac{\beta \mu_B^2}{3A} B \checkmark$$

The susceptibility is

$$\begin{aligned} \chi &= \frac{\partial M}{\partial B} \\ &= -N \frac{\beta \mu_B^2}{3A} \end{aligned}$$

Because $\chi < 0$ the magnetic field of the material opposes to the external magnetic field. This is a characteristic of diamagnetic materials \checkmark .

Problem 2

Item a

The pressure can be found according to

$$P = - \left. \frac{\partial \Xi}{\partial V} \right|_{T,\mu}$$

where Ξ is the grand canonical potential which in turn can be found as

$$\begin{aligned} \Xi &= -k_B T \log(Z_{GC}) \\ &= -\frac{V}{\beta \lambda^3} g_{5/2}(z) \end{aligned}$$

Then,

$$P = \frac{g_{5/2}(z)}{\beta \lambda^3} \checkmark$$

The number of particles is

$$\begin{aligned} N &= z \frac{\partial}{\partial z} \log Z_{GC} \\ &= \frac{V}{\lambda^3} g_{3/2}(z) \quad \checkmark \end{aligned}$$

Item b (Está bien planteado?)

We know

$$N = N_0 + N_\epsilon$$

where N_0 is the number of particles in the fundamental state and N_ϵ the number of particles in other states. By “definition” we have that when $T \rightarrow T_C^+$ then $N_0 = 0$ and $z = z_{\max} = \exp(\beta_C \epsilon_{\text{fundamental}})$. I will assume $\epsilon_{\text{fundamental}} = 0$ so that $z_{\max} = 1$. Considering all this we must have

$$\begin{aligned} N_\epsilon \Big|_{T \rightarrow T_C^+} &= N - N_0 \overset{0}{\rightarrow} \\ &= N(T = T_C, z = 1) \\ &= \frac{V}{\lambda_C^3} g_{3/2}(1) \\ &= \frac{V}{\lambda_C^3} \zeta(3/2) \end{aligned}$$

so in conclusion, at the critical point, $N = \frac{V}{\lambda_C^3} \zeta(3/2)$. Thus

$$x_c = \frac{1}{\zeta(3/2)} \quad \checkmark$$

Item c

For $\frac{V}{N\lambda^3} \gg x_c$ then

$$\frac{1}{g_{3/2}(z)} \gg \frac{1}{\zeta(3/2)} \Rightarrow g_{3/2}(z) \ll \zeta(3/2) \Rightarrow g_{3/2}(z) \approx z \ll 1$$

so we have

$$\begin{cases} P = \frac{z}{\beta\lambda^3} \\ N = \frac{V}{\lambda^3} z \end{cases}$$

and

$$P = \frac{Nk_B T}{V} \quad \checkmark$$

For the case $\frac{V}{N\lambda^3} < x_c$ then $z = 1$ so $g_{5/2}(z = 1) = \zeta(5/2)$ and

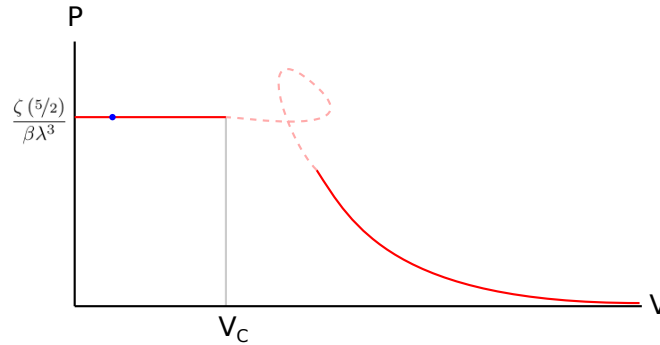
$$P = \frac{\zeta(5/2)}{\beta\lambda^3} \quad \checkmark$$

Item e

From item c we have

$$P = \begin{cases} \frac{Nk_B T}{V} & V \gg V_C \\ \frac{\zeta(5/2)}{\beta\lambda^3} & V < V_C \end{cases}$$

where $V_C = x_c N \lambda^3$ (obtained just solving for V from $\frac{V}{N\lambda^3} = x_c = \frac{1}{\zeta(3/2)}$). The plot is then something like this



and its interpretation as follows:

- The phase transition is of first order because if we begin at the blue dot and decrease the pressure by an infinitesimal amount, then V experiences a finite change. This implies that $V(T, P, N)$ is not continuous and because $V = \left. \frac{\partial^1 G}{\partial P^1} \right|_{T, N}$ we conclude that this is a first order phase transition ✓.
- For the region with $V < V_C$ we find multiple states all with the same P . This implies the coexistence of two phases (?).

Problem 3

The exact Hamiltonian for the Ising model is

$$\begin{aligned} \mathcal{H} &= -J \sum_{\langle i, j \rangle} s_i s_j - \mu B \sum_{\forall i} s_i \\ &= -\frac{J}{2} \sum_{\forall i} s_i \sum_{j \in \mathbb{V}_i} s_j - \mu B \sum_{\forall i} s_i \\ &= -\frac{J}{2} \sum_{\forall i} \sum_{j \in \mathbb{V}_i} s_i s_j - \mu B \sum_{\forall i} s_i \end{aligned}$$

where $\langle i, j \rangle$ denotes that the summation runs over all the pairs of near neighbors (this is the traditional notation) and \mathbb{V}_i is the set of near neighbors of i (this will be my notation which, from my point of view, is clearer). Note that each spin has different neighbors, thus $\mathbb{V}_i \neq \mathbb{V}_\ell$ for $i \neq \ell$.

The mean field approximation (Bragg-Williams) consist in approximating the term $s_i s_j$ as follows

$$\begin{aligned} s_i s_j &= ([s_i - \bar{s}] + \bar{s}) ([s_j - \bar{s}] + \bar{s}) \\ \text{Mean field } \rightarrow &\approx [s_i - \bar{s}] \bar{s} + [s_j - \bar{s}] \bar{s} + \bar{s}^2 + \cancel{[s_i - \bar{s}] [s_j - \bar{s}]} \\ &= \bar{s} s_i + \bar{s} s_j - \bar{s}^2 \quad \checkmark \end{aligned}$$

where \bar{s} is a number that we don't know at this stage and represents the mean value of the spins.

Introducing this into the Hamiltonian

$$\begin{aligned}
 \mathcal{H} &= -\frac{J}{2} \sum_{\forall i} \sum_{j \in \mathbb{V}_i} s_i s_j - \mu B \sum_{\forall i} s_i \quad \leftarrow \text{Exact Ising} \\
 \text{Mean field} \rightarrow &\approx -\frac{J}{2} \sum_{\forall i} \sum_{j \in \mathbb{V}_i} (s_i \bar{s} + s_j \bar{s} - \bar{s}^2) - \mu B \sum_{\forall i} s_i \\
 &= -\frac{J}{2} \left[\bar{s} \sum_{\forall i} s_i \underbrace{\sum_{j \in \mathbb{V}_i} 1}_{|\mathbb{V}|} + \bar{s} \sum_{\forall i} \sum_{j \in \mathbb{V}_i} s_j - \bar{s}^2 \sum_{\forall i} \underbrace{\sum_{j \in \mathbb{V}_i} 1}_{|\mathbb{V}|} \right] - \mu B \sum_{\forall i} s_i \\
 \sum_{\forall i} \sum_{j \in \mathbb{V}_i} s_j &= \sum_{\forall i} |\mathbb{V}| s_i \rightarrow &= -\frac{J}{2} \left[|\mathbb{V}| \sum_{\forall i} s_i \bar{s} + \bar{s} |\mathbb{V}| \sum_{\forall i} s_i - \bar{s}^2 \sum_{\forall i} |\mathbb{V}| \right] - \mu B \sum_{\forall i} s_i \\
 &= -J |\mathbb{V}| \bar{s} \sum_{\forall i} s_i + \frac{J}{2} \bar{s}^2 N |\mathbb{V}| - \mu B \sum_{\forall i} s_i \quad \checkmark
 \end{aligned}$$

where $|\mathbb{V}|$ is the number of near neighbors (note that, although $\mathbb{V}_i \neq \mathbb{V}_\ell$ for different i, ℓ because each has different neighbors, $|\mathbb{V}_i| = |\mathbb{V}_\ell| \stackrel{\text{def}}{=} |\mathbb{V}|$ because all spins have the same number of neighbors).

In the case of cells plus mean field the trick is, when we doing the approximation for $s_i s_j$ in mean field, to consider the next¹¹

$$\begin{aligned}
 s_i s_j &= \bar{s} s_i + \bar{s} s_j - \bar{s}^2 \\
 &= \left(\bar{s} s_i - \frac{\bar{s}^2}{2} \right) + \left(\bar{s} s_j - \frac{\bar{s}^2}{2} \right)
 \end{aligned}$$

Here, each of this terms depends only on s_i or s_j so each can be considered as the interaction of one spin s_i with one neighbor in the mean field approximation. Then, the Hamiltonian will be

$$\mathcal{H}_{\text{all the system}} = \sum_{\forall \text{cell}} \mathcal{H}_{\text{each cell}}$$

with

$$\begin{aligned}
 \mathcal{H}_{\text{one cell}} &= \mathcal{H}_{\text{inside cell}} + \mathcal{H}_{\text{cell-mean field}} + \mathcal{H}_{\text{cell-B external}} \\
 &= -\frac{J}{2} \sum_{\forall i \in \text{cell}} \sum_{j \in \mathbb{V}_i^{\text{internal}}} s_i s_j - J \sum_{\forall i \in \text{cell}} \sum_{j \in \mathbb{V}_i^{\text{external}}} \left(\bar{s} s_i - \frac{\bar{s}^2}{2} \right) - \mu B \sum_{\forall i \in \text{cell}} s_i \\
 &= -\frac{J}{2} \sum_{\forall i \in \text{cell}} \sum_{j \in \mathbb{V}_i^{\text{internal}}} s_i s_j - J |\mathbb{V}_{\text{external}}| \bar{s} \sum_{\forall i \in \text{cell}} s_i + \frac{J}{2} |\text{cell}| |\mathbb{V}_{\text{external}}| \bar{s}^2 - \mu B \sum_{\forall i \in \text{cell}} s_i \quad \checkmark \\
 &= \underbrace{-\frac{J}{2} \sum_{\forall i \in \text{cell}} \sum_{j \in \mathbb{V}_i^{\text{internal}}} s_i s_j}_{\mathcal{H}_{\text{inside cell}}} \underbrace{- J |\mathbb{V}_{\text{external}}| \left(\bar{s} \sum_{\forall i \in \text{cell}} s_i + \frac{|\text{cell}|}{2} \bar{s}^2 \right)}_{\mathcal{H}_{\text{cell-mean field}}} \underbrace{- \mu B \sum_{\forall i \in \text{cell}} s_i}_{\mathcal{H}_{\text{cell-B external}}}
 \end{aligned}$$

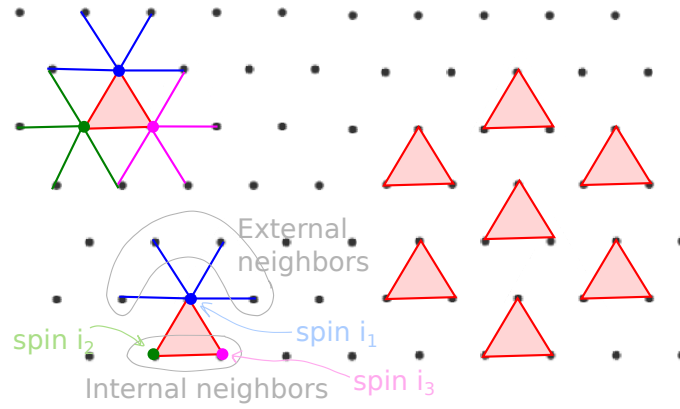
where

- cell Is the set of spins of this particular cell
- $|\text{cell}|$ Is the number of spins inside the cell
- $\mathbb{V}_i^{\text{internal}}$ The set of neighbors of i that are inside the cell
- $\mathbb{V}_i^{\text{external}}$ The set of neighbors of i that are outside the cell

This is the most general expression for the Hamiltonian of one cell using the mean field approximation for the Ising model.

In this exercise we have 3 spins per cell, each spin with 2 internal neighbors and 4 external neighbors, according to the next drawing:

¹¹This is what the professor told us to consider.



so

$$\begin{aligned}
 \mathcal{H}_{\text{one cell}} &= -\frac{J}{2} \sum_{i \in \{i_1, i_2, i_3\}} \sum_{j \in \mathbb{V}_i^{\text{internal}}} s_i s_j - 4J\bar{s} \sum_{i \in \{i_1, i_2, i_3\}} s_i + \frac{3}{2} 4J\bar{s}^2 - \mu B \sum_{i \in \{i_1, i_2, i_3\}} s_i \\
 &= -\frac{J}{2} (s_1 s_2 + s_1 s_3 + s_2 s_1 + s_2 s_3 + s_3 s_1 + s_3 s_2) + \dots \\
 &\quad \dots - 4J\bar{s} (s_1 + s_2 + s_3) + 6J\bar{s}^2 - \mu B (s_1 + s_2 + s_3) \\
 &= -J (s_1 s_2 + s_2 s_3 + s_3 s_1) - 4\bar{s} (s_1 + s_2 + s_3) + 6J\bar{s}^2 - \mu B (s_1 + s_2 + s_3) \\
 &= -J (s_1 s_2 + s_2 s_3 + s_3 s_1) - (\mu B - 4J\bar{s}) (s_1 + s_2 + s_3) + 6J\bar{s}^2 \checkmark \checkmark
 \end{aligned}$$

The generic expression for the Hamiltonian turned out to be correct. Nice ☺.

