Solution, Exam TFY4230
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1a)

$$\beta p V = \sum_k \ln\left(1+e^{-\beta(\varepsilon_k-\mu)}\right)$$

$$= \int d\varepsilon \underbrace{\sum_k \delta(\varepsilon-\varepsilon_k)}_{=g(\varepsilon)} \ln\left(1+e^{-\beta(\varepsilon-\mu)}\right)$$

$$= \int d\varepsilon\, g(\varepsilon) \ln\left(1+e^{-\beta(\varepsilon-\mu)}\right)$$

$$\langle N\rangle = \frac{\partial \ln Z_g}{\partial \beta\mu} = \frac{\partial(\beta p V)}{\partial(\beta\mu)}$$

$$= \int d\varepsilon\, g(\varepsilon) \frac{e^{-\beta(\varepsilon-\mu)}}{1+e^{-\beta(\varepsilon-\mu)}}$$

$$= \int d\varepsilon \frac{g(\varepsilon)}{e^{\beta(\varepsilon-\mu)}+1}$$

From the above, we have also

$$\langle N\rangle = \sum_k \langle n_k\rangle$$

where

$$\langle n_k\rangle = \frac{1}{e^{\beta(\varepsilon_k-\mu)}+1}$$

The Hamiltonian of the system is given $\hat{H} = \sum_k \varepsilon_k \hat{n}_k$ with eigenvalues $E = \sum_k \varepsilon_k n_k$; $n_k = 0, 1$.

$$U = \langle E \rangle = \sum_k \varepsilon_k \langle n_k \rangle$$

$$= \sum_k \varepsilon_k \frac{1}{e^{\beta(\varepsilon_k - \mu)} + 1}$$

Gjennomgående feil
$U = -\frac{\partial \ln Z_g}{\partial \beta}$!! ..

$$= \int d\varepsilon \, \frac{g(\varepsilon)\, \varepsilon}{e^{\beta(\varepsilon - \mu)} + 1}$$

b)

To obtain the connection between U and pV, we transform the expression we found for $\beta p V$ by a partial integration:

$$\beta p V = \Big| G(\varepsilon) \ln\left(1 + e^{-\beta(\varepsilon - \mu)}\right) \Big|_0^\infty$$

$$+ \beta \int_0^\infty d\varepsilon \frac{G(\varepsilon)}{e^{\beta(\varepsilon - \mu)} + 1} = \beta \int_0^\infty d\varepsilon \frac{G(\varepsilon)}{e^{\beta(\varepsilon - \mu)} + 1}$$

NB!!

where $G'(\varepsilon) = g(\varepsilon)$

With a $g(\varepsilon)$ of the form

$$g(\varepsilon) = A\,\varepsilon^{\alpha}\,\theta(\varepsilon),$$ we have

$$G(\varepsilon) = \frac{1}{\alpha+1} A\,\varepsilon^{\alpha+1}\,\theta(\varepsilon)$$

$$g(\varepsilon)\,\varepsilon = A\,\varepsilon^{\alpha+1}\,\theta(\varepsilon)$$

Hence, we have $G(\varepsilon) = \frac{g(\varepsilon)\,\varepsilon}{\alpha+1}$

$$pV = \int_0^\infty d\varepsilon\,\frac{G(\varepsilon)}{e^{\beta(\varepsilon-\mu)}+1} = \frac{1}{\alpha+1}\int_0^\infty d\varepsilon\,\frac{g(\varepsilon)\,\varepsilon}{e^{\beta(\varepsilon-\mu)}+1}$$

$$= \frac{1}{\alpha+1}\,U = K\,U$$

$$K = \frac{1}{\alpha+1}$$

In the present case, $\alpha = 0 \Rightarrow$

$$K = 1$$

c)

$$pV = V\,\frac{2\pi m}{h^2}\int_0^{\infty} d\varepsilon\,\frac{\varepsilon}{e^{\beta(\varepsilon-\mu)}+1}$$

T = 0:

$$\frac{1}{e^{\beta(\varepsilon-\mu)}+1} = \begin{cases} 1 & ; \quad \varepsilon < \mu \\ 0 & ; \quad \varepsilon > \mu \end{cases}$$

$$p = \frac{2\pi m}{h^2}\int_0^{\mu} d\varepsilon\,\varepsilon = \underline{\frac{\pi m}{h^2}\mu^2}$$

$$\langle N\rangle = V\,\frac{2\pi m}{h^2}\int_0^{\mu} d\varepsilon = V\,\frac{2\pi m}{h^2}\,\mu$$

$$\mu = \rho\,\frac{h^2}{2\pi m}$$

$$p = \frac{\pi m}{h^2}\left(\frac{h^2}{2\pi m}\right)^2 \rho^2 =$$

$$= \underline{\frac{h^2}{4\pi m}\,\rho^2}$$

We see that since $p \sim h^2$, $p \neq 0$ at $T = 0$ is a quantum effect.

