EKSAMEN I STATMEK 8.12.87

Løsningsforslag

Oppgave 1

a $H(p,q) = cQ^2 + H'(p,q)$

↑ avhenger ikke av Q

Kvadratiske ledd i Hamiltonfunksjonen bidrar hvert med $\frac{1}{2}k_BT$ til den indre energi

Bevis

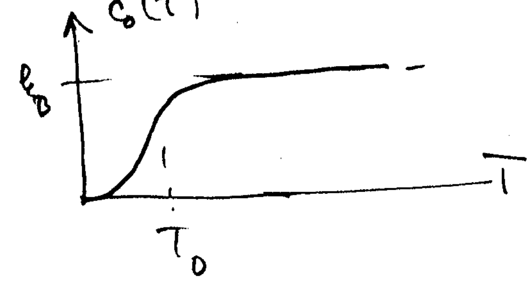
$$U = \langle H \rangle = \langle cQ^2 \rangle + \langle H' \rangle$$

$$\langle cQ^2 \rangle = \frac{\int dQ\, cQ^2 \int (dp\,dq)'\, e^{-\beta c Q^2 - \beta H'}}{\int dQ \int (dp\,dq)'\, e^{-\beta c Q^2 - \beta H'}}$$

$$= -\frac{\partial}{\partial \beta} \ln \int_{-\infty}^{\infty} dQ\, e^{-\beta c Q^2} = -\frac{\partial}{\partial \beta} \sqrt{\frac{\pi}{\beta c}}$$

$$= \frac{1}{2\beta} = \frac{k_B T}{2} \quad \text{qed.}$$

b



For $T < \frac{E_1 - E_0}{k_B} = \frac{\hbar\omega}{k_B} \equiv T_0$ vil $c_Q(T)$ raskt gå mot null når $T \to 0$ siden $e^{-\frac{E_1 - E_0}{k_B T}}$ raskt går mot null

Frihetsgraden fryses med. Når $T \to 0$ nærmer en seg klassisk grense. To kvadratiske ledd i $H(p,q)$ for harm. osc. Altså $c_Q(T) \to k_B$.

c Middelenergi for <u>en</u> oscillator

$$u = \langle H \rangle = \frac{\sum_n \varepsilon_n e^{-\beta \varepsilon_n}}{\sum_n e^{-\beta\varepsilon_n}} = -\frac{\partial}{\partial\beta} \ln \sum_{n=0}^{\infty} e^{-\beta\hbar\omega(n+\frac{1}{2})}$$

$$= -\frac{\partial}{\partial\beta} \ln \frac{e^{-\beta\hbar\omega/2}}{1-e^{-\beta\hbar\omega}} = \frac{1}{2}\hbar\omega \coth \frac{1}{2}\beta\hbar\omega$$

Varmekapasitet

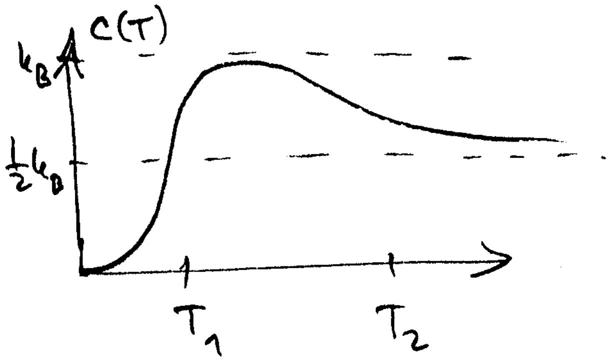
$$c_0(T) = \frac{\partial u}{\partial T} = \frac{d\beta}{dT}\frac{\partial u}{\partial\beta} = k_B \left(\frac{\frac{1}{2}\beta\hbar\omega}{\sinh\frac{1}{2}\beta\hbar\omega} \right)^2$$

$T \to 0$: $c_0(T) \simeq k_B \left(\frac{\hbar\omega}{k_B T}\right)^2 e^{-\frac{\hbar\omega}{k_B T}} \longrightarrow 0$

ok.