Now, the partition function of one cell is going to be

$$Z_{\text{cell}} = \sum_{\forall s_1, s_2, s_3 = \pm 1} e^{-\beta \mathcal{H}_{\text{one cell}}(s_1, s_2, s_3)}$$

where $\forall s_1, s_2, s_3 = \pm 1$ means that $[s_1 \ s_2 \ s_3] \in \{[-1 \ -1 \ -1], [-1 \ -1 \ 1], [-1 \ 1 \ -1], \dots, [1 \ 1 \ 1]\}$, they are in total $2^3 = 8$ combinations. Thus¹²

$$\begin{aligned}
 Z_{\text{cell}} &= e^{-\beta 6J\bar{s}^2} \left(e^{-\beta[-3J+3(\mu B-4J\bar{s})]} + 3e^{-\beta[J+(\mu B-4J\bar{s})]} + 3e^{-\beta[J-(\mu B-4J\bar{s})]} + e^{-\beta[-3J-3(\mu B+4J\bar{s})]} \right) \\
 &= e^{-\beta 6J\bar{s}^2} \left(e^{3\beta J} e^{-3\beta(\mu B-4J\bar{s})} + 3e^{-\beta J} e^{-\beta(\mu B-4J\bar{s})} + 3e^{-\beta J} e^{\beta(\mu B-4J\bar{s})} + e^{3\beta J} e^{3\beta(\mu B+4J\bar{s})} \right) \\
 &= e^{-6\beta J\bar{s}^2} \left(2e^{3\beta J} \cosh(3\beta [\mu B - 4J\bar{s}]) + 6e^{-\beta J} \cosh(\beta [\mu B - 4J\bar{s}]) \right) \checkmark
 \end{aligned}$$

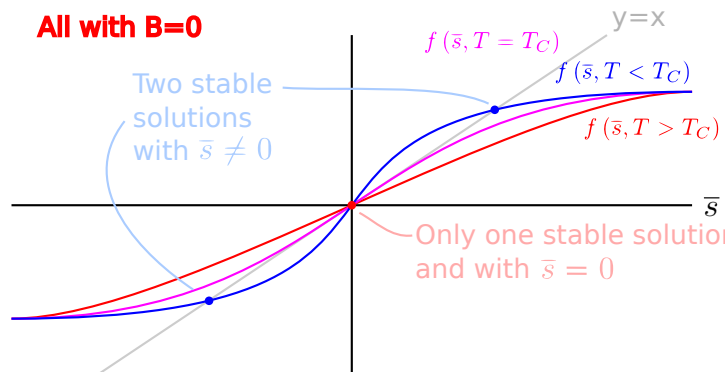
The value of \bar{s} is given by¹³

$$\bar{s} = \frac{1}{|\text{cell}| \beta \mu} \frac{\partial}{\partial B} \log Z_{\text{cell}}$$

This equation is of the form

$$\bar{s} = f(\bar{s}, B, T)$$

(where $f(\bar{s}) = \frac{1}{|\text{cell}| \beta \mu} \frac{\partial}{\partial B} \log Z_{\text{cell}}$). If the system is going to have a phase transition then we must hope the graphical solutions of the previous equation to be something like this (for $B = 0$):



¹²This calculation is very easy but has to be done with much care, because it is very easy to get confused just because it has many terms.

¹³This is magic, I don't know where this came from.

(the professor told us to assume the graphic of $f(\bar{s})$ to be more or less like that). Then, as shown in the plot,

$$\left. \frac{\partial f}{\partial \bar{s}} \right|_{B=0, \bar{s}=0} \begin{cases} < 1 & T > T_C \\ = 1 & T = T_C \\ > 1 & T < T_C \end{cases}$$

If we want to find a condition for T_C (as we are asked for by the *consigna*) then we see what happens if we impose $\left. \frac{\partial f}{\partial \bar{s}} \right|_{B=0, \bar{s}=0, T=T_C} = 1$. The calculus is

$$\begin{aligned} \log Z_{\text{cell}} &= \log \left[e^{-6\beta J \bar{s}^2} (2e^{3\beta J} \cosh(3\beta [\mu B - 4J\bar{s}]) + 6e^{-\beta J} \cosh(\beta [\mu B - 4J\bar{s}])) \right] \\ &= -6\beta J \bar{s}^2 + \log (2e^{3\beta J} \cosh(3\beta [\mu B - 4J\bar{s}]) + 6e^{-\beta J} \cosh(\beta [\mu B - 4J\bar{s}])) \end{aligned}$$

so

$$\frac{\partial \log Z_{\text{cell}}}{\partial B} = \frac{2e^{3\beta J} \sinh(3\beta [\mu B - 4J\bar{s}]) (3\beta\mu) + 6e^{-\beta J} \sinh(\beta [\mu B - 4J\bar{s}]) (\beta\mu)}{2e^{3\beta J} \cosh(3\beta [\mu B - 4J\bar{s}]) + 6e^{-\beta J} \cosh(\beta [\mu B - 4J\bar{s}])}$$

and

$$\frac{1}{|\text{cell}| \beta\mu} \frac{\partial}{\partial B} \log Z_{\text{cell}} = \frac{1}{3\beta\mu} \frac{2e^{3\beta J} \sinh(3\beta [\mu B - 4J\bar{s}]) (3\beta\mu) + 6e^{-\beta J} \sinh(\beta [\mu B - 4J\bar{s}]) (\beta\mu)}{2e^{3\beta J} \cosh(3\beta [\mu B - 4J\bar{s}]) + 6e^{-\beta J} \cosh(\beta [\mu B - 4J\bar{s}])}$$

Now we impose $B = 0$ so

$$\left(\frac{1}{|\text{cell}| \beta\mu} \frac{\partial}{\partial B} \log Z_{\text{cell}} \right) \Big|_{B=0} = \frac{e^{3\beta J} \sinh(12\beta J \bar{s}) + e^{-\beta J} \sinh(4\beta J \bar{s})}{e^{3\beta J} \cosh(12\beta J \bar{s}) + e^{-\beta J} \cosh(4\beta J \bar{s})} \checkmark$$

This is $f(\bar{s}, T, B = 0)$. Now we calculate

$$\begin{aligned} \left. \frac{\partial f}{\partial \bar{s}} \right|_{B=0} &= \frac{12\beta J e^{3\beta J} \sinh(12\beta J \bar{s}) + 4\beta J e^{-\beta J} \sinh(4\beta J \bar{s})}{e^{3\beta J} \cosh(12\beta J \bar{s}) + e^{-\beta J} \cosh(4\beta J \bar{s})} + \dots \\ &\dots - \frac{e^{3\beta J} \sinh(12\beta J \bar{s}) + e^{-\beta J} \sinh(4\beta J \bar{s})}{[e^{3\beta J} \cosh(12\beta J \bar{s}) + e^{-\beta J} \cosh(4\beta J \bar{s})]^2} [12\beta J e^{3\beta J} \cosh(12\beta J \bar{s}) + 4\beta J e^{-\beta J} \cosh(4\beta J \bar{s})] \end{aligned}$$

and impose $\bar{s} = 0$ and $T = T_C$ so

$$\begin{aligned} \left. \frac{\partial f}{\partial \bar{s}} \right|_{B=0, \bar{s}=0, T=T_C} &= \frac{12\beta_C J e^{3\beta_C J} + 4\beta_C J e^{-\beta_C J}}{e^{3\beta_C J} + e^{-\beta_C J}} - \frac{e^{3\beta_C J} + e^{-\beta_C J}}{e^{3\beta_C J} + e^{-\beta_C J}} (12\beta_C J e^{3\beta_C J} + 4\beta_C J e^{-\beta_C J}) \\ &\stackrel{?}{=} \frac{12\beta_C J e^{3\beta_C J} + 4\beta_C J e^{-\beta_C J}}{e^{3\beta_C J} + 3e^{-\beta_C J}} \checkmark \end{aligned}$$

I don't know how the professor did to arrive to the last result. I will assume I have made a mistake in some step during the derivation.

Now, calling $x = 2J\beta_C$ the previous expression becomes

$$\begin{aligned} \left. \frac{\partial f}{\partial \bar{s}} \right|_{B=0, \bar{s}=0, T=T_C} &= \frac{6xe^{\frac{3}{2}x} + 2xe^{-\frac{1}{2}x}}{e^{\frac{3}{2}x} + 3e^{-\frac{1}{2}x}} \\ \text{Multiply and divide by } e^{\frac{x}{2}} &\rightarrow = \frac{6xe^{2x} + 2x}{e^{2x} + 3} \\ &= 2xe^x \frac{3e^x + e^{-x}}{e^x + 3e^{-x}} \end{aligned}$$

I have some math error but I don't care, this is the way the exercise is solved. The last step is to equal that to 1 (as stated previously) and we are done.

4. 13/07/2016

Consigna

Problema 1

Considere un gas de electrones confinado a moverse en un plano de área A . Se aplica un campo magnético de módulo B en la dirección normal al plano. En estas condiciones, ignorando la interacción entre el espín de los electrones y el campo magnético, se obtiene que los niveles de energía monoparticulares son los de un oscilador armónico,

$$\epsilon = \hbar\omega \left(n + \frac{1}{2} \right) \quad n = 0, 1, 2, \dots$$

donde $\omega = \frac{|q_e|B}{mc}$. Cada nivel de energía tiene degeneración $g = 2A \frac{|q_e|B}{hc}$. El sistema se encuentra en equilibrio a temperatura T y fugacidad z .

- (a) Usando la fórmula de Euler-Maclaurin, $\sum_{n=0}^{\infty} f\left(n + \frac{1}{2}\right) \approx \int_0^{\infty} du f(u) + \frac{1}{24}f'(0)$, pruebe que la función de partición gran canónica del gas está dada por

$$\log Z \approx g \left[\frac{k_B T}{\hbar\omega} f_2(z) - \frac{1}{24} \frac{\hbar\omega}{k_B T} \frac{z}{1+z} \right]$$

Discuta el caso $B = 0$.

- (b) Calcule la magnetización $M = k_B T \left. \frac{\partial}{\partial B} \right|_{T,A,z} \log Z$ del gas en función de T, A, B y el número de partículas N a primer orden en B , y obtenga de ahí la susceptibilidad magnética del gas. Discuta los resultados.

Problema 2

Considere un gas de N partículas libres de espín 0 y masa m que se mueven en un espacio de d dimensiones. El gas está contenido en un recipiente de volumen V y se encuentra en equilibrio a temperatura T . Supondremos que $d \gg 1$, lo cual es una simplificación porque $g_\nu(z) \approx z$ para $\nu \gg 1$.

- (a) Calcule la fracción de partículas en el estado fundamental, la presión y la entropía por partícula del gas como funciones de T y $v = \frac{V}{N}$, y gráfíquelas a T constante. Discuta sus resultados.
- (b) Calcule el calor cedido por partícula cuando el gas condensa completamente de manera cuasiestática e isotérmica.

Problema 3

Considere una cadena unidimensional de Ising formada por N espines en presencia de un campo magnético.

- (a) Encuentre las ecuaciones del grupo de renormalización correspondientes a decimar el sistema sumando sobre todos los sitios que no son múltiplos de 3.
- (b) Particularizando al caso donde el campo magnético es nulo, obtenga los puntos fijos y estudie su estabilidad.

