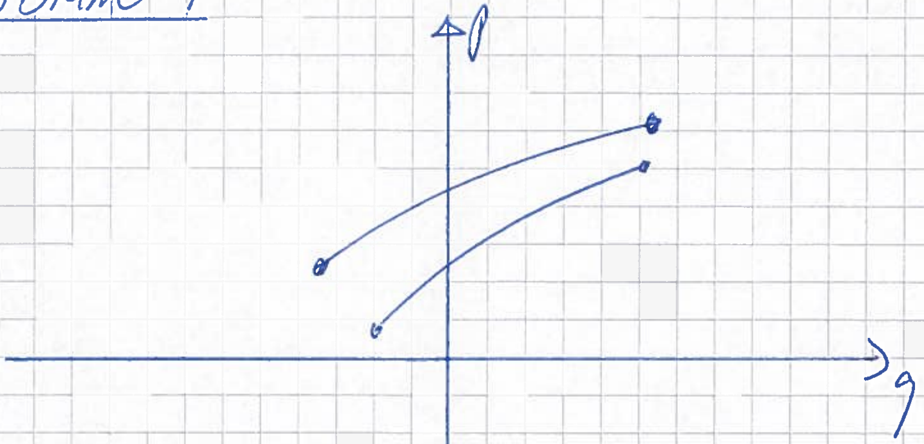
TFY 4230 14.05.2019

Problem 1

a)



$$\left.\begin{aligned} \dot{p} &= -\frac{\partial H}{\partial q} \\ \dot{q} &= \frac{\partial H}{\partial p} \end{aligned}\right\} \Rightarrow \underbrace{\frac{dp}{dq} = -\frac{\partial H/\partial q}{\partial H/\partial p}}_{\text{Slope of a given line in phase-space.}}$$

If two lines approach each other, then their slopes will also approach each other. Hence, the lines will never cross.

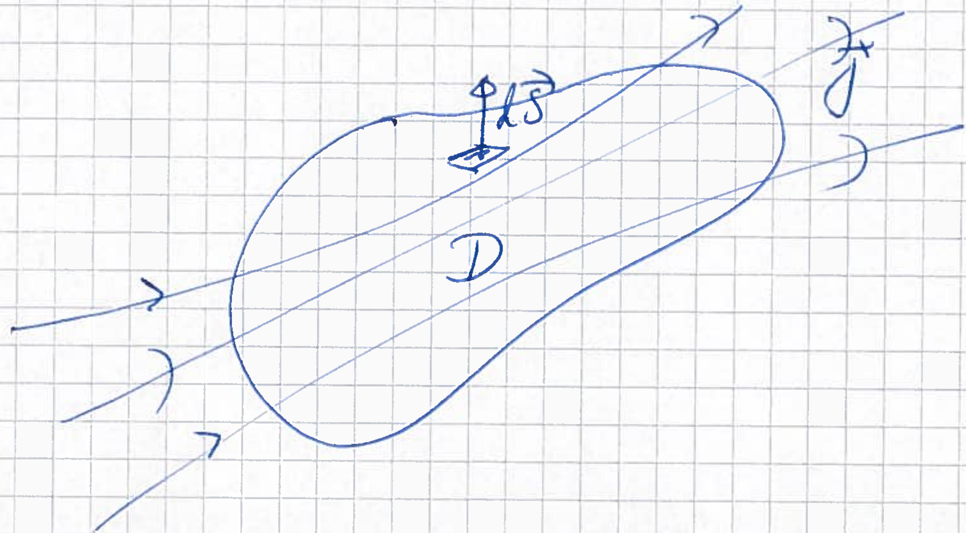
b) This means that points in phase-space never vanish and never appear.

