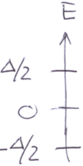
Tvístiga kerfi



Kórsumma
$$Z = 2\cosh\left(\frac{\beta\Delta}{2}\right)$$

Innri orkan

$$U = -\frac{d}{d\beta}(\ln Z) = -\frac{2\frac{\Delta}{2}\sinh\left(\frac{\beta\Delta}{2}\right)}{2\cosh\left(\frac{\beta\Delta}{2}\right)}$$

$$= \boxed{-\frac{\Delta}{2}\tanh\left(\frac{\beta\Delta}{2}\right)}$$

Varmarýmd

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V = k_B\left(\frac{\beta\Delta}{2}\right)^2 \frac{1}{\cosh^2\left(\frac{\beta\Delta}{2}\right)}$$

$$\boxed{= k_B\left(\frac{\beta\Delta}{2}\right)^2 \operatorname{sech}\left(\frac{\beta\Delta}{2}\right)}$$

Helmholtz fallið

$$F = -k_B T \ln Z = -k_B T \ln\left\{2\cosh\left(\frac{\beta\Delta}{2}\right)\right\}$$

og óreiðan

$$S = \frac{U-F}{T} = -\frac{\Delta}{2T}\tanh\left(\frac{\beta\Delta}{2}\right) + k_B \ln\left\{2\cosh\left(\frac{\beta\Delta}{2}\right)\right\}$$

Hreintóna sveifill

$$Z = \frac{e^{-\frac{\beta\hbar\omega}{2}}}{1-e^{-\beta\hbar\omega}}$$

$$U = -\frac{d}{d\beta}\ln Z = \frac{\hbar\omega}{2} + \frac{\hbar\omega e^{-\beta\hbar\omega}}{1-e^{-\beta\hbar\omega}}$$

$$= \boxed{\hbar\omega\left\{\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega}-1}\right\}}$$

$$\rightarrow C_V = \left(\frac{\partial U}{\partial T}\right)_V \quad \boxed{= k_B (\beta\hbar\omega)^2 \frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega} - 1)^2}}$$

Ef $\beta\hbar\omega \ll 1$ p.e. $T \rightarrow \infty$

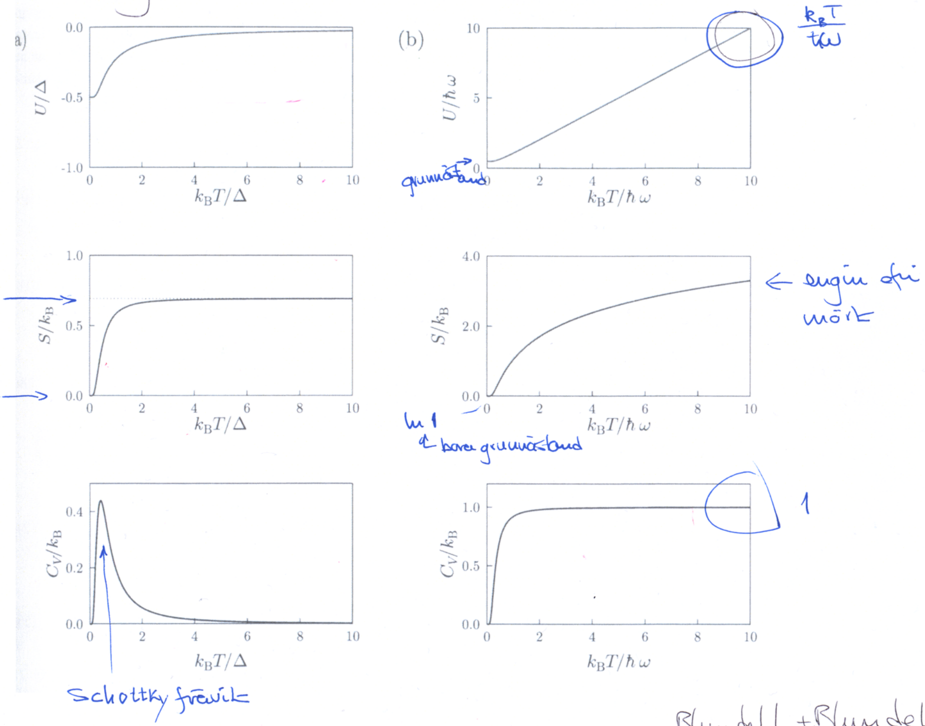
$$(e^{\beta\hbar\omega} - 1) = (1 + \beta\hbar\omega + \cdots - 1) \simeq \beta\hbar\omega$$ Mjög fallegt form

$$\rightarrow \boxed{\lim_{T\to\infty} C_V = k_B} \quad \text{og} \quad \boxed{U \rightarrow \frac{\hbar\omega}{2} + k_BT \simeq k_BT}$$

$$F = -k_BT \ln Z = \boxed{\frac{\hbar\omega}{2} + k_BT \ln\left(1 - e^{-\beta\hbar\omega}\right)}$$

$$S = \frac{U-F}{T} = \boxed{k_B\left\{\frac{\beta\hbar\omega}{e^{\beta\hbar\omega} - 1} - \ln\left(1 - e^{-\beta\hbar\omega}\right)\right\}}$$