Resolución

Problem 1

Item a

I have solved a similar exercise in problem 1 from 01/07/2015, see page 26. In that exercise I have found that

$$\log Z_{GC} = g \sum_{i=0}^{\infty} \log \left(1 + ze^{-\beta \hbar \omega (i + \frac{1}{2})} \right)$$

without making any approximation. I will continue from here. We can identify

$$f \left(n + \frac{1}{2} \right) = \log \left(1 + ze^{-\beta \hbar \omega (n + \frac{1}{2})} \right)$$

so that (using the Euler-Maclaurin formula from the *consigna*)

$$\sum_{i=0}^{\infty} \log \left(1 + ze^{-\beta \hbar \omega (i + \frac{1}{2})} \right) \approx \underbrace{\int_0^{\infty} du \log \left(1 + ze^{-\beta \hbar \omega u} \right)}_{\frac{\Gamma(2)}{\beta \hbar \omega} f_2(z)} + \left. \frac{1}{24} \frac{\partial f}{\partial n} \right|_{n=0}$$

The first integral can be calculated as

$$\begin{aligned} \int_0^{\infty} du u^a \log \left(1 + ze^{-bu} \right) &= \frac{1}{b^{a+1}} \int_0^{\infty} dx x^a \log \left(1 + ze^{-x} \right) \leftarrow x \stackrel{\text{def}}{=} bu \Rightarrow \begin{cases} du = \frac{dx}{b} \\ u = \frac{x}{b} \end{cases} \\ \text{Integration by parts} \rightarrow &= \frac{1}{b^{a+1}} \left[\frac{x^{a+1}}{a+1} \log \left(1 + ze^{-x} \right) \right]_{x=0}^{x=\infty} - \int_0^{\infty} dx \frac{x^{a+1}}{a+1} \frac{ze^{-x}(-1)}{1+ze^{-x}} \\ f_{\nu}(z) \stackrel{\text{def}}{=} \frac{1}{\Gamma(\nu)} \int_0^{\infty} dx \frac{x^{\nu-1}}{z^{-1}e^x + 1} \rightarrow &= \frac{\Gamma(a+2)}{b^{a+1}(a+1)} \underbrace{\frac{1}{\Gamma(a+2)} \int_0^{\infty} \frac{x^{a+1} dx}{z^{-1}e^x + 1}}_{f_{a+2}(z)} \\ &= \frac{\Gamma(a+2)}{b^{a+1}(a+1)} f_{a+2}(z) \end{aligned}$$

and the derivative is

$$\begin{aligned} \left. \frac{\partial f}{\partial n} \right|_0 &= \left. \frac{ze^{-\beta \hbar \omega (n + \frac{1}{2})} (-\beta \hbar \omega)}{1 + ze^{-\beta \hbar \omega (n + \frac{1}{2})}} \right|_0 \\ &= -\beta \hbar \omega \frac{z}{1+z} \end{aligned}$$

so finally

$$\begin{aligned} \log Z &\approx g \left[\frac{1}{\beta \hbar \omega} f_2(z) - \frac{1}{24} \beta \hbar \omega \frac{z}{1+z} \right] \checkmark \\ &= 2A \frac{|q_e| B}{hc} \left[\frac{mc}{\beta \hbar |q_e| B} f_2(z) - \frac{1}{24} \frac{\beta \hbar |q_e| B}{mc} \frac{z}{1+z} \right] \\ \lambda \stackrel{\text{def}}{=} \sqrt{\frac{2\pi \hbar^2}{mk_B T}} \rightarrow &= 2A \left[\frac{1}{\lambda^2} f_2(z) - \frac{1}{24} \frac{\beta |q_e|^2 B^2}{2\pi mc^2} \frac{z}{1+z} \right] \end{aligned}$$

Evaluating this for $B = 0$ it is obtained

$$\begin{aligned} \log Z &= 2A \left(\frac{1}{\sqrt{\frac{2\pi \hbar^2}{k_B T m}}} \right)^2 f_2(z) \\ &= \frac{2A}{\lambda^2} f_2(z) \checkmark \end{aligned}$$

which is nothing more than an ideal free fermions gas.

Item b

The magnetization is going to be

$$\begin{aligned}
 M &= k_B T \left. \frac{\partial}{\partial B} \right|_{T,A,z} \log Z \\
 &= k_B T \left. \frac{\partial}{\partial B} \right|_{T,A,z} \left(2A \left[\frac{1}{\lambda^2} f_2(z) - \frac{1}{24} \frac{\beta |q_e|^2 B^2}{2\pi m c^2} \frac{z}{1+z} \right] \right) \\
 &= \cancel{2A k_B T} \frac{1}{12} \frac{\beta |q_e|^2 B}{2\pi m c^2} \frac{z}{1+z} \\
 &= -\frac{A}{12\pi} \frac{|q_e|^2}{m c^2} \frac{z}{1+z} B \checkmark
 \end{aligned}$$

Now we must find $z = z(N)$ (we are asked for $M = M(T, A, B, N)$). Because we have obtained $M = f(z) B$ which already is at first order in B , then we need z to zero order in B .

For this we can consider

$$\begin{aligned}
 N &= z \frac{\partial}{\partial z} \log Z \\
 &= z \frac{\partial}{\partial z} \left(2A \left[\frac{1}{\lambda^2} f_2(z) - \frac{1}{24} \frac{\beta |q_e|^2 B^2}{2\pi m c^2} \frac{z}{1+z} \right] \right) \\
 &= \frac{2A}{\lambda^2} f_1(z) \checkmark
 \end{aligned}$$

where the term that has been canceled is because it is quadratic in B , and we are interested only in constant terms.

For inverting $f_1(z)$ we consider its definition

$$\begin{aligned}
 f_1(z) &\stackrel{\text{def}}{=} \int_0^\infty \frac{dx}{z^{-1} e^x + 1} \\
 &= \int_0^\infty \frac{z e^{-x}}{1 + z e^{-x}} dx \\
 &= - \int_0^\infty \frac{\partial}{\partial x} \log(1 + z e^{-x}) dx \\
 &= - \log(1 + z e^{-x}) \Big|_{x=0}^{x=\infty} \\
 &= \log(1 + z) \checkmark
 \end{aligned}$$

Replacing this into the expression for N we obtain $N = \frac{2A}{\lambda^2} \log(1 + z)$ from where

$$z = e^{\frac{N\lambda^2}{2A}} - 1 \checkmark$$

Finally we can introduce this in M so

$$M = -\frac{A}{12\pi} \frac{|q_e|^2}{m c^2} \frac{e^{\frac{N\lambda^2}{2A}} - 1}{e^{\frac{N\lambda^2}{2A}}} B \checkmark$$

and the susceptibility will be

$$\begin{aligned}
 \chi &= \frac{\partial M}{\partial B} \\
 &= -\frac{A}{12\pi} \frac{|q_e|^2}{m c^2} \frac{e^{\frac{N\lambda^2}{2A}} - 1}{e^{\frac{N\lambda^2}{2A}}} \checkmark
 \end{aligned}$$

Because $\chi < 0$ the material is a diamagnetic. Also, if we take $h \rightarrow 0$ then $\lambda \rightarrow 0$ so $\chi \xrightarrow{h \rightarrow 0} 0$. This tells us that the effect is purely a quantum phenomenon \checkmark .

Problem 2

Item a (Consultar varias cosas!)

The partition function is, due to the theorem in page 55,

$$\log Z_{GC} = \sum_{\forall \text{ monoparticular state } i} \log Z_i \qquad Z_i = \sum_{\forall \text{ allowed particles } n} (z e^{-\beta \epsilon_i})^n$$

Because the particles have spin zero, we are dealing with bosons. Then the allowed number of particles n can range from 0 to ∞ . Thus

$$Z_i = \sum_{n=0}^{\infty} (ze^{-\beta\epsilon_i})^n$$

Geometric series $\rightarrow = \frac{1}{1 - ze^{-\beta\epsilon_i}}$

and

$$\begin{aligned} \log Z &= - \sum_{\forall \text{ monoparticular state } i} \log(1 - ze^{-\beta\epsilon_i}) \\ \epsilon_i = \epsilon(\mathbf{q}, \mathbf{p}) &\rightarrow = - \sum_{\forall \text{ allowed } \mathbf{q}, \mathbf{p}} g(\mathbf{q}, \mathbf{p}) \log(1 - ze^{-\beta\epsilon(\mathbf{q}, \mathbf{p})}) \\ \mathbf{q} \text{ and } \mathbf{p} \text{ are independent} &\rightarrow = - \sum_{\forall \mathbf{q}} \sum_{\forall \mathbf{p}} \log(1 - ze^{-\beta\epsilon(\mathbf{q}, \mathbf{p})}) \end{aligned}$$

where $g(\mathbf{q}, \mathbf{p}) = 1$ is the degeneration for each \mathbf{q}, \mathbf{p} and the allowed values for \mathbf{q} and \mathbf{p} are from a quantum point of view, they are not the classical variables¹⁴. Now it comes the magic, we apply the next tricks:

$$\begin{aligned} \log Z &= - \sum_{\forall \mathbf{q}, \mathbf{p} \approx \text{classical}} \log(1 - ze^{-\beta\epsilon(\mathbf{q}, \mathbf{p})}) - \sum_{\forall \mathbf{q}, \mathbf{p} \neq \text{classical}} \log(1 - ze^{-\beta\epsilon(\mathbf{q}, \mathbf{p})}) \\ \text{Ask for this} &\rightarrow \approx - \int_{\forall \mathbf{q}} \int_{\forall \mathbf{p}} \frac{d^d q d^d p}{h^d} \log(1 - ze^{-\beta\epsilon(\mathbf{q}, \mathbf{p})}) - \log(1 - ze^{-\beta\epsilon_{\text{fundamental state}}}) \end{aligned}$$

where we have considered that the only “not classical” state is the fundamental. Also, d are the number of dimensions of the space.

We are told that the particles are free, which implies that the energy levels are

$$\begin{cases} \epsilon(\mathbf{q}, \mathbf{p}) = \frac{\mathbf{p}^2}{2m} & \forall \mathbf{q}, \mathbf{p} \approx \text{classical} \\ \epsilon_{\text{fundamental}} = 0 & \text{Non classical states} \end{cases}$$

so the previous equation writes

$$\begin{aligned} \log Z &= - \int_{\forall \mathbf{q}} \int_{\forall \mathbf{p}} \frac{d^d q d^d p}{h^d} \log(1 - ze^{-\beta \frac{\mathbf{p}^2}{2m}}) - \log(1 - z) \\ &= - \underbrace{\frac{V}{h^d} \int_{\forall \mathbf{p}} d^d p \log(1 - ze^{-\beta \frac{\mathbf{p}^2}{2m}})}_{\boxed{A}} - \log(1 - z) \end{aligned}$$

Now for solving the integral we can consider the change of variables $\begin{cases} r^2 = \mathbf{p}^2 \\ \theta_{d-1} = \text{the other stuff} \end{cases}$ so that we pass from Cartesian to spherical coordinates and use the happy relation¹⁵ $d^d p \stackrel{\odot}{=} \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2})} r^{d-1} dr$ so

$$\begin{aligned} \boxed{A} &= \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2})} \int_0^{\infty} dr r^{d-1} \log(1 - ze^{-\beta \frac{r^2}{2m}}) \\ x \stackrel{\text{def}}{=} r^2 &\Rightarrow \begin{cases} dr = dx \frac{1}{2\sqrt{x}} \\ r = \sqrt{x} \end{cases} \rightarrow = \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2})} 2 \int_0^{\infty} dx \underbrace{x^{-\frac{1}{2}} x^{\frac{d-1}{2}}}_{x^{\frac{d}{2}-1}} \log(1 - ze^{-\frac{\beta}{2m}x}) \\ \int_0^{\infty} du u^a \log(1 - ze^{-bu}) &= \frac{\Gamma(a+1)}{b^{a+1}} g_{a+1}(z) \rightarrow = \frac{\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2})} \frac{\Gamma(\frac{d}{2})}{(\frac{\beta}{2m})^{\frac{d}{2}}} g_{d/2}(z) \end{aligned}$$

¹⁴To be sincere I don't really understand this step. Maybe when I course Teo 2 I will understand. At least for now it is black magic.

¹⁵The integration over the $r = 1$ d -sphere has already been performed.

so the partition function finally is

$$\begin{aligned} \log Z &= -\frac{V}{h^d} \left(\frac{2\pi m}{\beta} \right)^{\frac{d}{2}} g_{d/2}(z) - \log(1-z) \\ &= -V \left(\frac{m}{2\pi\hbar^2\beta} \right)^{\frac{d}{2}} g_{d/2}(z) - \log(1-z) \\ \lambda \stackrel{\text{def}}{=} \sqrt{\frac{2\pi\hbar^2}{mk_B T}} &\rightarrow = +\frac{V}{\lambda^d} g_{d/2}(z) - \log(1-z) \checkmark \end{aligned}$$

where the + sign was forced, I don't know where have I made the mistake.