Regarding each point in analogy with a particle, we have a continuity equation for these points in phase-space:

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot (\rho \vec{v}) = 0$$

where ρ is density of points in phase-space

This comes about as follows: Since no points in (p,q) disappear or appear, it means that any change of the # of points in a sub-domain D of (p,q) must be due to a net flow of points in or out of D



$$\frac{d}{dt}\iiint_D dV\, \rho(p,q,t) = -\oiint_S d\vec{S}\cdot\vec{j}$$

S is a closed surface encompassing D

$$\iiint_D dV\,\frac{\partial\rho}{\partial t} = -\iiint_D dV\,(\vec{\nabla}\cdot\vec{j})$$ Gauss' theorem

Should be valid for any D $\Rightarrow$

$$\frac{\partial\rho}{\partial t} + \vec{\nabla}\cdot\vec{j} = 0$$

$\vec{j} = \rho\vec{v}$, where $\vec{v}$ is velocity in phase space (p,q). Q.E.D.

c) $$\frac{\partial \rho}{\partial t} + \sum_i \left(\frac{\partial}{\partial q_i} (\rho \dot{q}_i) + \frac{\partial}{\partial p_i} (\rho \dot{p}_i) \right) = 0$$

$$\vec{\nabla} \cdot (\rho \vec{v}) = \vec{\nabla}_q \cdot (\rho \dot{\vec{q}}) + \vec{\nabla}_p \cdot (\rho \dot{\vec{p}})$$

Consider now the terms inside $\sum_i$:

$$\frac{\partial \rho}{\partial q_i} \dot{q}_i + \rho \frac{\partial \dot{q}_i}{\partial q_i} + \frac{\partial \dot{p}_i}{\partial p_i} \rho + \frac{\partial \rho}{\partial p_i} \dot{p}_i$$

$$= \frac{\partial \rho}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial \rho}{\partial p_i} \frac{\partial H}{\partial q_i}$$

$$+ \rho \underbrace{\left(\frac{\partial^2 H}{\partial q_i \partial p_i} - \frac{\partial^2 H}{\partial p_i \partial q_i} \right)}_{=0}$$

Define

$$\{A, B\} \equiv \sum_i \left(\frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial B}{\partial q_i} \right)$$

Thus we obtain

$$\frac{\partial \rho}{\partial t} + \sum_i \left(\frac{\partial \rho}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial \rho}{\partial p_i} \frac{\partial H}{\partial q_i} \right)$$

$$= \underline{\frac{\partial \rho}{\partial t} + \{\rho, H\} = 0}$$

d)

$$\frac{\partial \rho}{\partial t} = 0 \Rightarrow$$

$$\{\rho, H\} = 0$$

$$\rho = \rho(\{q_i, p_i\})$$

If we now assume that

$$\rho(\{q_i, p_i\}) = \rho(B(\{q_i, p_i\}))$$

then $\{\rho, H\}$

$$= \frac{d\rho}{dB} \{B, H\}$$

which we require to be zero.

Choosing $B = H$ guarantees this.

$\Rightarrow$ we can choose

$$\underline{\underline{\rho(\{q_i, p_i\}) = \rho(H)}}$$

ρ can be regarded as a probability distribution of states in phase-space if we normalize it. Then, we can compute physically observable quantities $O(\{q_i, p_i\})$ as averages over ρ:

$$\langle O \rangle = \sum_{\{q_i, p_i\}} \rho(H)\, O$$

as soon as we specify the Hamiltonian (a microscopic description) of the system. This provides the connection

Microscopic physics $\Longrightarrow$ macroscopic physics

More generally, given H and $\rho(H)$

$$\langle O \rangle = \sum_{\text{states}} \rho(H)\, O$$

which is also suitable for quantum mechanical systems.

Problem 2

a) $$M = \sum_i \langle \sigma_i \rangle = \left\langle \sum_i \sigma_i \right\rangle$$

$$\left\langle \sum_i \sigma_i \right\rangle = \frac{1}{Z} \sum_{\{\sigma_i\}} \left(\sum_i \sigma_i \right) e^{-\beta H}$$

$$= \frac{1}{Z} \sum_{\{\sigma_i\}} \frac{\partial}{\partial \beta B} \left(e^{-\beta H} \right)$$

$$= \frac{1}{Z} \frac{\partial}{\partial \beta B} Z = \underline{\underline{\frac{\partial \ln Z}{\partial \beta B}}}$$

$$He = \langle H \rangle$$

$$= \frac{1}{Z} \sum_{\{\sigma_i\}} H e^{-\beta H}$$

$$= \frac{1}{Z} \sum_{\{\sigma_i\}} \left(-\frac{\partial}{\partial \beta} \right) e^{-\beta H}$$

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

b) $$Z = \left(Z_{1\text{-dimer}} \right)^{N_d}$$

since the dimers are independent, where $Z_{1\text{-dimer}}$ is the partition function of a single spin-dimer.