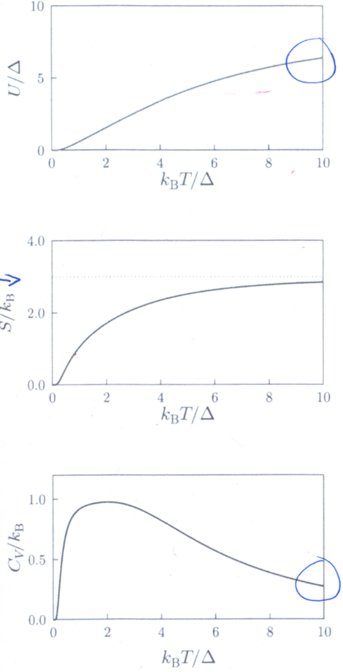
Tvístiga kerfi — Hreintóna sveifill



Blundell + Blundell

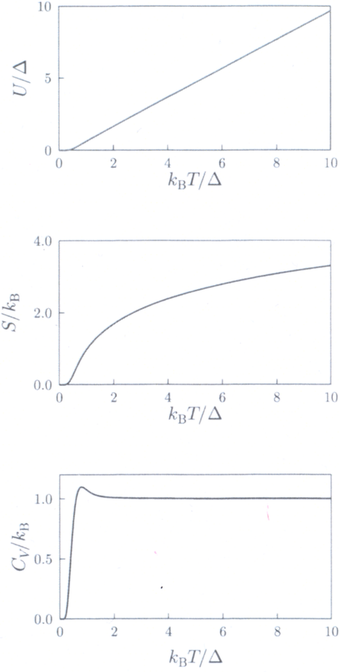
20-Stiga kerfi

tvíatómasameind - Snúningur



efri aðfella

(b)



Blundell + Blundell

Tvíatóma sameindir - snúningar

$$Z = \sum_{J=0}^{\infty} (2J+1)\, e^{-\beta\Delta J(J+1)}$$

fyrir hátt T, lítið $\beta\Delta$ má nálga

$$\simeq \int_0^{\infty} (2J+1)\, e^{-\beta\Delta J(J+1)}\, dJ$$

$$= \int_0^{\infty} dJ \left\{ \frac{d}{dJ} e^{-\beta\Delta J(J+1)} \right\} \left(-\frac{1}{\beta\Delta}\right)$$

$$= -\left\{ \frac{1}{\beta\Delta} e^{-\beta\Delta J(J+1)} \Big|_0^{\infty} \right\} = \frac{1}{\beta\Delta}$$

og því

$$\boxed{U = -\frac{d}{d\beta}\ln Z = \frac{1}{\beta} = k_B T}$$

$$\rightarrow \boxed{C_V = k_B}$$

fyrir hátt T

Röðirnar eru vel samleitnar og hægt að summa tölulega

Grunn hugmyndin

Nota Körsummuna

$$\boxed{Z = \sum_{\alpha} e^{-\beta E_\alpha}}$$

Reikna ástandaföllin
(functions of state)

$\downarrow$

t.d.

U, F

S, p, H, G

$C_V \ldots\ldots$

Bera saman $k_B T$ og „Δ"

Ef $k_B T << \Delta_1$ mun kerfið sitja í grunnástandinu

Ef $k_B T >> \Delta_n$ fyrir öll n þá eru öll ástöndin með jafna sætni

Ef $N \to \infty$ og $k_B T >> \Delta_n$ þá vex $\langle E \rangle \sim T$

Óháðir þættir í orkurófi

Til dæmis sveiflur og snúningar fyrir tvíatóma sameindina

$$E_{\cdot\cdot nJ} = E_{\cdot\cdot} + \hbar\omega(n+\tfrac{1}{2}) + \Delta J(J+1)$$

þá er kórsumman

$$Z = \sum_{\cdot\cdot}\sum_{n}\sum_{J} \exp\left[-\beta E_{\cdot\cdot} - \beta\hbar\omega(n+\tfrac{1}{2}) - \beta\Delta J(J+1)\right]$$

$$= \sum_{\cdot\cdot} e^{-\beta E_{\cdot\cdot}} \sum_{n} \exp\left\{-\beta\hbar\omega(n+\tfrac{1}{2})\right\} \sum_{J} \exp\left\{-\beta\Delta J(J+1)\right\}$$

$$= \boxed{Z_{\cdot\cdot}\cdot Z_{n}\cdot Z_{J}}$$

margfeldi kórsummanna fyrir hvern þátt

Meðseglun

$\frac{1}{2}$- tölu spuni í ytra segulsviði

$|\uparrow\rangle$ með orku $+\mu_B B$

$|\downarrow\rangle$ – " – $-\mu_B B$

Spuni samsíða eða andsamsíða $\vec{B} = B\hat{z}$

$\mu_B = \frac{e\hbar}{2m}$, $E = -\vec{m}\cdot\vec{B}$

Fyrir rafeind með hleðslu $-e$ er $\perp$ andsamsíða segulvoginu $\vec{m}$.

