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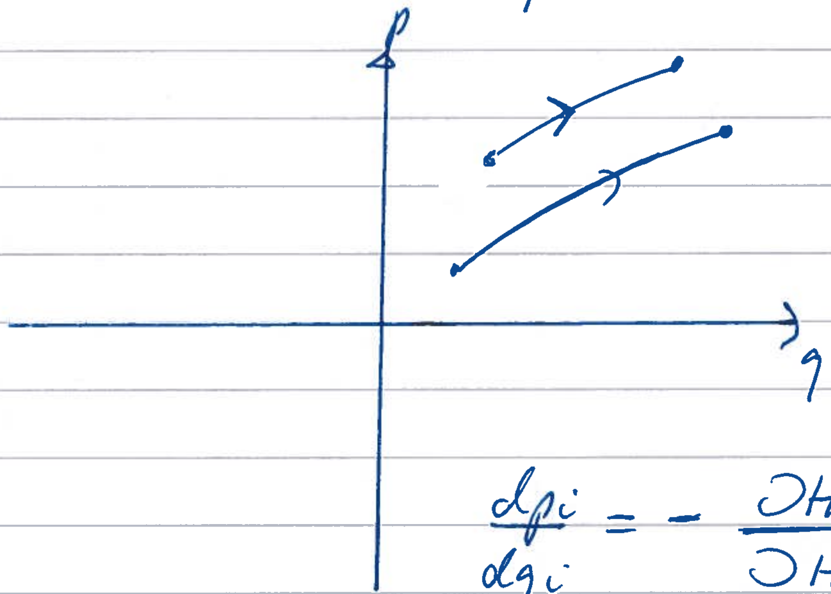
Oppgave 1a

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}$$

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}$$



$$\frac{dp_i}{dq_i} = -\frac{\partial H/\partial q_i}{\partial H/\partial p_i}$$

This equation applies to every point in phase space, and each point is governed by the same Hamiltonian. If two point approach each other, when they flow along two separate lines, the lines along which they move will gradually acquire the same slope, since H is the same. Hence, they never cross.

This is, in fact, a general property of any set of quantities whose flow is determined by a set of 1. order differential equations.

Note however, that even if the points in the figure above do not cross in (q,p)-space, they <u>do</u> „cross" when projected down on q-space!

Formulating the dynamics entirely in terms of $\{q_i\}$ gives a second order differential equation for $\{q_i\}$ (Newton's equation)

For second-order diff. equations, we have no „no-crossing theorem"

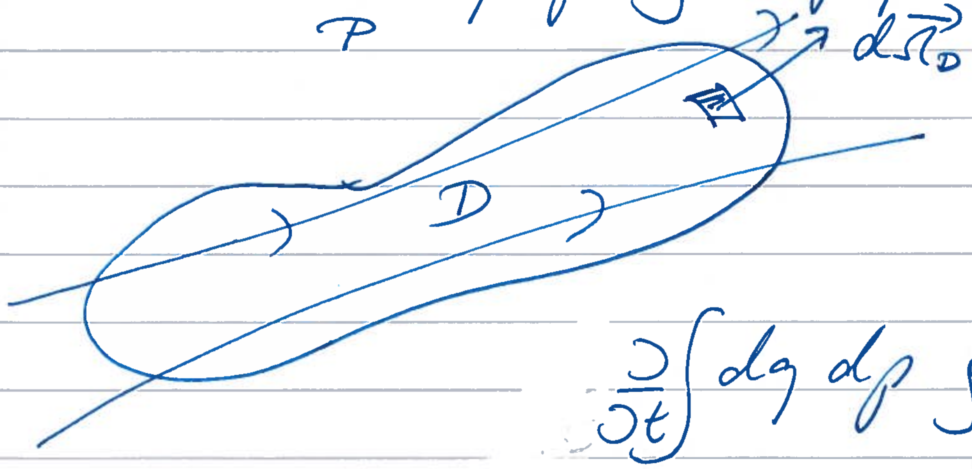
1(b) Number of points in phase-space do not dissappear. That means that any number of points flowing out of the region D in phase space, must be accompanied by a corresponding loss of exactly the same number of points in D. A current $\vec{j}$ of points (let us think about these points as particles) therefore leads to a reduction of particles inside D