Because the *consigna* says that $d \gg 1$ and $g_\nu(z) \approx z$ then

$$\log Z = \frac{V}{\lambda^d} z - \log(1-z)$$

The number of particles of the system is gonna be

$$\begin{aligned} N &= z \frac{\partial \log Z}{\partial z} \\ &= \frac{V}{\lambda^d} z + \frac{z}{1-z} \end{aligned}$$

Here we identify (using eq. (1))

$$N(T, z) = \begin{cases} \frac{V}{\lambda^d} z & T \geq T_C \\ N_0(T, z_{\max}) + \frac{V}{\lambda^d} & T < T_C \quad z = 1 \end{cases} \quad (2)$$

Note that I have thrown away the term $\frac{z}{1-z}$ by hand because it always gives troubles. This term corresponds to N_0 but, because of something related to the thermodynamic limit, it is wrong. Or something like this. The fraction in the fundamental is going to be, for $T < T_C$,

$$\begin{aligned} \frac{N_0}{N} &= 1 - \frac{N_\epsilon}{N} \\ &= 1 - \frac{1}{N} \frac{V}{\lambda^d} \\ v = \frac{V}{N} &\rightarrow = 1 - \frac{v}{\lambda^d} \checkmark \\ \lambda \stackrel{\text{def}}{=} \sqrt{\frac{2\pi\hbar^2}{mk_B T}} &\rightarrow = 1 - v \left(\frac{mk_B T}{2\pi\hbar^2} \right)^d \end{aligned}$$

and for $T \geq T_C$ this fraction is "by definition" null. So

$$\frac{N_0}{N} = \begin{cases} 0 & T \geq T_C \\ 1 - \frac{v}{\lambda^d} & T < T_C \equiv \frac{v}{\lambda^d} < 1 \end{cases}$$

Pressure can be obtained from

$$P = - \left. \frac{\partial \Xi}{\partial V} \right|_{T, N}$$

where Ξ is the grand canonical potential, which is

$$\begin{aligned} \Xi &= -k_B T \log Z \\ &= -k_B T \frac{V}{\lambda^d} z \end{aligned}$$

thus

$$\begin{aligned} P &= k_B T \left. \frac{\partial \log Z}{\partial V} \right|_{T, N} \\ &\stackrel{?}{=} \frac{k_B T}{V} \log Z \checkmark \\ &= \frac{k_B T}{\lambda^d} z \checkmark \end{aligned}$$

If we are above the critical temperature then $\frac{N}{V} = \frac{z}{\lambda^d}$ (see (2)) and

$$P = \frac{k_B T}{v} \rightarrow T \geq T_C$$

Thus

$$P = \begin{cases} \frac{k_B T}{v} & T \geq T_C \\ \frac{k_B T}{\lambda^d} & T < T_C \end{cases}$$

The entropy can be found considering that the grand canonical potential is $\Xi \stackrel{\text{def}}{=} U - TS - \mu N$ so

$$S = \frac{1}{T}U - \frac{1}{T}\Xi - \frac{1}{T}\mu N$$

where each quantity can be obtained from $\begin{cases} U = - \left. \frac{\partial}{\partial \beta} \right|_{V,z} \log Z_{GC} \\ \Xi = k_B T \log Z_{GC} \\ \mu = k_B T \log z \end{cases}$. The internal energy is

$$\begin{aligned} U &= - \left. \frac{\partial}{\partial \beta} \right|_{V,z} \left(\frac{V}{\lambda^d} z \right) = - \left. \frac{\partial}{\partial \beta} \right|_{V,z} \left(V \left(\frac{m}{2\pi\hbar^2\beta} \right)^{\frac{d}{2}} z \right) \leftarrow \lambda \stackrel{\text{def}}{=} \sqrt{\frac{2\pi\hbar^2}{mk_B T}} \\ &= -Vz \left(\frac{m}{2\pi\hbar^2} \right)^{\frac{d}{2}} \left(-\frac{d}{2} \right) \beta^{-\frac{d}{2}-1} \\ &= Vz \frac{d}{2} \frac{k_B T}{\lambda^d} \checkmark \end{aligned}$$

The grand canonical potential is

$$\begin{aligned} \Xi &= -k_B T \log Z \\ &= -k_B T \frac{V}{\lambda^d} z \end{aligned}$$

Then

$$\begin{aligned} S &= \frac{1}{T} Vz \frac{d}{2} \frac{k_B T}{\lambda^d} + \frac{1}{T} k_B T \frac{V}{\lambda^d} z - \frac{1}{T} k_B T \log z N \\ &= k_B \left(\frac{Vz}{\lambda^d} \left(1 + \frac{d}{2} \right) - N \log z \right) \end{aligned}$$

and the entropy per particle is

$$s = k_B \left(\frac{vz}{\lambda^d} \left(1 + \frac{d}{2} \right) - \log z \right) \checkmark$$

Because we don't like z we would like to replace it by $z = z(v, T)$. From (2) it can be replaced so that

$$s(v, T) = \begin{cases} k_B \left(1 + \frac{d}{2} - \log \frac{\lambda^d}{v} \right) & T \geq T_C \\ k_B \frac{v}{\lambda^d} \left(1 + \frac{d}{2} \right) & T < T_C \quad z = 1 \end{cases} \checkmark$$

Item b

The liberated heat is

$$\begin{aligned}
 Q_{\text{liberated}} &= -Q_{\text{absorbed}} \\
 &= -\int \delta Q_{\text{absorbed}} \\
 \text{quasi-static } \rightarrow &= -\int T dS \\
 \text{Isothermal } \rightarrow &= -T \int dS \\
 &= T (S_{\text{normal phase}} - S_{\text{condensed phase}}) \\
 &= T \left(k_B \left(1 + \frac{d}{2} - \log \frac{\lambda^d}{v} \right) \Big|_{\text{critical point}} - k_B \frac{v}{\lambda^d} \left(1 + \frac{d}{2} \right) \Big|_{\text{completely condensed}} \right) \\
 &= k_B T \left(1 + \frac{d}{2} \right) \checkmark
 \end{aligned}$$

because $\frac{\lambda^d}{v} \Big|_{\text{critical point}} = 1$ and $\frac{v}{\lambda^d} \Big|_{\text{completely condensed}} = 0$ (this can be seen in the formula for $\frac{N_0}{N}$).

Problem 3 (have no idea)

Item a

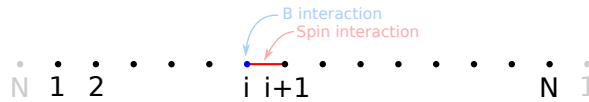
The Hamiltonian for Ising is

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - \mu B \sum_{\forall i} \sigma_i$$

where $\langle i, j \rangle$ denotes that the summation runs over all pairs of first neighbors, once per each pair. For the 1D cyclic case this is just

$$\mathcal{H} = -\sum_{i=1}^N (J \sigma_i \sigma_{i+1} - \mu B \sigma_i)$$

which can be better visualized considering the next drawing:



When the summation is standing at i it counts the spin interaction between i and the “next” neighbor $i + 1$ and the interaction with the external B of the i -th spin. Because the string is closed, then when $i = N$ we are counting the spin interaction between i_N and i_1 .

Because then we want to apply the renormalization group theory, I don’t know why right now but, the next equivalent expression for the Hamiltonian is better

$$\begin{aligned}
 \mathcal{H} &= -\sum_{i=1}^N \left(J \sigma_i \sigma_{i+1} - \frac{\mu B}{2} (\sigma_i + \sigma_{i+1}) \right) \\
 \mathcal{H} &= -\sum_{i=1}^{N/3} [J (\sigma_{3i} \sigma_{3i+1} + \sigma_{3i+1} \sigma_{3i+2} + \sigma_{3i+2} \sigma_{3i+3}) - \mu B (\sigma_{3i} + \sigma_{3i+1} + \sigma_{3i+2})]
 \end{aligned}$$

The Hamiltonian for Ising is (closed chain)

$$\begin{aligned}
 \mathcal{H} &= \sum_{i=1}^N \left(-\frac{J}{2} s_i s_{i-1} - \mu B s_i \right) \\
 \text{Simetrized } \rightarrow &= \sum_{i=1}^N \left(-\frac{J}{2} s_i s_{i-1} - \frac{\mu B}{2} (s_i + s_{i-1}) \right) \\
 k = \frac{i}{3} \rightarrow &= \sum_{k=1}^{N/3} \left(-\frac{J}{2} [s_{3k-3} s_{3k-2} + s_{3k-2} s_{3k-1} + s_{3k-1} s_{3k}] - \mu B (s_{3k-3} + 2s_{3k-2} + 2s_{3k-1} + s_{3k}) \right) \checkmark
 \end{aligned}$$

5. 23/11/2015 - Segundo intento

La consigna se puede encontrar en la página 3.

Resolution

Problem 1

Item a

The partition function for bosons is

$$\log Z = - \sum_{\forall \text{monoparticle state}} \log(1 - ze^{-\beta\epsilon_i})$$

ϵ_i is the energy of each monoparticle state. In this case, each monoparticle state will be given by the allowed values of \mathbf{q} , \mathbf{p} and s . So

$$\begin{aligned} \log Z &= - \sum_{\forall \mathbf{q}, \mathbf{p}, s} \log(1 - ze^{-\beta\epsilon(\mathbf{q}, \mathbf{p}, s)}) \\ &= - \sum_{\forall \mathbf{q}} \sum_{\forall \mathbf{p}} \sum_{\forall s} \log(1 - ze^{-\beta\epsilon(\mathbf{q}, \mathbf{p}, s)}) \end{aligned}$$

where the second equality holds because there exist no restrictions connecting \mathbf{q} , \mathbf{p} nor s , thus the allowed values for $\{\mathbf{q}, \mathbf{p}, s\}$ are just the allowed values for \mathbf{q} , the allowed values for \mathbf{p} and those of s .

The next step is a little bit magical. I don't know the justification but it seems that

$$\begin{aligned} \log Z &= \log Z_0 + \log Z_\epsilon \\ &= -\log(1 - ze^{-\beta\epsilon_{\text{fundamental}}}) - \sum_{\substack{\forall \mathbf{q} \\ \text{except the fundamental}}} \sum_{\forall \mathbf{p}} \sum_{\forall s} \log(1 - ze^{-\beta\epsilon(\mathbf{q}, \mathbf{p}, s)}) \\ \text{Magical step} \rightarrow &\approx -\log(1 - ze^{-\beta\epsilon_{\text{fundamental}}}) - \underbrace{\int_{\forall \mathbf{q}} \int_{\forall \mathbf{p}} \sum_{\forall s} \frac{d^d q d^d p}{h^d} \log(1 - ze^{-\beta\epsilon(\mathbf{q}, \mathbf{p}, s)})}_{[A]} \end{aligned}$$

where d is the number of dimensions. In this case the fundamental level is

$$\epsilon_{\text{fundamental}} = \epsilon(0, 0, +1) = -\mu_B B$$

so

$$\log Z = -\log(1 - ze^{\beta\mu_B B}) - \underbrace{\int_{\forall \mathbf{q}} \int_{\forall \mathbf{p}} \sum_{\forall s} \frac{d^d q d^d p}{h^d} \log(1 - ze^{-\beta\epsilon(\mathbf{q}, \mathbf{p}, s)})}_{[A]}$$

Now we have to rearrange and calculate the integral. This is

$$\begin{aligned} h^d [A] &= \sum_{s \in \{-1, 0, 1\}} \int_{\forall \mathbf{q}} \int_{\forall \mathbf{p}} d^d q d^d p \log\left(1 - ze^{-\frac{\beta}{2m}\mathbf{p}^2 - \frac{\beta m\omega^2}{2}\mathbf{q}^2 + \beta\mu_B B s}\right) \\ z_s \stackrel{\text{def}}{=} ze^{\beta\mu_B B s} \rightarrow &= \sum_{s \in \{-1, 0, 1\}} \int_{\forall \mathbf{q}} \int_{\forall \mathbf{p}} d^d q d^d p \log\left(1 - z_s e^{-\frac{\beta}{2m}\mathbf{p}^2 - \frac{\beta m\omega^2}{2}\mathbf{q}^2}\right) \\ \left\{ \begin{array}{l} \mathbf{Q} \stackrel{\text{def}}{=} \sqrt{\frac{\beta m\omega^2}{2}} \mathbf{q} \\ \mathbf{P} \stackrel{\text{def}}{=} \sqrt{\frac{\beta}{2m}} \mathbf{p} \end{array} \right. \rightarrow &= \left(\frac{2}{\beta m\omega^2}\right)^{\frac{d}{2}} \left(\frac{2m}{\beta}\right)^{\frac{d}{2}} \sum_{s \in \{-1, 0, 1\}} \int_{\forall \mathbf{Q}} \int_{\forall \mathbf{P}} d^d Q d^d P \log(1 - z_s e^{-\mathbf{Q}^2 - \mathbf{P}^2}) \end{aligned}$$

Now, because the integrand is of the form $f(|\mathbf{Q} + \mathbf{P}|)$ we consider to change variables to spherical coordinates in $2d$ dimensions (d for \mathbf{Q} and another d for \mathbf{P}). Then we will use $\begin{cases} r^2 \stackrel{\text{def}}{=} \mathbf{Q}^2 + \mathbf{P}^2 \\ \theta_{2d-1} = \text{other angular coordinates} \end{cases}$ so that

$$d^d Q d^d P = \frac{2\pi^d}{\Gamma(d)} r^{2d-1} dr$$

and then

$$\begin{aligned}
 h^d \boxed{A} &= \left(\frac{2}{\beta\omega}\right)^d \sum_{s \in \{-1,0,1\}} \frac{2\pi^d}{\Gamma(d)} \int_0^\infty dr r^{2d-1} \log(1 - z_s e^{-r^2}) \\
 x \stackrel{\text{def}}{=} r^2 \Rightarrow \begin{cases} r = \sqrt{x} \\ dr = \frac{1}{2\sqrt{x}} dx \end{cases} \rightarrow &= \left(\frac{2}{\beta\omega}\right)^d \sum_{s \in \{-1,0,1\}} \frac{2\pi^d}{\Gamma(d)} \int_0^\infty dx \frac{1}{2} x^{-\frac{1}{2}} x^{\frac{2d-1}{2}} \log(1 - z_s e^{-x}) \\
 &= \left(\frac{2}{\beta\omega}\right)^d \sum_{s \in \{-1,0,1\}} \frac{\pi^d}{\Gamma(d)} \int_0^\infty dx x^{d-1} \log(1 - z_s e^{-x}) \\
 \int_0^\infty du u^a \log(1 - ze^{-bu}) = -\frac{\Gamma(a+2)}{b^{a+1}(a+1)} g_{a+2}(z) \rightarrow &= -\left(\frac{2}{\beta\omega}\right)^d \sum_{s \in \{-1,0,1\}} \frac{\pi^d}{\Gamma(d)} \frac{\Gamma(d+1)}{d} g_{d+1}(z_s) \\
 \frac{\Gamma(x+1)}{\Gamma(x)} = x \rightarrow &= -\left(\frac{2\pi}{\beta\omega}\right)^d \sum_{s \in \{-1,0,1\}} g_{d+1}(z_s)
 \end{aligned}$$