$p \sim U$

Due to the Pauli-principle, $U > 0, T = 0$, because all except one particle has to have an ε_k with $\varepsilon_k > 0$.
The finite pressure at $T = 0$ thus originates with the fact that at most one fermion can occupy a single-particle state.

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a)

$$H = -\vec{h} \cdot \sum_{i=1}^{N} \vec{S}_i$$

Ising case $\quad H = -h\sum_{i=1}^{N} \sigma_i \quad ; \quad \sigma_i = \pm 1$

Heisenberg case $\quad H = -hS\sum_{i=1}^{N} \cos\theta_i \; ; \; \theta_i \in [0, \pi)$

$$Z = \sum_{\{\vec{S}_i\}} e^{-\beta H}$$

$$= \sum_{\{\sigma_i\}} e^{\beta h S \sum_{i=1}^{N} \sigma_i} \qquad \text{(Ising)}$$

$$= \sum_{\{\theta_i, \varphi_i\}} e^{\beta h S \sum_i \cos\theta_i} \qquad \text{(Heisenberg)}$$

Ising - case :

$$Z = \prod_{i=1}^{N} \left(\sum_{\sigma_i = \pm 1} e^{\beta h S \sigma_i} \right)$$

$$= \prod_{i=1}^{N} \left(2\cosh(\beta h S) \right)$$

$$= \left(2\cosh(\beta h S) \right)^N$$

$$\cosh x = \frac{1}{2}\left(e^{x} + e^{-x}\right)$$

Heisenberg-case:

$$Z = \sum_{\{\theta_i, \varphi_i\}} e^{\beta h S \sum_{i=1}^{N} \cos\theta_i}$$

$$= \prod_{i=1}^{N} \sum_{\varphi_i} \sum_{\theta_i} e^{\beta h S \cos\theta_i}$$

$$= \prod_{i=1}^{N} 2\pi \int_0^{\pi} d\theta_i \sin\theta_i \, e^{\beta h S \cos\theta_i}$$

$$= \prod_{i=1}^{N} 2\pi \int_{-1}^{1} dx_i \, e^{-\beta h S x_i} \quad ; \; x_i = -\cos\theta_i$$

$$dx_i = \sin\theta_i \, d\theta_i$$

$$= \prod_{i=1}^{N} \left(-\frac{2\pi}{\beta h S} \cdot \Big|_{-1}^{1} e^{-\beta h S x_i} \right)$$

$$= \prod_{i=1}^{N} \left(\frac{2\pi}{\beta h S} \cdot 2\sinh(\beta h S) \right)$$

$$= \left(4\pi \frac{\sinh(\beta h S)}{\beta h S} \right)^N$$

b)

$$H_e = -\frac{\partial \ln Z}{\partial \beta}$$

$$= -N \frac{\partial \ln(F(\beta h S))}{\partial \beta}$$

$$= -NhS \frac{\partial \ln F(x)}{\partial x} \quad ; \quad x = \beta h S$$

$$= -NhS \frac{F'(x)}{F(x)}$$

Ising-case: $F(x) = 2\cosh x$

$$F'(x) = 2\sinh x$$

$$\frac{F'}{F} = \tanh x$$

$$H_e = -NhS \tanh(\beta h S)$$

Heisenberg-case: $F(x) = 4\pi \frac{\sinh x}{x}$

$$F'(x) = \frac{4\pi}{x^2}(x\cosh x - \sinh x)$$

$$H_e = -NhS\left(\frac{x\coth x - 1}{x}\right) \quad ; \quad x = \beta h S$$

c) $C_h = -k_B \beta^2 \left(\frac{\partial H_e}{\partial \beta}\right)_h$

$$= -k_B \beta^2 \frac{\partial}{\partial \beta}\left(-\frac{1}{Z}\frac{\partial Z}{\partial \beta}\right)_h$$

$$= +k_B \beta^2 \left(\frac{1}{Z}\frac{\partial^2 Z}{\partial \beta^2} - \left(\frac{1}{Z}\frac{\partial Z}{\partial \beta}\right)^2\right)$$

$$\frac{1}{Z}\frac{\partial Z}{\partial \beta} = -\langle H \rangle$$

$$\frac{1}{Z}\frac{\partial^2 Z}{\partial \beta^2} = \langle H^2 \rangle$$

$$\underline{\underline{C_h = k_B \beta^2 \left[\langle H^2 \rangle - \langle H \rangle^2\right]}}$$

