Physics 552: Final

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Problem 1: One dimensional harmonic chain (20 pts.)

Consider a one-dimensional chain with length L containing N atoms coupled by nearest-neighbor harmonic forces. Compute the Debye frequency for this system. Calculate also the heat capacity and estimate its limit as $T \to 0$.

$$\omega^2 = \left(\frac{\pi c}{L}\right)^2 \alpha^2 \qquad \alpha = 0, 1, 2, \ldots$$

Debye frequency:

$$\nu = \frac{L}{\pi c}\omega \qquad d\nu = \frac{L}{\pi c} d\omega \quad \Rightarrow \int_0^{\omega_D} d\omega \left(\frac{L}{\pi c}\right) = N$$

$$\omega_D = \frac{N \pi c}{L}$$

heat capacity:

$$\bar{E} = \sum_{\alpha=0} \hbar\omega_\alpha + \sum_\alpha \frac{e^{-\beta\hbar\omega_\alpha}}{1 - e^{-\beta\hbar\omega_\alpha}} \hbar\omega_\alpha$$

$$\bar{E} = \sum_\alpha \hbar\omega_\alpha + \sum_\alpha \frac{\hbar\omega_\alpha}{e^{\beta\hbar\omega_\alpha} - 1} \to \frac{L}{\pi c}\int d\omega \left[\frac{\hbar\omega}{2} + \frac{\hbar\omega}{(e^{\beta\hbar\omega} - 1)}\right]$$

$$C = \frac{\partial \bar{E}}{\partial T} = -\frac{\partial \bar{E}}{\partial \beta}\left(-\frac{1}{k_B T^2}\right)$$

$$\frac{\partial \bar{E}}{\partial \beta} = -\frac{\hbar L}{\pi c}\int_0^{\omega_D} d\omega\, \omega \frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega} - 1)^2}\, \hbar\omega$$

$$= -\frac{\hbar^2 L}{\pi c}\int_0^{\omega_D} \omega^2 d\omega \frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega} - 1)^2}$$

$x = \beta\hbar\omega$

$x_D = \beta\hbar\omega_D$

as $T \to 0$ $\beta \to \infty$

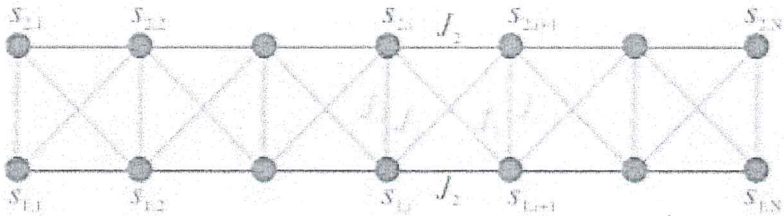
$x_D \to \infty$

$$= -\frac{\hbar^2 L}{\pi c}\int_0^\infty \frac{x^2 dx}{\beta^3 \hbar^3} \frac{e^x}{(e^x - 1)^2}$$

$$C = \frac{\cancel{\hbar^2} L\, k_B^{\cancel{3}\,2} T^{\cancel{3}}}{\pi c \hbar^{\cancel{3}}\, \cancel{k_B} \cancel{T^2}}\int_0^\infty \frac{x^2 dx\, e^x}{(e^x - 1)^2} = \frac{k_B T L}{\hbar \pi c}\int_0^\infty \frac{x^2 dx\, e^x}{(e^x - 1)^2}$$

Problem 2: Ising ladder (20 pts.)

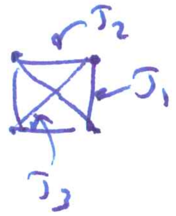
Consider an Ising ladder, made up of two chains running parallel to each other, as shown.



The Hamiltonian is: $H = -J_1 \sum_{\langle i,j \rangle_|} \sigma_i \sigma_j - J_2 \sum_{\langle i,j \rangle_-} \sigma_i \sigma_j - J_3 \sum_{\langle i,j \rangle_X} \sigma_i \sigma_j$. The three summations correspond to the set of bonds with different directions (vertical, horizontal, diagonal with respect to the figure).