Introducing this back into the expression for the partition function we finally obtain

$$\begin{aligned}
 \log Z &= -\log(1 - ze^{\beta\mu_B B}) + \left(\frac{2\pi}{h\beta\omega}\right)^d \sum_{s \in \{-1,0,1\}} g_{d+1}(z_s) \\
 &= -\log(1 - ze^{\beta\mu_B B}) + \left(\frac{k_B T}{\hbar\omega}\right)^d \sum_{s \in \{-1,0,1\}} g_{d+1}(ze^{\beta\mu_B B s}) \quad \checkmark
 \end{aligned}$$

The number of particles N will be

$$N = \begin{cases} N_\epsilon & T \geq T_C \\ N_0 + N_\epsilon & T < T_C \end{cases}$$

where

$$\begin{aligned}
 N_\epsilon &= z \frac{\partial}{\partial z} \log Z_\epsilon \\
 &= z \frac{\partial}{\partial z} \left[\left(\frac{k_B T}{\hbar\omega}\right)^d \sum_{s \in \{-1,0,1\}} g_{d+1}(ze^{\beta\mu_B B s}) \right] \\
 &= \left(\frac{k_B T}{\hbar\omega}\right)^d \sum_{s \in \{-1,0,1\}} g_d(ze^{\beta\mu_B B s})
 \end{aligned}$$

and the expression for N_0 should be

$$\begin{aligned}
 N_0 &= z \frac{\partial}{\partial z} \log Z_0 \\
 &= z \frac{\partial}{\partial z} [-\log(1 - ze^{\beta\mu_B B})] \\
 &= \frac{ze^{\beta\mu_B B}}{1 - ze^{\beta\mu_B B}} \\
 &= \frac{1}{z^{-1}e^{-\beta\mu_B B} - 1}
 \end{aligned}$$

so

$$N = \begin{cases} \left(\frac{k_B T}{\hbar\omega}\right)^d \sum_{s \in \{-1,0,1\}} g_d(ze^{\beta\mu_B B s}) & T \geq T_C \\ \frac{1}{z^{-1}e^{-\beta\mu_B B} - 1} + \left(\frac{k_B T}{\hbar\omega}\right)^d [g_d(e^{-2\beta\mu_B B}) + g_d(e^{-\beta\mu_B B}) + g_d(1)] & T < T_C \quad z = z_{\max} = e^{-\beta\mu_B B} \end{cases} \quad (3)$$

What the professor did for finding N was directly $N = z \frac{\partial}{\partial z} \log Z = \frac{1}{z^{-1}e^{-\beta\mu_B B} - 1} + \left(\frac{k_B T}{\hbar\omega}\right)^d \sum_{s \in \{-1,0,1\}} g_d(ze^{\beta\mu_B B s})$. I really don't know which answer is correct (I guess that the professor's one) because sometimes the answer is just $N = N_\epsilon$, and sometimes it's not.

Item b

First of all we must find the critical temperature. For this task we use the fact that $N(z_{\max}, T_C) = N_\epsilon$ because $N = \begin{cases} N_\epsilon & T \geq T_C \\ N_0 + N_\epsilon & T < T_C \end{cases}$. Remember that $z = \begin{cases} z(T) & T > T_C \\ z_{\max} = e^{\beta\epsilon_{\text{fundamental}}} & T \leq T_C \end{cases}$. Then

$$\begin{aligned} N(z_{\max}, T_C) &= \left(\frac{k_B T_C}{\hbar\omega}\right)^d \sum_{s \in \{-1,0,1\}} g_d(z_{\max} e^{\beta\mu_B B s}) \\ &= \left(\frac{k_B T_C}{\hbar\omega}\right)^d \sum_{s \in \{-1,0,1\}} g_d(e^{-\beta\mu_B B} e^{\beta\mu_B B s}) \\ &= \left(\frac{k_B T_C}{\hbar\omega}\right)^d \sum_{s \in \{-1,0,1\}} g_d(e^{\beta\mu_B B(s-1)}) \\ N &= \left(\frac{k_B T_C}{\hbar\omega}\right)^d [g_d(e^{-2\beta\mu_B B}) + g_d(e^{-\beta\mu_B B}) + g_d(1)] \end{aligned}$$

so the critical temperature is

$$T_C = \left(\frac{N}{g_d(e^{-2\beta\mu_B B}) + g_d(e^{-\beta\mu_B B}) + g_d(1)}\right)^{\frac{1}{d}} \frac{\hbar\omega}{k_B}$$

When $B \rightarrow 0$ the previous equation writes

$$\begin{aligned} T_C &= \left(\frac{N}{3g_d(1)}\right)^{\frac{1}{d}} \frac{\hbar\omega}{k_B} \\ &= \left(\frac{N}{3\zeta(d)}\right)^{\frac{1}{d}} \frac{\hbar\omega}{k_B} \checkmark \end{aligned}$$

When $B \rightarrow \infty$ this is

$$\begin{aligned} T_C &= \left(\frac{N}{g_d(0) + g_d(0) + g_d(1)}\right)^{\frac{1}{d}} \frac{\hbar\omega}{k_B} \\ &= \left(\frac{N}{\zeta(d)}\right)^{\frac{1}{d}} \frac{\hbar\omega}{k_B} \checkmark \end{aligned}$$

Item c

The magnetization is obtained according to

$$\begin{aligned} M &= \frac{1}{N\beta} \frac{\partial}{\partial B} \log Z_{GC} \\ &= \frac{1}{N\beta} \frac{\partial}{\partial B} \left[-\log(1 - ze^{\beta\mu_B B}) + \left(\frac{k_B T}{\hbar\omega}\right)^d \sum_{s \in \{-1,0,1\}} g_{d+1}(ze^{\beta\mu_B B s}) \right] \\ &= \frac{1}{N} \left[\frac{\mu_B}{z^{-1}e^{-\beta\mu_B B} - 1} + \left(\frac{k_B T}{\hbar\omega}\right)^d \sum_{s \in \{-1,0,1\}} \frac{g_d(ze^{\beta\mu_B B s})}{ze^{\beta\mu_B B s}} \mu_B \right] \\ &= \frac{\mu_B}{N} \left[N_0 + \left(\frac{k_B T}{\hbar\omega}\right)^d (-g_d(ze^{-\beta\mu_B B}) + g_d(ze^{\beta\mu_B B})) \right] \end{aligned}$$

Note that is important to replace $N_0 = \frac{1}{z^{-1}e^{-\beta\mu_B B} - 1}$ at this stage because if not, then when we impose $T < T_C$ (and $z = z_{\max}$) this factor goes to infinity. We don't like that.

Now yes, because temperature is below critical then $z = e^{-\beta\mu_B B}$ so

$$\begin{aligned} M &= \frac{\mu_B}{N} \left[N_0 + \left(\frac{k_B T}{\hbar\omega}\right)^d (-g_d(e^{-2\beta\mu_B B}) + g_d(1)) \right] \\ &= \mu_B \left[\frac{N_0}{N} + \frac{1}{N} \left(\frac{k_B T}{\hbar\omega}\right)^d (-g_d(e^{-2\beta\mu_B B}) + \zeta(d)) \right] \end{aligned}$$

The fraction $\frac{N_0}{N}$ can be obtained from $N = N_0 + N_\epsilon \Rightarrow 1 = \frac{N_0}{N} + \frac{N_\epsilon}{N}$ so

$$\begin{aligned} \frac{N_0}{N} &= 1 - \frac{N_\epsilon}{N} \\ &= 1 - \frac{\left(\frac{k_B T}{\hbar \omega}\right)^d [g_d(e^{-2\beta\mu_B B}) + g_d(e^{-\beta\mu_B B}) + g_d(1)]}{\left(\frac{k_B T_C}{\hbar \omega}\right)^d [g_d(e^{-2\beta\mu_B B}) + g_d(e^{-\beta\mu_B B}) + g_d(1)]} \\ &= 1 - \left(\frac{T}{T_C}\right)^d \end{aligned}$$

where we have used (3) to replace N_ϵ and N . Thus

$$M = \mu_B \left[\left(\frac{T}{T_C}\right)^d + \frac{1}{N} \left(\frac{k_B T}{\hbar \omega}\right)^d (-g_d(e^{-2\beta\mu_B B}) + \zeta(d)) \right]$$

The professor has expressed this result in a different way, I think its only a matter of how he wrote things and both answers are OK. For the professor approach you can see my previous resolution of this exercise in page 8.

Problem 2

Item a

The condition for F to be minimum at ψ is

$$dF = 0$$

where

$$dF = \frac{\partial F}{\partial \psi} d\psi + \frac{\partial F}{\partial \psi^*} d\psi^*$$

The first term is

$$\begin{aligned} \frac{\partial F}{\partial \psi} d\psi &= \int d^3r \left[\frac{\hbar^2}{2m} \frac{\partial}{\partial \psi} |\vec{\nabla} \psi|^2 + \frac{a(T - T_C)}{2} \frac{\partial}{\partial \psi} |\psi|^2 + \frac{b}{4} \frac{\partial}{\partial \psi} |\psi|^4 \right] d\psi \\ \frac{\partial}{\partial \psi} |\vec{\nabla} \psi|^2 = \nabla^2 \psi^* \rightarrow &= \int d^3r \left[\frac{\hbar^2}{2m} (\nabla^2 \psi^*) + \frac{a(T - T_C)}{2} \left(\psi \frac{\partial \psi^*}{\partial \psi} + \psi^* \right) + \frac{b}{4} 2 |\psi|^2 \left(\psi \frac{\partial \psi^*}{\partial \psi} + \psi^* \right) \right] d\psi \\ &= \int d^3r \left[\frac{\hbar^2}{2m} (\nabla^2 \psi^*) d\psi + \frac{a(T - T_C)}{2} (\psi d\psi^* + \psi^* d\psi) + \frac{b}{2} |\psi|^2 (\psi d\psi^* + \psi^* d\psi) \right] \\ &= \int d^3r \left[\frac{\hbar^2}{2m} (\nabla^2 \psi^*) d\psi + \left[\frac{a(T - T_C)}{2} + \frac{b}{2} |\psi|^2 \right] (\psi d\psi^* + \psi^* d\psi) \right] \end{aligned}$$

while the second one

$$\begin{aligned} \frac{\partial F}{\partial \psi^*} d\psi^* &= \int d^3r \left[\frac{\hbar^2}{2m} \frac{\partial}{\partial \psi^*} |\vec{\nabla} \psi|^2 + \frac{a(T - T_C)}{2} \frac{\partial}{\partial \psi^*} |\psi|^2 + \frac{b}{4} \frac{\partial}{\partial \psi^*} |\psi|^4 \right] d\psi^* \\ \frac{\partial}{\partial \psi^*} |\vec{\nabla} \psi|^2 = \nabla^2 \psi \rightarrow &= \int d^3r \left[\frac{\hbar^2}{2m} (\nabla^2 \psi) + \frac{a(T - T_C)}{2} \left(\psi + \psi^* \frac{\partial \psi}{\partial \psi^*} \right) + \frac{b}{4} 2 |\psi|^2 \left(\psi + \psi^* \frac{\partial \psi}{\partial \psi^*} \right) \right] d\psi^* \\ &= \int d^3r \left[\frac{\hbar^2}{2m} (\nabla^2 \psi) d\psi^* + \frac{a(T - T_C)}{2} (\psi d\psi^* + \psi^* d\psi) + \frac{b}{2} |\psi|^2 (\psi d\psi^* + \psi^* d\psi) \right] \\ &= \int d^3r \left[\frac{\hbar^2}{2m} (\nabla^2 \psi) d\psi^* + \left[\frac{a(T - T_C)}{2} + \frac{b}{2} |\psi|^2 \right] (\psi d\psi^* + \psi^* d\psi) \right] \end{aligned}$$

Thus

$$\begin{aligned} dF &= \int d^3r \left[\frac{\hbar^2}{2m} (\nabla^2 \psi^*) d\psi + \left[\frac{a(T - T_C)}{2} + \frac{b}{2} |\psi|^2 \right] (\psi d\psi^* + \psi^* d\psi) + \dots \right. \\ &\quad \left. \dots + \frac{\hbar^2}{2m} (\nabla^2 \psi) d\psi^* + \left[\frac{a(T - T_C)}{2} + \frac{b}{2} |\psi|^2 \right] (\psi d\psi^* + \psi^* d\psi) \right] \\ &= \int d^3r \left[\frac{\hbar^2}{2m} (\nabla^2 \psi^* d\psi + \nabla^2 \psi d\psi^*) + \left[a(T - T_C) + b |\psi|^2 \right] (\psi d\psi^* + \psi^* d\psi) \right] \\ &= \int d^3r \left[\left(\frac{\hbar^2}{2m} \nabla^2 \psi^* + \left[a(T - T_C) + b |\psi|^2 \right] \psi^* \right) d\psi + \left(\frac{\hbar^2}{2m} \nabla^2 \psi + \left[a(T - T_C) + b |\psi|^2 \right] \psi \right) d\psi^* \right] \\ z + z^* = 2\text{Re}(z) \rightarrow &= \int d^3r \ 2\text{Re} \left(\left(\frac{\hbar^2}{2m} \nabla^2 \psi + \left[a(T - T_C) + b |\psi|^2 \right] \psi \right) d\psi^* \right) \end{aligned}$$

If $dF = 0$ then its integrand must be null (why?) so

$$\left(\frac{\hbar^2}{2m} \nabla^2 \psi + [a(T - T_C) + b|\psi|^2] \psi \right) d\psi^* = 0$$

Because $d\psi^*$ is not null then $(\dots) = 0$ so

$$\frac{\hbar^2}{2m} \nabla^2 \psi + a(T - T_C) \psi + b|\psi|^2 \psi = 0$$

I don't know why but the professor arrive to the same but with the negative of the first term...