This shows that the heat-capacity of the system originates with the energy-fluctuations of the system. This follows from the fact that

$\langle H^2 \rangle - \langle H \rangle^2 = \langle (H - \langle H \rangle)^2 \rangle$

which is the variance of the energy, i.e. a measure of the magnitude of the fluctuations in the energy around its average value.

d) Specific heat

$$C_h = \left(\frac{\partial H_e}{\partial T}\right)_h = -k_B \beta^2 \left(\frac{\partial H_e}{\partial \beta}\right)_h$$

Ising-case:

$$C_h = -k_B \beta^2 (-NhS)\, hS \left(\frac{\partial H_e}{\partial x}\right)_h \; ; \quad x = \beta h S$$

$$= N k_B (\beta h S)^2 \underbrace{\frac{d \tanh x}{dx}}_{= \frac{1}{\cosh^2 x}}$$

$$= \frac{N k_B (\beta h S)^2}{\cosh^2(\beta h S)} \overset{x \gg 1}{\simeq} 4 N k_B\, x^2 e^{-2x} \; ; \quad x = \beta h S$$

$$\xrightarrow{T \to 0} 0$$

Heisenberg-case

$$C_h = N k_B (\beta h S)^2 \underbrace{\frac{d}{dx}\left(\coth x - \frac{1}{x}\right)}_{\frac{1}{x^2} - \frac{1}{\sinh^2 x}}$$

$$= N k_B\, x^2 \left(\frac{1}{x^2} - \frac{1}{\sinh^2 x}\right) \; ; \quad x = \beta h S$$

$x \gg 1 \Rightarrow$

$\underline{\underline{C_h = N k_B}}$

For the Ising case, the specific heat vanishes at $T \to 0$

For the Heisenberg case, it is nonzero.

The reason for this is that spin-fluctuations (which give energy fluctuations and therefore specific heat) are frozen out in the Ising model at low T:

$\downarrow \to \uparrow$ or $\uparrow \to \downarrow$

Such a spin-flip requires a finite energy $2hS$, which is not available at low T.

In the Heisenberg-model, spins can point in any direction, and even arbitrarily small deviations from the direction of the magnetic field is allowed. This gives energy fluctuations and therefore specific heat at arbitrarily low T. There is an energy-gap in the spin-excitation spectrum of the Ising-model, but there is no such gap in the Heisenberg-model

3a

$$U = \langle H \rangle = \frac{1}{Z} \frac{1}{h^{2N} N!} \int d\Gamma \, H e^{-\beta H}$$

$$= \frac{1}{Z} \left(-\frac{\partial}{\partial \beta}\right) \underbrace{\frac{1}{h^{2N} N!} \int d\Gamma \, e^{-\beta H}}_{= Z}$$

$$U = -\frac{1}{Z} \frac{\partial Z}{\partial \beta} = - \frac{\partial \ln Z}{\partial \beta}$$

b)
$$Z = \frac{1}{h^{2N} N!} \int \cdots \int \prod_{i=1}^{N} d^2 p_i \, d^2 r_i \, e^{-\beta \sum_{i=1}^{N} \left(\frac{\vec{p}_i^{\,2}}{2m} + V_0 r_i\right)}$$

$$= \frac{1}{h^{2N} N!} \prod_{i=1}^{N} \int d^2 p_i \, e^{-\beta \frac{\vec{p}_i^{\,2}}{2m}} \int d^2 r_i \, e^{-\beta V_0 r_i}$$

$$= \frac{1}{h^{2N} N!} \Bigg(\underbrace{\int d^2 p \, e^{-\beta \frac{\vec{p}^{\,2}}{2m}}}_{= I} \Bigg)^N \Bigg(\underbrace{\int d^2 r \, e^{-\beta V_0 r}}_{= Q} \Bigg)^N$$

$$I = \int_{-\infty}^{\infty} dp_x \int_{-\infty}^{\infty} dp_y \, e^{-\frac{\beta}{2m}(p_x^2 + p_y^2)}$$

$$= I_0^2 \, ; \quad I_0 = \int_{-\infty}^{\infty} dp_x \, e^{-\frac{\beta}{2m} p_x^2}$$