1. Draw the ordered states you would expect for the following cases. If you expect competing ordered states indicate both, and also the limits in which one would dominate over the other. (5 pts.) → ferro $\begin{matrix}+++\\+++\end{matrix}$ or $\begin{matrix}---\\---\end{matrix}$
   1. $J_3 = 0, J_1 > 0 J_2 > 0.$ → ferro
   2. $J_3 = 0, J_1 < 0, J_2 < 0.$ → antiferro $\begin{matrix}+-+\\-+-\end{matrix}$ (J_3 small)
   3. $J_3 < 0, J_1 < 0, J_2 < 0.$ → competing: J_3 small, J_3 large $(J_3 \gg J)$ $\begin{matrix}+-+\\+-+\end{matrix}$
2. Write down the elements of the transfer matrix for this system.
3. Solve this system within mean-field theory, for the case $J_3 = 0, J_1 < 0, J_2 < 0.$

2. transfer matrix



$\sigma_{L1} \to \bullet \qquad \bullet \, \sigma_{R1}$

$\sigma_{L2} \to \bullet \qquad \bullet \, \sigma_{R2}$

R \ L	1 1	1 −1	−1 1	−1 −1
1 1	$e^{2J_2+2J_3+J_1}$	1	1	$e^{-2J_2-2J_3+J_1}$
1 −1	1	$e^{2J_2-2J_3-J_1}$	$e^{-2J_2+2J_3-J_1}$	1
−1 1	1	$e^{-2J_2+2J_3-J_1}$	$e^{2J_2-2J_3-J_1}$	1
−1 −1	$e^{-2J_2-2J_3+J_1}$	1	1	$e^{2J_2+2J_3+J_1}$

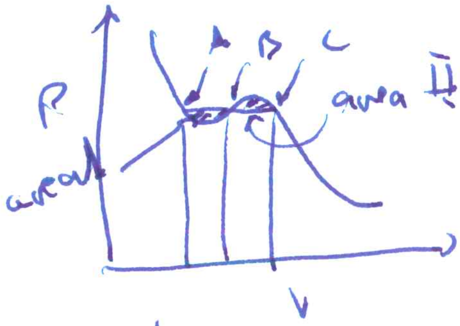
$$\bar{\bar{T}} = e^{J_2(\sigma_{L1}\sigma_{R1} + \sigma_{L2}\sigma_{R2}) + J_3(\sigma_{L1}\sigma_{R2} + \sigma_{L2}\sigma_{R1}) + \frac{J_1}{2}(\sigma_{L1}\sigma_{L2} + \sigma_{R1}\sigma_{R2})}$$

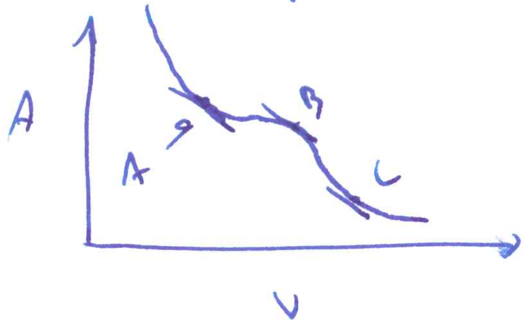
$$Q = \mathrm{Tr}\, \bar{\bar{T}}^N$$

part 3 on worksheet +

Problem 3: Maxwell Construction (20 pts.)

Deduce the Maxwell construction using stability properties of the Helmholtz free energy rather than the Gibbs free energy.





$$P = -\frac{\partial A}{\partial V}$$

$$G = A + PV$$

$$A = G - PV$$

(stability)

$$\frac{\partial P}{\partial V} = -\frac{\partial^2 A}{\partial V^2} < 0$$

$$G_C - G_A = 0$$

$$A_C - A_A = P_A(V_C - V_A)$$

$$\int_A^B P\,dV = P_A(V_B - V_A) - \text{area I}$$

$$\int_B^C P\,dV = P_A(V_C - V_B) + \text{area II}$$

change in A: $\int_A^C P\,dV = P(V_C - V_A)$

so area I and area II must cancel

Problem 4: Bose-Fermi mixture (20 pts.)

Consider a system of non-interacting bosons and fermions with the same masses in a box of side length L. The bosons are spin-1, the fermions are spin-3/2. Calculate the partition function, the average number of particles, and the pressure for this system. Estimate the temperature at which the bosons would condense.

$$\varepsilon_{\vec{l}} = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 (l_x^2 + l_y^2 + l_z^2) \quad \text{for both}$$

$$Q = Q_{\text{Boson}} \, Q_{\text{fermion}}$$

$$Q_{\text{Boson}} = \prod_{\vec{l}} \left(\frac{1}{1 - e^{-\beta(\varepsilon_{\vec{l}} - \mu)}} \right)^3 \qquad Q_{\text{fermion}} = \prod_{\vec{l}} \left(1 + e^{-\beta(\varepsilon_{\vec{l}} - \nu)}\right)^4$$