Item b

By art of magic we have that

$$\psi = \sqrt{n_0} e^{i\mathbf{k} \cdot \mathbf{r}}$$

where c is a constant, $\mathbf{k} = \frac{\mathbf{p}}{\hbar} = \frac{m}{\hbar} \mathbf{v}$ and \mathbf{r} is the position. Introducing this into $-\frac{\hbar^2}{m} \nabla^2 \psi + a(T - T_C) \psi + b|\psi|^2 \psi = 0$ we obtain

$$\frac{\hbar^2}{m} \mathbf{k}^2 \sqrt{n_0} e^{i\mathbf{k} \cdot \mathbf{r}} + a(T - T_C) \sqrt{n_0} e^{i\mathbf{k} \cdot \mathbf{r}} + bn_0 \sqrt{n_0} e^{i\mathbf{k} \cdot \mathbf{r}} = 0$$

so

$$\begin{aligned} n_0 &= -\frac{a(T - T_C) + \frac{\hbar^2}{m} \mathbf{k}^2}{b} \\ \mathbf{k} = \frac{m}{\hbar} \mathbf{v} \rightarrow &= -\frac{a(T - T_C) + m\mathbf{v}^2}{b} \checkmark \end{aligned}$$

so

$$\psi = \sqrt{\frac{a(T_C - T) - m\mathbf{v}^2}{b}} \exp\left(i\frac{m}{\hbar} \mathbf{v} \cdot \mathbf{r}\right) \checkmark$$

For finding the maximum value for \mathbf{v} we impose $n_0 > 0$ so

$$|\mathbf{v}| < \sqrt{\frac{a(T_C - T)}{m}} \checkmark$$

Item c

The specific heat can be found using

$$\begin{aligned} C_V &= \left. \frac{\partial E}{\partial T} \right|_{V,N} \\ &= T \left. \frac{\partial S}{\partial T} \right|_{V,N} \\ S = - \left. \frac{\partial F}{\partial T} \right|_{V,N} &\rightarrow = -T \left. \frac{\partial^2 F}{\partial T^2} \right|_{V,N} \end{aligned}$$

From here it is nothing more than doing the math.

6. 29/06/2016 - Segundo intento

La consigna se puede encontrar en la página 13.

Resolution

Problem 1

Item a

Because it is a gas of fermions the partition function will be

$$\log Z = \sum_{\forall \text{monoparticular states}} \log(1 + ze^{-\beta\epsilon_i})$$

The energy levels will be given by

$$\epsilon_i = \frac{\mathbf{p}^2}{2m} + \Delta \mathbf{1}\{\mathbf{q} \in V_\Delta\}$$

where $\mathbf{1}\{x\}$ is the *indicator function* defined as $\mathbf{1}\{x\} \stackrel{\text{def}}{=} \begin{cases} 1 & \text{If } x \text{ is true} \\ 0 & \text{else} \end{cases}$ and V_Δ is the half volume with potential Δ . All the monoparticular states for each fermion are the all the possible combinations of \mathbf{q}, \mathbf{p} and s allowed for each particle. Thus

$$\begin{aligned} \log Z &= \sum_{\forall \mathbf{q}, \mathbf{p}, s} \log \left(1 + ze^{-\beta \left[\frac{\mathbf{p}^2}{2m} + \Delta \mathbf{1}\{\mathbf{q} \in V_\Delta\} \right]} \right) \\ &= \sum_{\forall \mathbf{q}} \sum_{\forall \mathbf{p}} \sum_{\forall s} \log \left(1 + ze^{-\beta \left[\frac{\mathbf{p}^2}{2m} + \Delta \mathbf{1}\{\mathbf{q} \in V_\Delta\} \right]} \right) \end{aligned}$$

where this holds due to the fact that \mathbf{q}, \mathbf{p} and s are all independent of each other. The next step is to consider the spin degeneration and replace the summation over s with g_s ,

$$\log Z = \sum_{\forall \mathbf{q}} \sum_{\forall \mathbf{p}} g_s \log \left(1 + ze^{-\beta \left[\frac{\mathbf{p}^2}{2m} + \Delta \mathbf{1}\{\mathbf{q} \in V_\Delta\} \right]} \right)$$

being $g_s = 2s + 1$. This double summation can be approximated by an integral of the form

$$\begin{aligned}
 \log Z &\approx g_s \int_{\forall \mathbf{q} \in V_\Delta} \int_{\forall \mathbf{p}} \frac{d^d p d^d q}{h^d} \log \left(1 + z e^{-\beta \left[\frac{p^2}{2m} + \Delta \mathbf{1}_{\{\mathbf{q} \in V_\Delta\}} \right]} \right) \\
 &= g_s \int_{\forall \mathbf{q} \in V_\Delta} \int_{\forall \mathbf{q} \notin V_\Delta} \int_{\forall \mathbf{p}} \frac{d^d p d^d q}{h^d} \log \left(1 + z e^{-\beta \left[\frac{p^2}{2m} + \Delta \mathbf{1}_{\{\mathbf{q} \in V_\Delta\}} \right]} \right) \\
 &= g_s \left[\int_{\forall \mathbf{q} \in V_\Delta} \int_{\forall \mathbf{p}} \frac{d^d p d^d q}{h^d} \log \left(1 + z e^{-\beta \left[\frac{p^2}{2m} + \Delta \right]} \right) + \int_{\forall \mathbf{q} \notin V_\Delta} \int_{\forall \mathbf{p}} \frac{d^d p d^d q}{h^d} \log \left(1 + z e^{-\beta \frac{p^2}{2m}} \right) \right] \\
 \int_{\forall \mathbf{q} \in V_\Delta} d^d q = V_\Delta &\rightarrow = \frac{g_s}{h^d} \left[V_\Delta \int_{\forall \mathbf{p}} d^d p \log \left(1 + z e^{-\beta \left[\frac{p^2}{2m} + \Delta \right]} \right) + (V - V_\Delta) \int_{\forall \mathbf{p}} d^d p \left(1 + z e^{-\beta \frac{p^2}{2m}} \right) \right] \\
 z_\Delta \stackrel{\text{def}}{=} z e^{-\beta \Delta} &\rightarrow = \frac{g_s}{h^d} \left[V_\Delta \int_{\forall \mathbf{p}} d^d p \log \left(1 + z_\Delta e^{-\beta \frac{p^2}{2m}} \right) + (V - V_\Delta) \int_{\forall \mathbf{p}} d^d p \left(1 + z e^{-\beta \frac{p^2}{2m}} \right) \right] \\
 d^d p = \frac{2\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}\right)} r^{d-1} dr &\rightarrow = \frac{g_s}{h^d} \frac{2\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}\right)} \left[V_\Delta \int_0^\infty dr r^{d-1} \log \left(1 + z_\Delta e^{-\beta \frac{r^2}{2m}} \right) + (V - V_\Delta) \int_0^\infty dr r^{d-1} \left(1 + z e^{-\beta \frac{r^2}{2m}} \right) \right] \\
 x \stackrel{\text{def}}{=} r^2 \Rightarrow \begin{cases} r = \sqrt{x} \\ dr = \frac{dx}{2\sqrt{x}} \end{cases} &\rightarrow = \frac{g_s}{h^d} \frac{2\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}\right)} \left[V_\Delta \int_0^\infty \frac{dx}{2} x^{-\frac{1}{2}} x^{\frac{d-1}{2}} \log \left(1 + z_\Delta e^{-\frac{\beta}{2m} x} \right) + (V - V_\Delta) \int_0^\infty \frac{dx}{2} x^{-\frac{1}{2}} x^{\frac{d-1}{2}} \left(1 + z e^{-\frac{\beta}{2m} x} \right) \right] \\
 &= \frac{g_s}{h^d} \frac{\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}\right)} \left[V_\Delta \int_0^\infty dx x^{\frac{d}{2}-1} \log \left(1 + z_\Delta e^{-\frac{\beta}{2m} x} \right) + (V - V_\Delta) \int_0^\infty dx x^{\frac{d}{2}-1} \left(1 + z e^{-\frac{\beta}{2m} x} \right) \right] \\
 &= \frac{g_s}{h^d} \frac{\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}\right)} \frac{\Gamma\left(\frac{d}{2} + 1\right)}{\left(\frac{\beta}{2m}\right)^{\frac{d}{2}} \frac{d}{2}} [V_\Delta f_{d/2+1}(z_\Delta) + (V - V_\Delta) f_{d/2+1}(z)]
 \end{aligned}$$

In the last step I have used eq. (4). Now we can apply $\frac{\Gamma(x+1)}{\Gamma(x)} = x$ so everything cancels out and finally

$$\begin{aligned}
 \log Z &= g_s \left(\frac{2\pi m}{h^2 \beta} \right)^{\frac{d}{2}} [V_\Delta f_{d/2+1}(z_\Delta) + (V - V_\Delta) f_{d/2+1}(z)] \\
 &= \frac{g_s}{\lambda^d} [V_\Delta f_{d/2+1}(z_\Delta) + (V - V_\Delta) f_{d/2+1}(z)]
 \end{aligned}$$

For the special case when $V_\Delta = \frac{V}{2}$ and $d = 3$ (as the *consigna* says) this is (replace $z_\Delta = z e^{-\beta \Delta}$)

$$\log Z = g_s \frac{V}{2\lambda^3} [f_{5/2}(z e^{-\beta \Delta}) + f_{5/2}(z)] \quad \checkmark$$

Now we calculate the number of particles of the system. This is

$$\begin{aligned}
 N &= z \frac{\partial}{\partial z} \log Z \\
 &= g_s \frac{V}{2\lambda^3} [f_{3/2}(z e^{-\beta \Delta}) + f_{3/2}(z)]
 \end{aligned}$$

Because the Fermi energy is the chemical potential at temperature $T = 0$ we will use the Sommerfeld's approximation

$f_\nu(z) \approx \frac{(\log z)^\nu}{\Gamma(\nu+1)}$ which is valid for $z \gg 1$ (i.e. at $T \rightarrow 0$). Then

$$\begin{aligned} N &\approx g_s \frac{V}{2\lambda^3} \left[\frac{(\log(ze^{-\beta\Delta}))^{\frac{3}{2}}}{\Gamma(5/2)} + \frac{(\log z)^{\frac{3}{2}}}{\Gamma(5/2)} \right] \\ z = e^{\beta\mu} &\rightarrow = g_s \frac{V}{2\lambda^3} \left[\frac{(\log(e^{\beta(\mu-\Delta)}))^{\frac{3}{2}}}{\Gamma(5/2)} + \frac{(\log e^{\beta\mu})^{\frac{3}{2}}}{\Gamma(5/2)} \right] \\ \lambda = \sqrt{\frac{2\pi\hbar^2\beta}{m}} &\rightarrow = g_s \frac{V}{2} \left(\frac{m}{2\pi\hbar^2\beta} \right)^{\frac{3}{2}} \left[\frac{(\beta(\mu-\Delta))^{\frac{3}{2}}}{\Gamma(5/2)} + \frac{(\beta\mu)^{\frac{3}{2}}}{\Gamma(5/2)} \right] \\ \mu(T \rightarrow 0) = \epsilon_F &\rightarrow = g_s \frac{V}{2\Gamma(5/2)} \left(\frac{m}{2\pi\hbar^2} \right)^{\frac{3}{2}} \left[(\epsilon_F - \Delta)^{\frac{3}{2}} + \epsilon_F^{\frac{3}{2}} \right] \end{aligned}$$

Calling $a \stackrel{\text{def}}{=} \frac{N}{g_s \frac{V}{2\Gamma(5/2)} \left(\frac{m}{2\pi\hbar^2} \right)^{\frac{3}{2}}}$ the previous equation is

$$\epsilon_F^{\frac{3}{2}} + (\epsilon_F - \Delta)^{\frac{3}{2}} = a$$

For $\Delta = 0$ we could consider

$$\begin{aligned} \epsilon_{F0} &= \left(\frac{a}{2} \right)^{\frac{2}{3}} \\ &= \left(\frac{N\Gamma(5/2)}{g_s V} \right)^{\frac{2}{3}} \frac{2\pi\hbar^2}{m} \end{aligned}$$