$$Z_{1\text{-}dim} = \sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} e^{\beta(J\sigma_1\sigma_2 + B(\sigma_1+\sigma_2))}$$

$$= \underline{e^{\beta(J+2B)} + e^{\beta(J-2B)} + 2e^{-\beta J}}$$

$Z = (Z_{1\text{-}dim})^{Nd}$; independent dims

$$H_e = -\frac{\partial \ln Z}{\partial \beta} = -Nd \frac{\partial \ln Z_{1\text{-}dim}}{\partial \beta}$$

$$= -Nd \frac{A}{K}$$

$$K = e^{\beta(J+2B)} + e^{\beta(J-2B)} + 2e^{-\beta J}$$

$$A = (J+2B)e^{\beta(J+2B)} + (J-2B)e^{\beta(J-2B)} - 2Je^{-\beta J}$$

K, A may also be written:

$$K = 2[e^{\beta J}\cosh(2\beta B) + e^{-\beta J}]$$

$$A = 2[J\cosh(2\beta B) + 2B\sinh(2\beta B) - Je^{-\beta J}]$$

Hence,

$$H_e = -Nd\left(\frac{J\cosh(2\beta B) + 2B\sinh(2\beta B) - Je^{-\beta J}}{e^{\beta J}\cosh(2\beta B) + e^{-\beta J}}\right)$$

Specific heat:

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

Define $\quad X' \equiv \left(\frac{\partial X}{\partial \beta}\right)_B$

$$C_B = -N\alpha\,(-k_B)\,\beta^2\, H_c'$$

$$= N\alpha\, k_B\, \beta^2 \left(\frac{A'K - AK'}{K^2}\right)$$

Define $x = e^{\beta(J+2B)}$; $y = e^{\beta(J-2B)}$; $z = e^{-\beta J}$

$a = J+2B$; $b = J-2B$; $c = J$

$A = ax + by - 2cz$; $A' = a^2x + b^2y + 2c^2z$

$K = x + y + 2z$; $K' = A$

$A'K - AK' = A'K - A^2$

$$= (a^2x + b^2y + 2c^2z)(x+y+2z)$$
$$- (ax+by-2cz)(ax+by-2cz)$$

$$= \underline{xy\,(a-b)^2 + 2xz\,(a+c)^2 + 2yz\,(b+c)^2}$$

$a - b = 4B$ $\qquad xy = e^{2\beta J}$

$a + c = 2(J+B)$ $\qquad xz = e^{2\beta B}$

$b + c = 2(J-B)$ $\qquad yz = e^{-2\beta B}$

$$A'K - A^2 = \underline{16B^2 e^{2\beta J} + 8(J+B)^2 e^{2\beta B} + 8(J-B)^2 e^{-2\beta B}}$$

$$C_B = N k_B \beta^2 \,\frac{16B^2 e^{2\beta J} + 8(J+B)^2 e^{2\beta B} + 8(J-B)^2 e^{-2\beta B}}{\left(e^{\beta(J+2B)} + e^{\beta(J-2B)} + 2e^{-\beta J}\right)^2}$$

c)

$$M = N\alpha \frac{\partial}{\partial(B\beta)} \ln Z_{1\text{-dim}}$$

$$= \frac{N\alpha}{\beta} \frac{1}{Z_{1\text{-dim}}} \frac{\partial Z_{1\text{-dim}}}{\partial B}$$

$$\frac{\partial Z_{1\text{-dim}}}{\partial B} = 2\beta \left(e^{\beta(J+2B)} - e^{\beta(J-2B)} \right)$$

$$= 2\beta e^{\beta J} \left(e^{2\beta B} - e^{-2\beta B} \right)$$

$$= 4\beta e^{\beta J} \sinh(2\beta B)$$

$$M = 4N\alpha \frac{e^{\beta J} \sinh(2\beta B)}{e^{\beta(J+2B)} + e^{\beta(J-2B)} + 2e^{-\beta J}}$$

Per spin: Divide by $2N\alpha$

Can be compactified a little:

$$M = 2N\alpha \cdot \left(\frac{e^{\beta J} \sinh(2\beta B)}{e^{\beta J} \cosh(2\beta B) + e^{-\beta J}} \right)$$