$T \to \infty$: $c_0(T) \simeq k_B$

d



Lave T, $T < T_1 = \frac{\hbar\omega}{k_B}$:

Omtrent som harmonisk oscillator

Høye T, $T > T_2 = \frac{U_0}{k_B}$:

Nærmer seg fri rotator om <u>en</u> akse: Ett kvadratisk ledd i klassisk Hamiltonfunksjon: $c(T) \simeq \frac{1}{2}k_B$

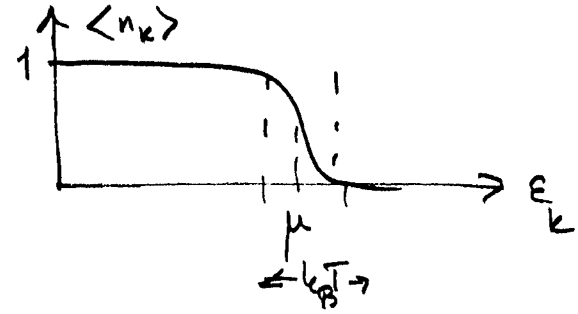
$$T_1 = \frac{0.03\,\text{eV} \cdot 1.6 \cdot 10^{-19}\,\text{J/eV}}{1.38 \cdot 10^{-23}\,\text{J/K}} \approx 350\,\text{K}$$

$$T_2 = \frac{U_0}{k_B} = \frac{0.14\,\text{eV} \cdot 1.6 \cdot 10^{-19}\,\text{J/eV}}{1.38 \cdot 10^{-23}\,\text{J/K}} \approx 1600\,\text{K}$$

Det spørs om etanmolekylet holder i hop ved høyere temperaturer!

Oppgave 2

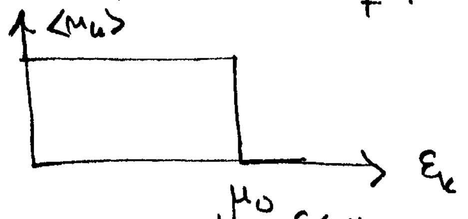
a



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

Bare fermionene i et energiområde $\sim k_BT$ rundt μ_0 deltar aktivt i fysiske prosesser. De under dette området er medfrosset. De over finnes ikke. Brøkdelen av "aktive" ~~elektroner~~ fermioner er av størrelsesorden $\frac{k_BT}{\mu_0} \equiv T/T_F$ $\quad (\mu_0 = \mu(T=0))$

b Må bestemme T_F.



$$\langle n_k \rangle = \begin{cases} 1 & \varepsilon_k < \mu_0 \\ 0 & \varepsilon_k > \mu_0 \end{cases}$$

$$\rho = 2\pi g_s \left(\frac{2m}{h^2}\right)^{3/2} \underbrace{\int_0^{\mu_0} d\varepsilon \sqrt{\varepsilon}}_{\frac{2}{3}\mu_0^{3/2}}$$

$$\Downarrow$$

$$T_F = \frac{\mu_0}{k_B} = \frac{h^2}{2mk_B}\left(\frac{3\rho}{4\pi g_s}\right)^{2/3}$$

Innsatt ($\rho \approx 10^{44}\, m^{-3}$ etc.) for nøytronstjerne

$$T_F \sim 4 \cdot 10^{11} K \qquad \frac{T}{T_F} \sim \frac{10^8}{4 \cdot 10^{11}} \sim 2 \cdot 10^{-4}$$

Slike nøytronstjerner er kalde, tross i de hundre millioner gradene!

Oppgave 3

a Ved $T=0$ er systemet (i likevekt!) sikkert i én av de g grunntilstandene, og med samme sannsynlighet i hver av dem. Altså $p_i = \frac{1}{g}$ $(i=1,\ldots,g)$

Altså: $S(T=0) = -k_B \sum_{i=1}^{g} \frac{1}{g} \ln \frac{1}{g} = k_B \ln g$

b (i) $J=0, h=0$; $g = 2^N$ (alle tilst. er gr. tilst.!)

$$s = \frac{S(T=0)}{N} = \frac{k_B}{N} \ln 2^N = k_B \ln 2$$

(ii) $J=0$, $h>0$; $g=1$ (spinn opp for alle spinn gr.t.)