The *consigna* says that $\Delta \ll \frac{\hbar^2}{2m} \left(\frac{N}{V} \right)^{\frac{2}{3}} \sim \epsilon_{F0}$. Thus, we can consider

$$(\epsilon_F - \Delta)^{\frac{3}{2}} \approx \epsilon_{F0}^{\frac{3}{2}} - \frac{3}{2} \epsilon_{F0}^{\frac{1}{2}} \Delta + \dots$$

so $\epsilon_F^{\frac{3}{2}} + (\epsilon_F - \Delta)^{\frac{3}{2}} = a$ becomes

$$\epsilon_F^{\frac{3}{2}} + \epsilon_{F0}^{\frac{3}{2}} - \frac{3}{2} \epsilon_{F0}^{\frac{1}{2}} \Delta = a$$

and from here, apparently, it can be obtained

$$\epsilon_F \approx \epsilon_{F0} + \frac{\Delta}{2} \checkmark$$

Item b

From the previous item we know

$$\begin{aligned} N &= g_s \frac{V}{2\lambda^3} [f_{3/2}(ze^{-\beta\Delta}) + f_{3/2}(z)] \\ &= N_\Delta + N_0 \end{aligned}$$

For $T \gg \frac{\epsilon_F}{k_B}$ we have $z \rightarrow 0 \Rightarrow f_\nu(z) \approx z$ so

$$\begin{cases} N_\Delta = g_s \frac{V}{2\lambda^3} z e^{-\beta\Delta} \\ N_0 = g_s \frac{V}{2\lambda^3} z \\ N = g_s \frac{V}{2\lambda^3} [z e^{-\beta\Delta} + z] \end{cases}$$

so

$$\frac{N_\Delta}{N} = \frac{1}{1 + e^{\beta\Delta}} \checkmark \quad \frac{N_0}{N} = \frac{1}{e^{-\beta\Delta} + 1} \checkmark$$

When $T \rightarrow \infty$ it is easy to see that $\frac{N_\Delta}{N} = \frac{N_0}{N} = \frac{1}{2}$ what means that the particles distribute indifferently between the two sides of the volume.

For $T \rightarrow 0$ the case is $z \gg 1$ so Sommerfeld applies and, as we have find in the previous item,

$$\begin{aligned} N &= g_s \frac{V}{2\Gamma(5/2)} \left(\frac{m}{2\pi\hbar^2} \right)^{\frac{3}{2}} \left[(\epsilon_F - \Delta)^{\frac{3}{2}} + \epsilon_F^{\frac{3}{2}} \right] \\ &= N_\Delta + N_0 \end{aligned}$$

so

$$\frac{N_\Delta}{N} = \frac{(\epsilon_F - \Delta)^{\frac{3}{2}}}{(\epsilon_F - \Delta)^{\frac{3}{2}} + \epsilon_F^{\frac{3}{2}}} \checkmark \quad \frac{N_0}{N} = \frac{\epsilon_F^{\frac{3}{2}}}{(\epsilon_F - \Delta)^{\frac{3}{2}} + \epsilon_F^{\frac{3}{2}}} \checkmark$$

As $\Delta \rightarrow \epsilon_F$ we see that $\frac{N_\Delta}{N} \rightarrow 0$ and $\frac{N_0}{N} \rightarrow 1$, which means that all the particles will be at the zero potential side.

Item c

The energy is

$$\begin{aligned} U &= - \left. \frac{\partial}{\partial \beta} \right|_{V,z} \log Z \\ &= - \left. \frac{\partial}{\partial \beta} \right|_{V,z} \left(g_s \frac{V}{2\lambda^3} [f_{5/2}(ze^{-\beta\Delta}) + f_{5/2}(z)] \right) \\ \lambda = \sqrt{\frac{2\pi\hbar^2\beta}{m}} \rightarrow &= -g_s \frac{V}{2} \left(\frac{m}{2\pi\hbar^2} \right)^{\frac{3}{2}} \left. \frac{\partial}{\partial \beta} \right|_{V,z} \left(\beta^{-\frac{3}{2}} [f_{5/2}(ze^{-\beta\Delta}) + f_{5/2}(z)] \right) \\ &= -g_s \frac{V}{2} \left(\frac{m}{2\pi\hbar^2} \right)^{\frac{3}{2}} \left(-\frac{3}{2}\beta^{-\frac{5}{2}} [f_{5/2}(ze^{-\beta\Delta}) + f_{5/2}(z)] + \beta^{-\frac{3}{2}} f_{3/2}(ze^{-\beta\Delta}) (-\Delta) \right) \\ &= -g_s \frac{V}{2} \left(\frac{m}{2\pi\hbar^2} \right)^{\frac{3}{2}} \left(-\frac{3}{2}\beta^{-\frac{5}{2}} [f_{5/2}(ze^{-\beta\Delta}) + f_{5/2}(z)] - \beta^{-\frac{3}{2}} \Delta f_{3/2}(ze^{-\beta\Delta}) \right) \end{aligned}$$

The math is a high fiaca...

Problem 2

Item a

The particles have spin 0, thus they are bosons. In consequence the partition function is

$$\begin{aligned} \log Z &= - \sum_{\forall \text{monoparticular state}} \log(1 - ze^{-\beta\epsilon_i}) \\ &= - \sum_{\forall \{n_1, \dots, n_d\}} \log(1 - ze^{-\beta\epsilon(n_1, \dots, n_d)}) \end{aligned}$$

The monoparticular states are given by all the possible combinations of the quantum numbers n_1, \dots, n_d . Because this numbers are all independent one another then

$$\begin{aligned} \log Z &= - \sum_{n_1=0}^{\infty} \dots \sum_{n_d=0}^{\infty} \log(1 - ze^{-\beta\epsilon(n_1, \dots, n_d)}) \\ &= - \sum_{n_1=0}^{\infty} \dots \sum_{n_d=0}^{\infty} \log(1 - ze^{-\beta\hbar\omega(n_1 + \dots + n_d)}) \end{aligned}$$

From now on there are two approaches. One is to consider the change of variable for the summation $n = n_1 + \dots + n_d$ and include the degeneration $g = g(n, d)$ as follows

$$\log Z = - \sum_{n=0}^{\infty} g(n, d) \log(1 - ze^{-\beta\hbar\omega n})$$

This approach is the one I have followed in my previous resolution of this exercise, see page 18.

The other way is to consider the passage to the continuous right now in the next way

$$\begin{aligned} \log Z &= \log Z_{\text{fundamental}} + \log Z_{\text{non fundamental states}} \\ &\approx - \log(1 + z) - \underbrace{\int_{n_1=0}^{\infty} \dots \int_{n_d=0}^{\infty} dn_1 \dots dn_d \log(1 - ze^{-\beta\hbar\omega(n_1 + \dots + n_d)})}_{\boxed{A}} \end{aligned}$$

$$\begin{aligned}
 \boxed{A} &= 2 \int_{a_1=0}^{\infty} \dots \int_{a_d=0}^{\infty} d^d a \, a_1 \dots a_d \log \left(1 - z e^{-\beta \hbar \omega (a_1^2 + \dots + a_d^2)} \right) \leftarrow a_i \stackrel{\text{def}}{=} \sqrt{n_i} \Rightarrow \begin{cases} n_i = a_i^2 \\ dn_i = 2a_i da_i \end{cases} \\
 \text{Sphericals} \rightarrow &= 2 \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2})} \int_0^{\infty} dr \, r^{d-1} a_1 \dots a_d \log \left(1 - z e^{-\beta \hbar \omega r^2} \right)
 \end{aligned}$$

Not this way... I really don't know how to apply the approach for using the surface of the sphere that we are told in the *consigna*.

7. 13/07/2016

Consigna

Problema 1

Considere un gas de N electrones atrapados en una trampa armónica d -dimensional de frecuencia angular ω , sobre el que actúa un campo magnético uniforme de módulo B . Las energías monoparticulares son pues las del oscilador armónico en d dimensiones más un término $\mp\mu B$, donde μ es el momento magnético del electrón y el signo $- (+)$ corresponde a que el espín se oriente paralelo (antiparalelo) al campo. El sistema se encuentra a temperatura 0.

- ¿Qué condición debe satisfacer B para que todos los espines estén orientados paralelamente al campo?
- Calcule la energía de Fermi en el caso $B = 0$.
- Calcule la susceptibilidad magnética del gas. Discuta su resultado.

Ayuda: según cómo afronte el problema le será útil saber que el volumen de una esfera de radio 1 en un espacio de $2d$ dimensiones es $\frac{\pi^d}{d!}$, o bien que $\frac{(m+k)!}{m!} \approx m^k$ cuando $m \gg k$.

Problema 2

Considere un gas de partículas idénticas de espín 0 y masa m contenido en un recipiente cilíndrico de altura L , en presencia del campo gravitatorio terrestre.

- Calcule la función de partición gran canónica del sistema en términos de sus variables naturales y la función $g_{5/2}$.
- Pruebe que la temperatura crítica satisface $T_C > T_C^0$ donde T_C^0 es la temperatura crítica en ausencia de gravedad. Discuta cualitativamente por qué es así.
- Suponiendo que $mgL \ll k_B T_C^0$, donde g es la aceleración de la gravedad, calcule la temperatura crítica en términos de T_C^0 , incluyendo la primera corrección debida al campo gravitatorio.

Ayuda: $g_{3/2}(e^{-\alpha}) \approx \zeta(3/2) - 2\sqrt{\pi\alpha}$ para $\alpha \ll 1$.

Problema 3

Considere una cadena de Ising unidimensional, cerrada, sin campo magnético, formada por N espines y con constante de acoplo adimensional $\beta J = K$.

- Si ℓ es un divisor de N , pruebe que los espines ubicados en las posiciones $\ell, 2\ell, \dots, N$ (es decir, las posiciones múltiplos de ℓ) se comportan como una nueva cadena de Ising con constante de acoplo adimensional K' dada por

$$\tanh K' = (\tanh K)'$$

Ayuda: escriba las probabilidades en términos de la matriz de transferencia. Va a tener que calcular sus autovalores.

- Encuentre los puntos fijos y estudie su estabilidad.

Problem 1

Item a

First off all, as always, we need the partition function. Because electrons are fermions then

$$\log Z = \sum_{\forall \text{monoparticular state}} \log (1 + ze^{-\beta \epsilon_i})$$

Although the *consigna* says that the monoparticular energies are just $\epsilon = \hbar\omega (n_1 + \dots + n_d) + s\mu B$ ($s = \pm 1$ indicates the direction of the spin) I think they are

$$\epsilon = \frac{\mathbf{p}^2}{2m} + \hbar\omega (n_1 + \dots + n_d) + s\mu B$$

because we are dealing with a gas. Unfortunately, in the real exam I have used the first one ☹. Hope it's OK. Then we can calculate the partition function as

$$\begin{aligned} \log Z &= \sum_{\forall \mathbf{q}, \mathbf{p}, \{n_i\}, s} \log (1 + ze^{-\beta \epsilon(\mathbf{q}, \mathbf{p}, n_1, \dots, n_d, s)}) \\ &= \sum_{\forall \mathbf{q}} \sum_{\forall \mathbf{p}} \sum_{\forall \{n_i\}} \sum_{\forall s} \log (1 + ze^{-\beta \epsilon(\mathbf{q}, \mathbf{p}, n_1, \dots, n_d, s)}) \\ &\approx \int_{\forall \mathbf{q}} \int_{\forall \mathbf{p}} \frac{d^d q d^d p}{h^d} \sum_{\forall \{n_i\}} \sum_{\forall s} \log (1 + ze^{-\beta \epsilon(\mathbf{q}, \mathbf{p}, n_1, \dots, n_d, s)}) \end{aligned}$$

where the last approximation is due to the magical quantum mechanical stuff.