Per spin: Divide by $2N\alpha$

$$M = 2N\alpha \quad \frac{L_1}{L_2}$$

$$L_1 = e^{\beta J} \sinh(2\beta B)$$

$$L_2 = e^{\beta J} \cosh(2\beta B) + e^{-\beta J}$$

$$\chi = \left(\frac{\partial M}{\partial B}\right)_T = \beta \left(\frac{\partial M}{\partial \beta B}\right)_T$$

$$= 2N\alpha \, \beta \quad \frac{\partial}{\partial(\beta B)} \left(\frac{L_1}{L_2}\right)$$

Define $\frac{\partial X}{\partial(\beta B)} = X'$

$$\chi = 2N\alpha \beta \left(\frac{L_1' L_2 - L_1 L_2'}{L_2^2}\right)$$

$$L_1' = 2 e^{\beta J} \cosh(2\beta B)$$

$$L_2' = 2 e^{\beta J} \sinh(2\beta B)$$

$$L_1' L_2 - L_1 L_2'$$

$$= 2 e^{\beta J} \cosh(2\beta B) \left[e^{\beta J} \cosh(2\beta B) + e^{-\beta J} \right]$$

$$- e^{\beta J} \sinh(2\beta B) \cdot 2 e^{\beta J} \sinh(2\beta B)$$

$$= 2 e^{2\beta J} + 2 \cosh(2\beta B)$$

$$\chi = 4N\alpha\beta \frac{\left(\cosh(2\beta B) + e^{2\beta J}\right)}{\left(e^{\beta J}\cosh(2\beta B) + e^{-\beta J}\right)^2}$$

Per spin: Divide by $2N\alpha$

d) $J < 0$ $\qquad \beta \gg 1$

$$\chi \simeq \frac{4N\alpha\beta}{2} \frac{e^{2\beta(|J| + B)}}{\left(\frac{1}{2}e^{2\beta B} + e^{2\beta|J|}\right)^2}$$

$|J| > B$:

$$\chi \simeq 2N\alpha\beta\, e^{-2\beta(|J| - B)}$$

$\chi \to 0$, $T \to 0$. Dimers form spin-singlets with zero magnetization $\to \chi \to 0$

$B > |J|$:

$$\chi \simeq 8N\alpha\beta\, e^{-2\beta(B - |J|)}$$

$\chi \to 0$, $T \to 0$: B completely aligns spins as $T \to 0$, $\Rightarrow$ no further increase in M as B increases $\Rightarrow$ $\chi \to 0$

Problem 3

a) $$Z_g = \prod_k \left(1 + z e^{-\beta \varepsilon_k}\right)$$

$$z = e^{\beta\mu}$$

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

$$= \sum_{\vec{k}} \sum_{l=1}^{\infty} \frac{(-1)^{l-1}}{l} z^l e^{-\beta \varepsilon_k l}$$

$$= \sum_{l=1}^{\infty} \frac{(-1)^{l-1}}{l} z^l \underbrace{\sum_{\vec{k}} e^{-\beta\varepsilon_k l}}$$

$$= \int_0^\infty d\varepsilon \underbrace{g(\varepsilon)}_{= \frac{A}{(hc)^2}\varepsilon} e^{-\beta \varepsilon l}$$

$$\sum_k e^{-\beta\varepsilon_k l} = \frac{A}{(hc)^2} \underbrace{\int_0^\infty d\varepsilon \, \varepsilon \, e^{-\beta l \varepsilon}}$$

$$= \left(\frac{1}{\beta l}\right)^2 \underbrace{\int_0^\infty dx \, x \, e^{-x}}_{=1}$$

$$\beta p A = \frac{A}{(\beta h c)^2} \sum_{l=1}^{\infty} \frac{(-1)^{l-1}}{l^3} z^l$$

$$\beta p = \frac{1}{\lambda^2} \sum_{l=1}^{\infty} b_l z^l$$

$$\underline{\underline{b_l = \frac{(-1)^{l-1}}{l^3}}}$$

Fugacity coefficient

$$\underline{\underline{\lambda = \beta h c}}$$

λ: Ultra-relativistic thermal de Broglie-wavelength

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

$$= z \frac{\partial \beta p A}{\partial z}$$

$$\rho = \frac{\langle N \rangle}{A} \Rightarrow$$

$$\rho = z \frac{\partial (\beta p)}{\partial z} = \underline{\underline{\frac{1}{\lambda^2} \sum_{l=1}^{\infty} l b_l z^l}}$$