$$s = \frac{k_B}{N} \ln 1 = 0$$

(iii) $J>0$, $h=0$; $g=2$ (alle opp; alle ned)

$$s = \frac{k_B}{N} \ln 2 \approx 0$$

(iv) $J<0$, $h=0$; $g=2$ ($\uparrow\downarrow\uparrow$; $\downarrow\uparrow\downarrow$)

$$s = \frac{k_B}{N} \ln 2 \approx 0$$

(v) $J>0$, $h>0$; $g=1$ (alle opp)

$$s = 0$$

(vi) $J<0$, $h>0$; $g = \begin{cases} 1 & \text{sterkt felt} \\ 2 & \text{sterk vekselvirkn.} \end{cases}$

s = makroskopisk sett null ($N \sim 10^{23}$)

Kreves ikke

Mer finurlig: Et kubisk gitter i 3 dim. har $\frac{6}{2} = 3$ bånd (J-bånd) pr. spinn. Dvs at "grunntilstands" energiene er, pr. spinn

$$E_{AF} = E(\uparrow\downarrow\uparrow) = 3J + 0h$$

$$E_F = E(\uparrow\uparrow\uparrow) = -3J - 1h$$

Antiferromagnetiske grunntilst. ($g=2$) dersom $E_{AF} < E_F$: $6J < -h$

Ferromagn. gr tilst. (spinn opp, $g=1$) —"— $E_F < E_{AF}$: $6J > -h$

* Ennå mer finurlig: Når $6J = -h$, kan spinnene på det ene av to kubiske undergitter fleippes fritt (I 2 dim; ved $4J = -h$; "$2DJ = -h$")

Kreves absolutt ikke!

$$\begin{matrix} + & - & + & - \\ - & + & - & + \\ + & - & + & - \\ - & + & - & + \end{matrix} \quad \Longleftrightarrow \quad \begin{matrix} + & - & + & - \\ - & + & + & + \\ + & - & + & - \\ - & + & - & + \end{matrix}$$

begge er grunntilst. i 2D med $2DJ = -h$

Derved er $g = 2 \cdot 2^{N/2}$ og $s = \left(\frac{1}{2} + \frac{1}{N}\right) k_B \ln 2$

Oppgave 4

a
$$Z_N(T,h) = \sum_{\{\sigma\}} e^{\beta h \sum_{i=1}^{N} \sigma_i} = \left[\sum_{\sigma_i = \pm 1} e^{\beta h \sigma_i} \right]^N$$
$$= (2 \cosh \beta h)^N$$

$$m = \langle \sigma_i \rangle = \frac{\sum_{\sigma_i = \pm 1} \sigma_i e^{\beta h \sigma_i}}{\sum_{\sigma_i = \pm 1} e^{\beta h \sigma_i}} = \frac{2 \sinh \beta h}{2 \cosh \beta h} = \tanh \beta h$$

b
$$\tau_i = \sigma_{i-1} \sigma_i \implies \sigma_1 = \sigma_1$$
$$\sigma_2 = \underbrace{\sigma_1 \sigma_1}_{\equiv 1} \sigma_2 = \sigma_1 \tau_2$$
$$\sigma_3 = \sigma_1 \sigma_1 \sigma_2 \sigma_2 \sigma_3 = \sigma_1 \tau_2 \tau_3$$
$$\vdots$$

1-1 tydig
$$\{\sigma\} \Longleftrightarrow \{\sigma_1, \tau_2, \ldots \tau_N\}$$

$$Z_N(T, h_1, \ldots h_N) = \sum_{\sigma_1 = \pm 1} \sum_{\{\tau\}} e^{\beta J \sum_{i=2}^{N} \tau_i + \beta \sum_{i=1}^{N} h_i \sigma_1 \tau_2 \cdots \tau_i}$$

qed.

c

$$m_m = \langle \sigma_m \rangle = \frac{\sum_{\{\sigma\}} \sigma_m \, e^{\beta J \sum_{i=2}^{N} \sigma_{i-1}\sigma_i + \sum_{i=1}^{N} h_i \sigma_i}}{\sum_{\{\sigma\}} \quad \text{— '' —}}$$

$$= \frac{1}{\beta}\frac{\partial}{\partial h_m} \ln Z_N = \frac{1}{\beta} \frac{\partial Z_N / \partial h_m}{Z_N}$$