μ – chemical potential for bosons

ν – chemical potential for fermions

$$\Omega = -\frac{1}{\beta} \ln Q_{\text{Boson}} Q_{\text{fermion}} = - \cancel{\frac{1}{\beta}\sum_{\vec{l}}} \ln$$

$$= -\frac{1}{\beta}\left[-3\sum_{\vec{l}} \ln\left(1 - e^{-\beta(\varepsilon_{\vec{l}} - \mu)}\right) + 4 \sum_{\vec{l}} \ln\left(1 + e^{-\beta(\varepsilon_{\vec{l}} - \nu)}\right)\right]$$

$$\bar{N} = \bar{N}_b + \bar{N}_f \qquad \bar{N}_b = -\frac{\partial \Omega}{\partial \mu} = 3 \sum_{\vec{l}} \frac{1}{e^{\beta(\varepsilon_{\vec{l}} - \mu)} - 1}$$

$$\bar{N}_f = -\frac{\partial \Omega}{\partial \nu} = 4 \sum_{\vec{l}} \frac{1}{e^{\beta(\varepsilon_{\vec{l}} - \nu)} + 1}$$

$$P = -\frac{\Omega}{V}$$

condensation temperature: $\boxed{3 \bar{n}_b \lambda_T^3 = g_{3/2}(1)}$

Problem 5: Fokker-Planck equation in the short time limit

Consider the 'short time' relaxation of a Brownian particle. The Langevin equation for the velocity is $m\frac{\mathrm{d}v}{\mathrm{d}t} = -\gamma v + \xi(t)$, where m is the mass of the particle, γ is the friction constant, and $\xi(t)$ is a random force obeying $\langle \chi(t) \rangle = 0$, and $\langle \xi(t)\xi(t')\rangle = g\delta(t-t')$. Derive the Fokker-Planck equation valid for the probability $P(v,t)$. The probability that the velocity of the system is between v and $v + \mathrm{d}v$ at a given time t is $P(v,t)\mathrm{d}v$.

$g(v,t)_{\xi} \rightarrow \int_V \frac{\partial g(v,t)}{\partial t} d\vec{v} = -\int_A g(v,t)\,\dot{v}\, d\vec{\sigma}$

1D system $\Rightarrow$ Gauss' law $\Rightarrow$ $\frac{\partial g(v,t)}{\partial t} = -\frac{\partial[g(v,t)\dot{v}]}{\partial v}$

$\dot{v} = -\frac{\gamma}{m}v + \frac{\xi(t)}{m}$

$\frac{\partial g\dot{v}}{\partial v} = \frac{\partial}{\partial v}\left[-\frac{\gamma}{m}vg + \frac{\xi(t)}{m}g\right] = -\frac{\gamma}{m}g - \frac{\gamma}{m}v\frac{\partial g}{\partial v} + \frac{\xi(t)}{m}\frac{\partial g}{\partial v}$

$\Rightarrow \quad \frac{\partial g}{\partial t} = \frac{\gamma}{m}g + \frac{\gamma}{m}v\frac{\partial g}{\partial v} - \frac{\xi(t)}{m}\frac{\partial g}{\partial v}$

$\frac{\partial g}{\partial t} = -L_0 g - L_1(t)\, g \qquad L_0 = \frac{\gamma}{m} + \frac{\gamma}{m}v\frac{\partial}{\partial v}$

$L_1(t) = \frac{\xi(t)}{m}$

$g(t) = e^{-L_0 t}\sigma(t) \Rightarrow \frac{\partial g(t)}{\partial t} = -L_0 e^{-L_0 t}\sigma(t) + e^{-L_0 t}\frac{\partial \sigma(t)}{\partial t}$

$\Rightarrow \frac{\partial \sigma(t)}{\partial t} = -V_1(t)\,\sigma(t) \qquad V_1(t) = e^{L_0 t} L_1(t) e^{-L_0 t}$

$\sigma(t) = e^{-\int_0^t dt' V_1(t')}\sigma(0)$

$\langle \sigma(t) \rangle = \sum_{n=0}^{\infty} \frac{\langle [\int_0^t dt' V_1(t')]^n \rangle}{n!}\sigma(0)$