\# particles in D:

$$N_D = \int_D dq\, dp\, \rho(q, p, t)$$

Total number of points in entire phase-space P:

$$N = \int_P dq\, dp\, \rho(q, p, t)$$



$$\frac{\partial}{\partial t}\int_D dq\, dp\, \rho = -\oint_{\Omega_D} d\vec{\Omega} \cdot \vec{j}$$

Gauss' theorem:

$$\iint_{\Omega_D} d\vec{\Omega}_D \cdot \vec{j} = \iiint_D dp\,dq \;\; \vec{\nabla}\cdot(\vec{j})$$

$$\vec{j} = \rho\,\vec{v}$$

$$\int_D dp\,dq \left(\frac{\partial \rho}{\partial t} + \vec{\nabla}\cdot\vec{j} \right) = 0$$

Should apply to any „volume" $D \Longrightarrow$

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

c)

$$\frac{\partial \rho}{\partial t} + \sum_i \left[\frac{\partial}{\partial q_i}(\rho\,\dot{q}_i) + \frac{\partial}{\partial p_i}(\rho\,\dot{p}_i) \right]$$

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

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

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

$\Rightarrow$

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

$$= \frac{\partial \rho}{\partial t} + \{\rho, H\} = 0 \qquad \text{q.e.d.}$$

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

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

$$\sum_i \left(\frac{\partial \rho}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial \rho}{\partial p_i} \frac{\partial H}{\partial q_i} \right) = 0 \quad (*)$$

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

Then
$$\left.\begin{aligned} \frac{\partial \rho}{\partial q_i} &= \frac{d\rho}{dH} \frac{\partial H}{\partial q_i} \\ \frac{\partial \rho}{\partial p_i} &= \frac{d\rho}{dH} \frac{\partial H}{\partial p_i} \end{aligned}\right\} \Rightarrow$$

$(*) \Rightarrow$

$$\frac{d\rho}{dH} \{H, H\} = 0$$

More generally:

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

Then:

$$\left.\begin{aligned} \frac{\partial \rho}{\partial q_i} &= \frac{d\rho}{dB} \frac{\partial B}{\partial q_i} \\ \frac{\partial \rho}{\partial p_i} &= \frac{d\rho}{dB} \frac{\partial B}{\partial p_i} \end{aligned}\right\} \Longrightarrow$$

$\otimes \Rightarrow$

$$\frac{d\rho}{dB} \{B, H\} = 0$$

Equation holds for any B which is a constant of motion.

ρ is the density of points in phase-space. With the normalization

$$\int_P dq\, dp\ \rho = 1,$$ ρ may be interpreted as the probability distribution for finding a classical system of N particles in a state $\{q_i, p_i\}$

$$\varrho = \varrho(\{q_i, p_i\}) \Rightarrow \varrho(H)$$

facilitates a computation of macroscopically observable quantities

$$\langle A \rangle = \int_{P} dq\, dp\, A(\{q_i, p_i\})\, \varrho(H)$$

without having to solve the (impossibly difficult) problem of actually solving Hamilton's equations.