$\boxed{h_1 \neq 0;\, h_{i>1} = 0}$

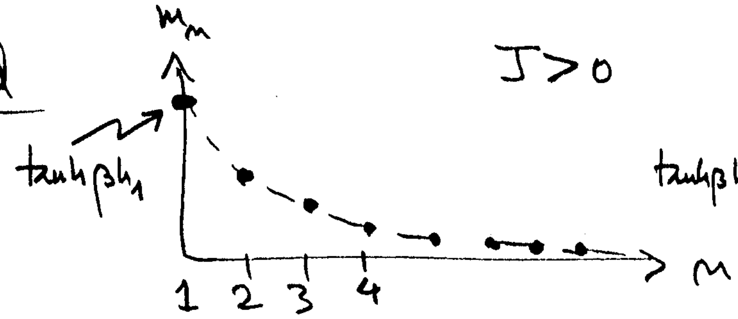
$$m_m = \frac{\sum_{\sigma_1 = \pm 1} \sum_{\{\tau\}} \sigma_1 \tau_2 \cdots \tau_m \, e^{\beta J \sum_{i=2}^{N} \tau_i + \beta h_1 \sigma_1}}{\sum_{\sigma_1 = \pm 1} \sum_{\{\sigma\}} \quad \text{— '' —}}$$

$$= \frac{\sum_{\sigma_1=\pm 1} \sigma_1 e^{\beta h_1 \sigma_1} \sum_{\tau_2 = \pm 1} \tau_2 e^{\beta J \tau_2} \cdots \sum_{\tau_m = \pm 1} \tau_m e^{\beta J \tau_m} \sum_{\tau_{m+1} = \pm 1} e^{\beta J \tau_{m+1}} \cdots}{\sum_{\sigma_1 = \pm 1} e^{\beta h_1 \sigma_1} \sum_{\tau_2 = \pm 1} e^{\beta J \tau_2} \cdots\cdots}$$

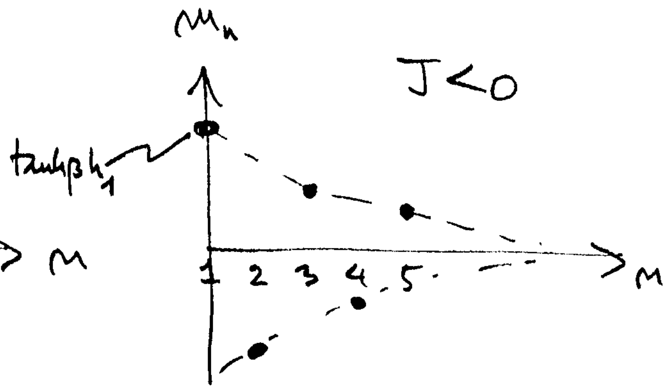
$$= \underset{1}{\tanh \beta h_1} \cdot \underset{2}{\tanh \beta J} \cdot \ldots \cdot \underset{m}{\tanh \beta J} \cdot \underset{m+1}{1} \cdot 1 \cdots \underset{N}{1}$$

$$\boxed{m_m = \tanh \beta h_1 \, \tanh^{m-1} \beta J}$$

d



Ferromagnetisk kjede



Antiferromagn. kjede.

Inntrengningsdybde = korrelasjonslengde $\equiv \xi$

$$\xi = -\frac{1}{\ln \tanh \beta J} \quad ; \quad m_n = \tanh \beta h_1 \; e^{-\frac{(n-1)}{\xi}}$$

Høye T $(\beta J \ll 1)$ $\quad \xi \simeq -\frac{1}{\ln \beta J} \to 0$

Lave T $(\beta J \gg 1)$ $\quad \xi \simeq \frac{-1}{\ln(1-2e^{-2\beta J})} \simeq \frac{1}{2} e^{2\beta J} \to \infty$

Alt dette er i tråd med direkte fysiske innsikt!