$$Z_1 = \exp\{\beta\mu_B B\} + \exp\{-\beta\mu_B B\} = 2\cosh(\beta\mu_B B)$$

Hugsum okkur N óháða spuna

spunarvíxlverkun ekki hér

$$\rightarrow Z_N = Z_1^N$$

Greinilega er ástandið $\cdots\downarrow\downarrow\downarrow\downarrow\cdots$ ekki líklegt
þó orkulega hagkvæmt

Væntanlega eru mjög mörg ástönd með heildarspuna ~ 0

$$F = U - \underbrace{TS}$$

vaxandi vægi með
vaxandi T

skiptir miklu máli
þegar T er lítið

$$F = -k_B T \ln Z_N = -N k_B T \ln\left\{2\cosh(\beta\mu_B B)\right\}$$

$$m = -\left(\frac{\partial F}{\partial B}\right)_T = N\mu_B \tanh(\beta\mu_B B)$$

<u>Seglun</u> $M = \frac{m}{V} = \frac{N\mu_B}{V}\tanh(\beta\mu_B B)$

<u>Vidtak</u> fyrir lítið segulsvið þegar $\beta\mu_B B \ll 1$

og $\tanh x \approx x$ ~~fást~~

$$M \simeq \frac{N\mu_B}{V}\beta\mu_B B = \mu_B\left(\frac{N}{V}\right)\left(\frac{\mu_B B}{k_B T}\right)$$

$\boxed{\bar{B} = \mu_0(\bar{H}+\bar{M})}$, og fyrir veika miðseglun $M \simeq \chi H$, $\chi \ll 1$

$$\to B \simeq \mu_0(1+\chi)H \simeq \mu_0\frac{1+\chi}{\chi}M \simeq \frac{\mu_0 M}{\chi}$$

$$\chi \simeq \frac{N}{V}\frac{\mu_0\mu_B^2}{k_B T}$$

<u>Lögmál Curie</u>

$$\chi \sim \frac{1}{T}$$

Ef $\qquad M \simeq \mu_B \left(\frac{N}{V}\right)\left(\frac{\mu_B B}{k_B T}\right)$

$$\rightarrow \quad m = VM \simeq \mu_B N \frac{\mu_B B}{k_B T} = \mu_B N \, \mu_B \beta B$$

$$\rightarrow \quad \boxed{\frac{m}{\mu_B N} = \beta \mu_B B}$$

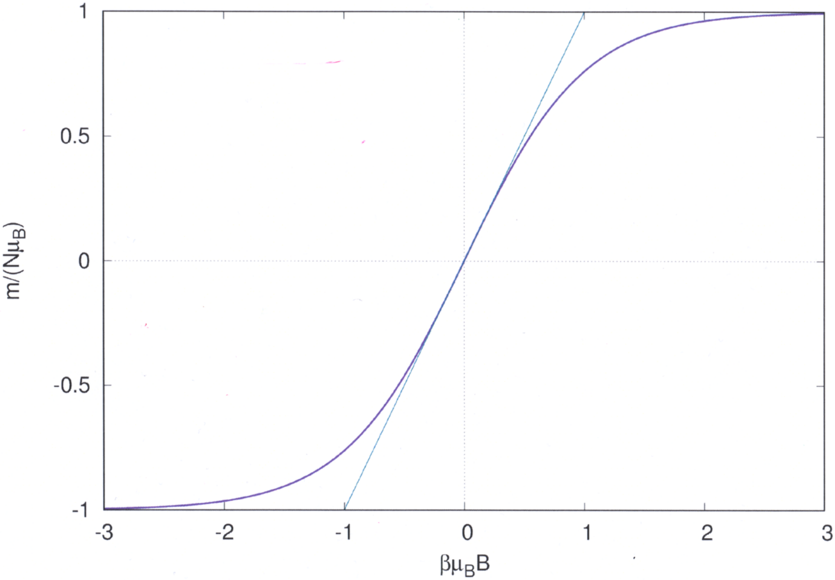
þar sem Curie lögmál er í lagi

annars

$$\boxed{\frac{m}{\mu_B N} = \tanh(\beta \mu_B B)}$$

teiknum

$\boxed{\text{Engin segulm (eða segulvægi) án ytra sviðs } B}$


1
0.5
0
-0.5
-1
m/(Nμ_B)
-3
-2
-1
0
1
2
3
βμ_BB