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Oppg 2a

$$H = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j - \vec{B} \cdot \sum_i \vec{S}_i$$

$$\vec{S}_i = \vec{m} + \delta\vec{S}_i$$

$$\vec{S}_i \cdot \vec{S}_j \cong \vec{m}^2 + \vec{m} \cdot (\delta\vec{S}_i + \delta\vec{S}_j)$$

$$= -\vec{m}^2 + \vec{m} \cdot (\vec{S}_i + \vec{S}_j)$$

$$H = J \sum_{\langle i,j \rangle} \vec{m}^2 - J \sum_{\langle i,j \rangle} \vec{m} \cdot (\vec{S}_i + \vec{S}_j) - \vec{B} \cdot \sum_i \vec{S}_i$$

$$= NzJm^2 - (2J\vec{m}z + \vec{B}) \cdot \sum_i \vec{S}_i$$

$$= NzJm^2 - \vec{B}_{eff} \cdot \sum_i \vec{S}_i$$

$$\vec{B}_{eff} = \vec{B} + 2Jz\vec{m}$$

This effective field is comprised of the external magnetic field $\vec{B}$ and the field $2Jz\vec{m}$ felt by $\vec{S}_i$ from the surrounding nearest-neighbor spins.

b) In MFA, we have reduced the problem to an effective problem of independent spins, where however $\vec{m}$ must be determined selfconsistently by minimizing the Gibbs energy G.

$$\frac{\partial G}{\partial \vec{m}} = 0$$

$$G = -\frac{1}{\beta} \ln Z \;;\; Z = (Z_1)^N$$

$$Z_1 = e^{-\beta J z m^2} \sum_{\vec{S}} e^{\beta \vec{B}_{eff} \cdot \vec{S}}$$

Summing over all values of $\vec{S}$ means integrating over all values of φ

$$\sum_{\vec{S}} \to \sum_{\varphi} = \frac{1}{2\pi} \int_0^{2\pi} d\varphi$$

$$\sum_{\vec{S}} e^{-\beta \vec{B}_{eff} \cdot \vec{S}} = \frac{1}{2\pi} \int_0^{2\pi} d\varphi \, e^{\beta B_{eff} S \cos\varphi}$$

Introduce $x = \beta B_{eff} S$

$$I_0(x) = \frac{1}{2\pi}\int_0^{2\pi} d\varphi \, e^{x\cos\varphi}$$

$\Rightarrow$

$$Z_1 = e^{-\beta J z m^2} I_0(x) \, ; \; x = \beta B_{eff} S$$

$$\underline{\underline{G = NJzm^2 - \frac{N}{\beta}\ln\left(I_0(x)\right)}}$$

Gibbs energy in the limit $T \to 0$ $(\beta \to \infty)$

$\beta \to \infty \Rightarrow x = \beta B_{eff} S \to \infty$

Must consider $I_0(x)$ for large x.

$x \gg 1$:

$$I_0(x) \simeq \frac{e^x}{\sqrt{2\pi x}}$$

$$G \simeq NJzm^2 - \frac{N}{\beta}\left(x - \frac{1}{2}\ln(2\pi x)\right)$$

$$\simeq NJzm^2 - \frac{N}{\beta} \cdot \beta B_{eff} S$$

$$= NJzS^2 - N(B + 2JzS)S = \underline{\underline{-NJzS^2 - NB}}$$

Comment:

The exact ground state energy is found by direct inspection of H: The ground state is the state where all spins are maximally aligned along $\vec{B}$, $\vec{S}_i = S\hat{z}$

$$H = -JNzS^2 - NBS = E_0^{Exact}$$

When all spins are maximally aligned along $\vec{B}$, we find in the mean-field approximation

$$E_0^{MFA} = NzJS^2 - (BNS + 2JzSNS)$$

$$= -JNzS^2 - BNS$$

$$E_0^{Exact} = E_0^{MFA}$$

The reason for this is that the fluctuation terms that we are ignoring in MFA are not present in the ground state (T=0).