$$= \sqrt{\frac{2\pi m}{\beta}}$$

$$I = 2\pi m k_B T \Rightarrow$$

$$\frac{I^N}{h^{2N}} = \left(\frac{2\pi m k_B T}{h^2}\right)^N = \frac{1}{\lambda^{2N}}$$

$$\lambda \equiv \frac{h}{\sqrt{2\pi m k_B T}} \Rightarrow$$

$$\left.\begin{aligned} Z &= \frac{1}{N!}\frac{1}{\lambda^{2N}} Q_1^N \\ Q_1 &= \int d^2r\, e^{-\beta V_0 r} \end{aligned}\right\} \quad \text{q.e.d}$$

c

$$Q_1 = 2\pi \int_0^R dr\, r\, e^{-\beta V_0 r}$$

$$= 2\pi R_0^2 \int_0^{R/R_0} dx\, x\, e^{-x}$$

$$= -2\pi R_0^2 \Big/_0^{R/R_0} e^{-x}(x+1)$$

$$= -2\pi R_0^2 \left[e^{-\frac{R}{R_0}}\left(\frac{R}{R_0}+1\right) - 1 \right]$$

$$Q_1 = 2\pi R_0^2 \left(1 - e^{-\frac{R}{R_0}}\left(\frac{R}{R_0}+1\right)\right)$$

$$\frac{R}{R_0} \gg 1 \Rightarrow Q_1 \simeq 2\pi R_0^2 = \frac{2\pi}{(\beta V_0)^2}$$

$$\frac{R}{R_0} \ll 1 \Rightarrow Q_1 = 2\pi R_0^2 \ \frac{1}{2}\left(\frac{R}{R_0}\right)^2 = \pi R^2 = V$$

This follows from:

$$1-(1+x)e^{-x} \simeq 1-(1+x)\left(1-x+\frac{x^2}{2}+\cdots\right)$$

$$\simeq 1-\left(1-x+\frac{x^2}{2}\right)-x(1-x)+\mathcal{O}(x^3)$$

$$= 1-1+x-\frac{x^2}{2}-x+x^2 = \frac{x^2}{2}.$$

$$\frac{R}{R_0} \ll 1 \Rightarrow Z \ \frac{V^N}{N!\,\lambda^{2N}} \Rightarrow$$

$$U = -\frac{\partial}{\partial\beta}\ln Z = N\frac{\partial \ln\lambda^2}{\partial\beta} = N\frac{\partial \ln\beta}{\partial\beta} = \frac{N}{\beta}$$

$$\underline{U = N k_B T} \ ; \ \frac{R}{R_0} \ll 1$$

$$\frac{R}{R_0} \gg 1 \Rightarrow Z = \frac{1}{N!}\frac{1}{\lambda^{2N}}\left(\frac{2\pi}{(\beta V_0)^2}\right)^N$$ ← NB!!

$$U = -\frac{\partial}{\partial\beta}\ln Z = N\frac{\partial\ln\lambda^2}{\partial\beta} + N\frac{\partial \ln\beta^2}{\partial\beta}$$

$$= N k_B T + 2 N k_B T$$

$$\underline{U = 3 N k_B T} \ ; \ \frac{R}{R_0} \gg 1$$

d) A naive application of the generalized equipartition theorem fails for the potential energy.

The correct answer, found from above, is

$$\langle V_0 r \rangle = 2 k_B T \quad ; \quad \frac{R}{R_0} \gg 1$$

A naive application yields

$\langle V_0 r \rangle = k_B T$, which is wrong.

The reason is that r actually contains two coordinates, (x, y). A correct application of the generalized equipartition principle requires that we are able to identify one generalized coordinate that does not appear elsewhere in the Hamiltonian.

Another way of seeing this, goes as follows. We may re-express the Hamiltonian in polar coordinates.

$$H = \sum_{i=1}^{N} H_i$$

$$H_i = \frac{p_{xi}^2 + p_{yi}^2}{2m} + V_0\left(\sqrt{x_i^2 + y_i^2}\right)$$

$$= \frac{p_{ri}^2}{2m} + \frac{p_{\theta i}^2}{2mr^2} + V_0 r_i$$

Here, p_r is the momentum associated with the radial motion of the particles and p_θ is its angular momentum.

We see that r appears in $\frac{p_\theta^2}{2mr^2}$ as well as $V_0 r$, precluding an application of the generalized equipartition principle to the term $V_0 r$.