Now we can consider the change of variable $m \stackrel{\text{def}}{=} n_1 + \dots + n_n$ so that

$$\log Z = \int_{\forall \mathbf{q}} \int_{\forall \mathbf{p}} \frac{d^d q d^d p}{h^d} \sum_{m=0}^{\infty} \sum_{\forall s} g(m, d) \log \left(1 + ze^{-\beta \left[\frac{\mathbf{p}^2}{2m} + \hbar\omega m + s\mu B \right]} \right)$$

where $g(m, d)$ is the degeneration, which is

$$g(m, d) = \binom{m + d - 1}{m}$$

because it is the number of ways that identical energy quanta can be distributed in numbered boxes n_1, n_2, \dots, n_d . Then

$$\begin{aligned} \log Z &= \frac{1}{(d-1)!} \int_{\forall \mathbf{q}} \int_{\forall \mathbf{p}} \frac{d^d q d^d p}{h^d} \sum_{m=0}^{\infty} \sum_{\forall s} \frac{(m + d - 1)!}{m!} \log \left(1 + ze^{-\beta \left[\frac{\mathbf{p}^2}{2m} + \hbar\omega m + s\mu B \right]} \right) \\ \text{Help from } \textit{consigna} \rightarrow &\approx \frac{1}{(d-1)!} \int_{\forall \mathbf{q}} \int_{\forall \mathbf{p}} \frac{d^d q d^d p}{h^d} \int_0^{\infty} dm \sum_{\forall s} m^{d-1} \log \left(1 + ze^{-\beta \left[\frac{\mathbf{p}^2}{2m} + \hbar\omega m + s\mu B \right]} \right) \end{aligned}$$

where I have used the help from *consigna* just because otherwise I don't know how to continue with the calculation. So

$$\begin{aligned} \log Z &= \frac{1}{(d-1)!} \int_{\forall \mathbf{q}} \int_{\forall \mathbf{p}} \frac{d^d q d^d p}{h^d} \int_0^{\infty} dm \sum_{\forall s} m^{d-1} \log \left(1 + ze^{-\beta \left[\frac{\mathbf{p}^2}{2m} + \hbar\omega m + s\mu B \right]} \right) \\ z_{ms} \stackrel{\text{def}}{=} ze^{-\beta(\hbar\omega m + s\mu B)} \rightarrow &= \frac{1}{(d-1)!} \int_{\forall \mathbf{q}} \int_{\forall \mathbf{p}} \frac{d^d q d^d p}{h^d} \int_0^{\infty} dm \sum_{\forall s} m^{d-1} \log \left(1 + z_{ms} e^{-\beta \frac{\mathbf{p}^2}{2m}} \right) \\ &= \frac{V}{(d-1)! h^d} \sum_{\forall s} \int_0^{\infty} dm m^{d-1} \int_{\forall \mathbf{p}} d^d p \log \left(1 + z_{ms} e^{-\beta \frac{\mathbf{p}^2}{2m}} \right) \\ d^d p = \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2})} r^{d-1} dr \rightarrow &= \frac{V}{(d-1)! h^d} \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2})} \sum_{\forall s} \int_0^{\infty} dm m^{d-1} \int_0^{\infty} dr r^{d-1} \log \left(1 + z_{ms} e^{-\beta \frac{r^2}{2m}} \right) \end{aligned}$$

where in the last equality I have just changed variable to spherical coordinates. Thus

$$\begin{aligned}
 \log Z &= \frac{V}{(d-1)!h^d} \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2})} \sum_{\forall s} \int_0^\infty dm m^{d-1} \int_0^\infty \frac{dx}{2} \underbrace{x^{-\frac{1}{2}} x^{\frac{d-1}{2}}}_{x^{\frac{d}{2}-1}} \log(1 + z_{ms} e^{-\beta \frac{x}{2m}}) \leftarrow x \stackrel{\text{def}}{=} r^2 \Rightarrow \begin{cases} r = \sqrt{x} \\ dr = \frac{dx}{2\sqrt{x}} \end{cases} \\
 &= \frac{V}{(d-1)!h^d} \frac{\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2})} \sum_{\forall s} \int_0^\infty dm m^{d-1} \frac{\Gamma(\frac{d}{2} + 1)}{\left(\frac{\beta}{2m}\right)^{\frac{d}{2}} \frac{d}{2}} f_{d/2+1}(z_{ms}) \\
 &= \frac{V}{(d-1)!} \underbrace{\left(\frac{2\pi m}{h^2 \beta}\right)^{\frac{d}{2}}}_{\lambda^{-d}} \sum_{\forall s} \int_0^\infty dm m^{d-1} \underbrace{\frac{\Gamma(\frac{d}{2} + 1)}{\Gamma(\frac{d}{2}) \frac{d}{2}}}_{=1} f_{d/2+1}(z_{ms}) \\
 &= \frac{V}{\lambda^d} \frac{1}{(d-1)!} \sum_{\forall s} \int_0^\infty dm m^{d-1} f_{d/2+1}\left(ze^{-\beta(\hbar\omega m + s\mu B)}\right)
 \end{aligned}$$

How to go on?

8. Resumen de fórmulas y cosas

Matemáticas

$$\text{Serie geométrica} \rightarrow \sum_{k=0}^{n-1} r^k = \frac{1-r^n}{1-r} \quad \frac{(m+k)!}{m!} \xrightarrow{m \gg k} m^k$$

$\sinh x = \frac{e^x - e^{-x}}{2}$	$\tanh x = \frac{\sinh x}{\cosh x}$	$\sinh x \xrightarrow{x \ll 1} x + \frac{x^3}{3!}$	$\frac{\partial \cosh x}{\partial x} = +\sinh x$	$\frac{\partial \tanh x}{\partial x} = \frac{2}{\cosh(2x) + 1} = \frac{1}{\cosh^2 x}$
$\cosh x = \frac{e^x + e^{-x}}{2}$	$\coth x = \frac{1}{\tanh x}$	$\coth x \xrightarrow{x \ll 1} \frac{1}{x} + \frac{x}{3}$	$\frac{\partial \coth x}{\partial x} = -\frac{1}{\sinh^2 x}$	

$$d^d p = \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2})} r^{d-1} dr \rightarrow \text{Pasaje a esféricas en } d \text{ dimensiones}$$

$$\frac{\Gamma(x+1)}{\Gamma(x)} = x \quad \Gamma(n) = (n-1)! \quad \begin{cases} \Gamma\left(\frac{3}{2}\right) = \frac{\pi^{1/2}}{2} \\ \Gamma\left(\frac{5}{2}\right) = \frac{3}{4}\pi^{1/2} \end{cases}$$

Truco para calcular gaussianas

$$I_\alpha = \int_0^\infty x^\alpha e^{-\gamma x^2} dx$$

$I_{\alpha=0} = \frac{1}{2}\sqrt{\frac{\pi}{\gamma}}$	$I_{\alpha=1} = \frac{1}{2\gamma}$
$I_{\alpha=2} = \frac{1}{2}\sqrt{\frac{\pi}{\gamma^3}}$	

$$I_{\alpha=n \in \mathbb{N}^\circ \text{ pares}} = -\frac{d^n I_{\alpha=0}}{d\gamma^n} \quad I_{\alpha=n \in \mathbb{N}^\circ \text{ impares}} = \frac{d^n I_{\alpha=1}}{d\gamma^n}$$

$\Psi = ae^{i\mathbf{k} \cdot \mathbf{r}} \rightarrow$ Partícula libre

$$\begin{cases} \delta |\vec{\nabla} \Psi|^2 = \vec{\nabla} \Psi^* \cdot \vec{\nabla} \delta \Psi + \vec{\nabla} \Psi \cdot \vec{\nabla} \delta \Psi^* \\ \delta |\Psi|^2 = \Psi^* \delta \Psi + \Psi \delta \Psi^* \\ \vec{\nabla} \Psi^* \cdot \vec{\nabla} \delta \Psi = -\nabla^2 \Psi^* \delta \Psi + \vec{\nabla} \cdot (\vec{\nabla} \Psi^* \delta \Psi) \end{cases}$$

Función g_ν

Se define

$$g_\nu(z) \stackrel{\text{def}}{=} \frac{1}{\Gamma(\nu)} \int_0^\infty dx \frac{x^{\nu-1}}{z^{-1}e^x - 1}$$

y la fórmula que siempre usamos es

$$\int_0^\infty du u^a \log(1 - ze^{-bu}) = -\frac{\Gamma(a+2)}{b^{a+1}(a+1)} g_{a+2}(z)$$

Tiene las siguientes propiedades

- Son todas crecientes.
- $\frac{\partial g_\nu}{\partial z} = \frac{g_{\nu-1}}{z}$.
- $g_\nu(z) \xrightarrow{z \rightarrow 0} z$.
- $g_\nu(z=1) \begin{cases} \infty & \nu \leq 1 \\ \zeta(\nu) & \nu > 1 \end{cases}$ donde $\zeta(\nu) = \sum_{n \in \mathbb{N}} \frac{1}{n^\nu}$ es la función zeta de Riemann.

Función f_ν

Se define

$$f_\nu(z) \stackrel{\text{def}}{=} \frac{1}{\Gamma(\nu)} \int_0^\infty dx \frac{x^{\nu-1}}{z^{-1}e^x + 1}$$

y la fórmula que usamos siempre es (ver deducción en pág. 35)

$$\int_0^\infty du u^a \log(1 + ze^{-bu}) = \frac{\Gamma(a+2)}{b^{a+1}(a+1)} f_{a+2}(z) \quad (4)$$

Sus propiedades son

- $f'_\nu(z) = \frac{f_{\nu-1}(z)}{z}$.
- $f_\nu(z) \xrightarrow{z \ll 1} z$ (o sea altas temperaturas).
- Para $z \gg 1$ (o sea bajas temperaturas) tenemos la aproximación de Sommerfeld que es

$$f_\nu(z) = \frac{(\log z)^\nu}{\Gamma(\nu+1)} \left[1 + \frac{\pi^2}{6} \frac{\nu(\nu-1)}{(\log z)^2} + \mathcal{O}((\log z)^{-3}) \right]$$

Ensamble gran canónico

$$Z_{GC} = \sum_{\forall \text{ estados}} e^{-\beta(\epsilon_i - \mu N_i)}$$

$$\langle N \rangle = z \frac{\partial}{\partial z} \log Z_{GC} \quad \langle N \rangle = \sum_{\forall \text{ monoparticular state}} \langle N_i \rangle \quad \text{with } \langle N_i \rangle = z \frac{\partial}{\partial z} \log Z_{\text{monoparticular } i}$$

$$M = \frac{1}{N\beta} \frac{\partial}{\partial B} \log Z_{GC}$$

$$U = - \left. \frac{\partial}{\partial \beta} \right|_{V,z} \log Z_{GC}$$

$$\Xi = \begin{cases} -PV \\ -k_B T \log Z_{GC} \end{cases}$$

$$\lambda \stackrel{\text{def}}{=} \sqrt{\frac{2\pi\hbar^2}{mk_B T}} = \sqrt{\frac{2\pi\hbar^2\beta}{m}} = \sqrt{\frac{\hbar^2\beta}{2\pi m}}$$

Teorema de partículas indistinguibles y no interactuantes.

Si se tiene un sistema de partículas indistinguibles y no interactuantes entre sí entonces su función de partición gran canónica se puede factorizar según

$$\log Z_{GC} = \sum_{\forall \text{ monoparticular state } i} \log Z_i \quad Z_i = \sum_{\forall \text{ allowed particles } n} (ze^{-\beta\epsilon_i})^n$$

donde $z \stackrel{\text{def}}{=} e^{\beta\mu}$ es la fugacidad (μ el potencial químico) y

$$\forall \text{ allowed particles } n = \begin{cases} \{0, 1\} & \text{Fermions} \\ \{0, 1, 2, \dots, \infty\} & \text{Bosons} \end{cases}$$

son las cantidades de partículas permitidas para cada estado monoparticular. Los estados monoparticulares son los estados en que puede estar cada una de las partículas¹⁶ (creo que son algo así como las celdas del espacio de fases).

Fermiones

$$\epsilon_F(V, N) \stackrel{\text{def}}{=} \lim_{T \rightarrow 0} \mu(T, V, N) \rightarrow \text{Is this ok?}$$

$$\log Z_{GC} = g_s \frac{V}{\lambda^d} f_{d/2+1}(z) \rightarrow \text{Ideal gas in } d \text{ dimensions}$$

¹⁶Spin up o down son, por ejemplo, dos estados monoparticulares.

Bosones

$$\log Z_{CG} = - \sum_{\forall \text{monoparticular state}} \log(1 - ze^{-\beta\epsilon_i})$$

$$N = \begin{cases} N_\epsilon & T \geq T_C \\ N_0 + N_\epsilon & T < T_C \end{cases}$$

$$z = \begin{cases} z(T) & T > T_C \\ z_{\max} = e^{\beta\epsilon_{\text{fundamental}}} & T \leq T_C \end{cases}$$

Ising

$$\mathcal{H} = \begin{cases} -J \sum_{\langle i,j \rangle} s_i s_j - \mu B \sum_{\forall i} s_i \\ -\frac{J}{2} \sum_{\forall i} \sum_{j \in J_i^+} s_i s_j - \mu B \sum_{\forall i} s_i \end{cases}$$

$$\mathcal{H}_{\text{mean field}} = -J |\mathbb{V}| \bar{s} \sum_{\forall i} s_i + \frac{J}{2} \bar{s}^2 N |\mathbb{V}| - \mu B \sum_{\forall i} s_i$$

$$\mathcal{H}_{\text{all system}} = \sum_{\forall \text{cells}} \mathcal{H}_{\text{cell } i}$$

$$\mathcal{H}_{\text{one cell}} = -\frac{J}{2} \sum_{\forall i \in \text{cell}} \sum_{j \in \mathbb{V}_i^{\text{internal}}} s_i s_j - J |\mathbb{V}_{\text{external}}| \left(\bar{s} \sum_{\forall i \in \text{cell}} s_i + \frac{|\text{cell}|}{2} \bar{s}^2 \right) - \mu B \sum_{\forall i \in \text{cell}} s_i$$

$$\langle s \rangle = \frac{1}{|\text{cell}| \beta \mu} \frac{\partial}{\partial B} \log Z_{\text{cell}} \quad \bar{s} = \langle s \rangle \quad \leftarrow \text{Autoconsistencia en campo medio}$$