MFA is therefore exact at T=0 (at least for $d \geq 2$).

c)

The magnetization of the system is determined self-consistently by minimizing G

$$\frac{\partial G}{\partial m} = 0$$

$$2NJzm - \frac{N}{\beta}\frac{I_0'}{I_0}\frac{\partial x}{\partial m} = 0$$

$$* = \beta B_{eff} S$$
$$= \beta S (B + 2Jzm)$$

$$\frac{\partial x}{\partial m} = 2\beta SJz$$

$$2NJzm - \frac{N}{\beta} 2\beta Jz S \frac{I_0'(x)}{I(x)} = 0$$

$B = 0$ and consider $x \ll 1$
($m \to 0$, but still nonzero)

For small x, $I_0 \simeq 1 + \frac{x^2}{4} + \cdots$

$$I_0' \simeq \frac{x}{2}$$

$$\frac{I_0'}{I_0} \simeq \frac{x}{2} = \frac{\beta S}{2} 2Jzm \quad (B = 0)$$

$$= \beta SJzm$$

$$m = S^2 \beta Jzm$$

$$\underline{k_B T_c = S^2 Jz}$$

Problem 3

$$\beta P = \sum_{l=1}^{\infty} B_l \rho^l$$

ⓐ Working in the grand canonical ensemble, we have that

$$\beta P V = \ln Z_g$$

$$Z_g = \sum_{N=0}^{\infty} \frac{Q_N}{\lambda^{3N} N!} e^{\beta \mu N}$$

$$= \sum_{N=0}^{\infty} z^N \frac{Q_N}{N!}$$

$$= Q_0 + z Q_1 + z^2 \frac{Q_2}{2!} + \dots; \quad Q_0 = 1$$

$$\ln Z_g = z Q_1 + \frac{z^2}{2}\left(Q_2 - Q_1^2\right) + \dots$$

Define

$$\chi(z) = \frac{\ln Z_g}{V} = \sum_{l=1}^{\infty} b_l z^l$$

$$= z b_1 + z^2 b_2 + z^3 b_3 + \dots$$

$$b_1 = 1 = \frac{1}{V} \int d^3x \cdot 1$$

$$= \frac{Q_1}{V}$$

$$\beta P = z b_1 + z^2 b_2 + b_3 z^3 + \dots$$

$$\rho = z b_1 + 2 b_2 z^2 + 3 b_3 z^3 + \dots$$

$$Z = a_1 \rho + a_2 \rho^2 + \cdots$$

$$\rho = b_1 (a_1 \rho + a_2 \rho^2 + \cdots)$$

$$+ 2b_2 (a_1 \rho^2 + 2 a_1 a_2 \rho^2 + \cdots) + \cdots$$

$$= a_1 b_1 \rho + (b_1 a_2 + 2 b_2 a_1) \rho^2 + \cdots$$

$$b_1 = 1 \quad \Rightarrow \quad a_1 = 1$$

$$a_2 + 2b_2 = 0 \Rightarrow a_2 = -2b_2$$

$$\beta p = \rho - 2b_2 \rho^2 + \cdots$$

$$= \rho + B_2 \rho^2 + \cdots$$

$$\underline{\underline{B_1 = 1}}$$

b) $l \geq 2$:

$$\frac{\partial^l (\beta p / \rho)}{\partial \rho^l} = (l-1)! \, B_l + O(\rho)$$

$$B_l = \frac{1}{(l-1)!} \frac{\partial^l (\beta p / \rho)}{\partial \rho^l}$$

when B_l are regardes as the coefficients of a Taylor-expansion in ρ of βp.

c) $$p = \frac{N k_B T}{V - Nb} - a\left(\frac{N}{V}\right)^2$$

$$\frac{N}{V} = \rho$$

$$\beta p = \frac{1}{\frac{1}{\rho} - b} - \beta a \rho^2$$

$$= \frac{\rho}{1 - \rho b} - \beta a \rho^2$$

$$= \rho \sum_{l=0}^{\infty} b^l \rho^l - \beta a \rho^2$$

$$= \sum_{l=1}^{\infty} b^{l-1} \rho^l - \beta a \rho^2$$

$$= \sum_{l=1}^{\infty} B_l \rho^l$$

$$B_1 = 1$$

$$B_2 = b - \beta a$$

$$B_l = b^{l-1} \quad ; \quad l \geq 3$$