b) $$\beta p = \frac{1}{\lambda^2}\left(z - \frac{1}{8}z^2 + \dots\right)$$

$$\varrho = \frac{1}{\lambda^2}\left(z - \frac{1}{4}z^2 + \dots\right)$$

$$\beta p - \varrho = \frac{1}{\lambda^2}\,\frac{1}{8}z^2 + \dots$$

$$\varrho\lambda^2 \simeq z + \dots \quad \Rightarrow \quad z^2 = \varrho^2\lambda^4 + \dots$$

$$\beta p - \varrho = \frac{1}{\lambda^2}\,\frac{1}{8}\varrho^2\lambda^4 + \dots$$

$$\beta p = \varrho + B_2\varrho^2 + \dots$$

$$\underline{B_2 = \frac{1}{8}\lambda^2} \qquad > 0$$

The pressure in an ideal Fermi-gas is higher than in an ideal classical gas, due to the Pauli-principle which acts like a repulsion. Hence $B_2 > 0$. Since $\lambda \sim h$ (Planck's constant), we see that the correction to the classical ideal gas equation of state $\beta p = \varrho$ is a <u>quantum effect.</u>

c) $\beta p = \rho \left(1 + \frac{1}{4} \rho \lambda^2 + \ldots \right)$

In general

$$\beta p = \frac{1}{\lambda^2} H(z)$$

$$\rho = \frac{1}{\lambda^2} z \frac{\partial H}{\partial z} = \frac{1}{\lambda^2} G(z)$$

$$G(z) = \rho \lambda^2$$

$$z = G^{-1}(\rho \lambda^2)$$

$$\beta p = \frac{1}{\lambda^2} H\left(G^{-1}(\rho \lambda^2) \right)$$

$$= \frac{1}{\lambda^2} R(\rho \lambda^2)$$

Hence, βp is a function of $\rho \lambda^2$ which may be Taylor-expanded around $\rho \lambda^2 = 0$.

We can truncate this power-series at low order in $\rho \lambda^2$ when

$$\underline{\rho \lambda^2 \ll 1}$$

$$\rho \sim \frac{1}{l_0^2}$$

l_0: Mean separation between particles

$$\rho \lambda^2 = \left(\frac{\lambda}{l_0}\right)^2$$

Truncate when

$$\lambda << l_0$$

i.e. when relativistic thermal de Broglie wavelength is much smaller than separation between particles

$$\beta h c << l_0$$

$$k_B T >> \frac{hc}{l_0}$$

High-temp limit, when quantum effects are small.

d)

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

$$T \to 0 \implies \beta \to \infty$$

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

$$\beta \to \infty \implies \ln\left(1 + e^{-\beta(\varepsilon-\mu)}\right) = 0; \quad \varepsilon > \mu$$

$$= \beta(\mu - \varepsilon); \quad \varepsilon < \mu$$

$$\beta p A = \beta \int_0^\mu d\varepsilon \frac{A}{(hc)^2} (\mu - \varepsilon)\, \varepsilon$$

$$p = \frac{1}{(hc)^2} \int_0^\mu d\varepsilon \, \varepsilon(\mu - \varepsilon)$$

$$= \frac{1}{(hc)^2} \left\{ \mu \frac{\mu^2}{2} - \frac{\mu^3}{3} \right\}$$

$$= \frac{1}{(hc)^2} \frac{1}{6} \mu^3$$

$$\langle N \rangle = \frac{\partial \ln Z_G}{\partial \beta\mu} = \sum_k \frac{1}{e^{\beta(\varepsilon_k - \mu)} + 1}$$

$$\langle N \rangle = \frac{A}{(hc)^2} \int_0^{\mu} d\varepsilon \ \varepsilon$$

$$\rho = \frac{1}{(hc)^2} \frac{\mu^2}{2}$$

$$\mu^2 = 2 (hc)^2 \rho$$

$$\mu = \sqrt{2} \ hc \ \rho^{1/2}$$

$$p = \frac{1}{(hc)^2} \frac{1}{6} 2^{\frac{3}{2}} (hc)^3 \rho^{\frac{3}{2}}$$

$$= \frac{\sqrt{2}}{3} hc \ \rho^{3/2}$$