$\int_0^t \dots \int_0^t dt_1 \dots dt_n \langle V_1(t_1) \dots V_1(t_n) \rangle$

cont'd worksheet 2

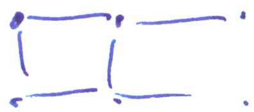
Worksheet 1: (number of sites => 2N)

mean-field:

easiest approach => solve ferromagnetic case

→ obtain $\bar{\sigma}$, and then assign $\bar{\sigma}$ to one sublattice, $-\bar{\sigma}$ to other sublattice

$$H = -J_1 \sum_{\langle ij \rangle} \sigma_i \sigma_j - J_2 \sum_{\langle\langle ij \rangle\rangle} \sigma_i \sigma_j$$



$$H_{MF} = -J_1 \sum_i \sigma_i \bar{\sigma} - 2J_2 \sum_i \sigma_i \bar{\sigma} + N J_1 \bar{\sigma}^2 + 2N J_2 \bar{\sigma}^2$$

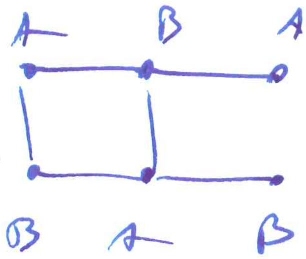
$$Q = \cancel{\sum \cdots \sum_{\sigma \ \sigma}} \left[\sum_\sigma e^{(J_1 \bar{\sigma} + 2J_2 \bar{\sigma})\sigma} \right]^{2N} e^{-N J_1 \bar{\sigma}^2 - 2N J_2 \bar{\sigma}^2}$$

~~free energy:~~ $\cancel{-2N \tanh}$ $= \cosh(\bar{\sigma}(2J_2 + J_1))^{2N} e^{-N\bar{\sigma}^2(J_1 + 2J_2)}$

free energy: $f = -\ln Q$

$$\frac{\partial f}{\partial \bar{\sigma}} = 0 \Rightarrow \boxed{\tanh(\bar{\sigma}(2J_2 + J_1)) = \frac{1}{2}\bar{\sigma}(J_1 + 2J_2)}$$

for antiferromagnetic case



$$\bar{\sigma}_A = \bar{\sigma}$$

$$\bar{\sigma}_B = -\bar{\sigma}$$

Worksheet 2:

n - odd $\quad \int dt_1 \dots dt_n \langle V_1(t_1) \dots V_1(t_n) \rangle = 0$

n - even $\quad \frac{2n!}{n!\,2^n} \int \dots \int dt_1 \dots dt_n \langle V_1(t_1) V_1(t_2) \rangle \dots$

$$\Rightarrow \sum_{n=0}^{\infty} \frac{\langle [\int_0^t dt' \, V_1(t')]^{2n} \rangle}{2n!} = \sum_{n=0}^{\infty} \frac{1}{n!} \left[\frac{\int_0^t \int_0^t dt_1 dt_2 \langle V_1(t_1) V_1(t_2) \rangle}{2 \cancel{n}} \right]^n$$

$$\Rightarrow \int_0^{t_1} \int_0^t dt_1 dt_2 \langle V_1(t_1) V_1(t_2) \rangle$$

$$= \frac{1}{m^2} \int_0^t \int_0^t dt_1 dt_2 \, e^{\lambda_0 t_1} \frac{\partial}{\partial v} e^{-\lambda_0 (t_1 - t_2)} \frac{\partial}{\partial v} e^{-\lambda_0 t_2} \langle \xi(t_1) \xi(t_2) \rangle$$

$$= \frac{g}{m^2} \int_0^t dt' \, e^{\lambda_0 t'} \frac{\partial^2}{\partial v^2} e^{-\lambda_0 t'}$$

$$\Downarrow$$

$$\sigma(t) = e^{\frac{g}{2m^2} \int_0^t dt' \, e^{\lambda_0 t'} \frac{\partial^2}{\partial v^2} e^{-\lambda_0 t'}} \sigma(0)$$

$$\frac{\partial \sigma}{\partial t} = \frac{g}{2m^2} e^{\lambda_0 t} \frac{\partial^2}{\partial v^2} e^{-\lambda_0 t} \sigma(t) = \frac{g}{2m^2} e^{\lambda_0 t} \frac{\partial^2}{\partial v^2} \varrho(t)$$

F.P.E. $\Rightarrow$

$$\boxed{\frac{\partial P(v,t)}{\partial t} = \frac{\gamma}{m} P(v,t) + \frac{\gamma}{m} v \frac{\partial P(v,t)}{\partial v} + \frac{g}{2m^2} \frac{\partial^2}{\partial v^2} P(v,t)}$$