Statistical Mechanics - Class Exercise 1

Exercise 0080 - The spreading of a free particle

Given a free classic particle $H=\frac{p^2}{2m}$, that has been prepared in time $t=0$ in a state represented by the probability function

$$\rho_{t=0}(x,p)\propto\exp\left(-a(x-x_0)^2-b(p-p_0)^2\right)$$

1. Normalize $\rho_{t=0}(x,p)$.
2. Calculate $\langle x\rangle$, $\langle p\rangle$, σ_x, σ_p, E
3. Express the random variables $\hat{x}_t,\hat{p}_t$ with $\hat{x}_{t=0},\hat{p}_{t=0}$
4. Express $\rho_t(x,p)$ with $\rho_{t=0}(x,p)$. (Hint: 'variables replacement').
5. Mention two ways to calculate the sizes appeared in paragraph (2) in time t. use the simple one to express $\sigma_x(t),\sigma_p(t)$ with $\sigma_x(t=0),\sigma_p(t=0)$ (that you've calculated in (2)).

Answer

1. We know that $\rho_{t=0}(x,p)=2\sqrt{ab}Ne^{-a(x-x_0)^2-b(p-p_0)^2}$

$$\begin{aligned}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\rho_{t=0}(x,p)\frac{dxdp}{2\pi}=&1\\ =&N\int_{-\infty}^{\infty}e^{-a(x-x_0)^2}dx\int_{-\infty}^{\infty}e^{-b(p-p_0)^2}\frac{dp}{2\pi}=N\frac{1}{2\sqrt{ab}}=1\\ &\to N=2\sqrt{ab}\end{aligned}$$

2. $\langle A(x,p)\rangle=\int\int\rho_{t=0}(x,p)A(x,p)\frac{dxdp}{2\pi}$

$$\begin{aligned}\langle x\rangle=&2\sqrt{ab}\int\int e^{-a(x-x_0)^2-b(p-p_0)^2}x\frac{dxdp}{2\pi}\\ =&\sqrt{\frac{a}{\pi}}\int e^{-a(x-x_0)^2}xdx=\sqrt{\frac{a}{\pi}}\int e^{-ax^2}(x+x_0)dx\\ =&x_0\sqrt{\frac{a}{\pi}}\int e^{-ax^2}dx+\sqrt{\frac{a}{\pi}}\int e^{-ax^2}xdx=x_0\end{aligned}$$

In the same way $\langle p\rangle=p_0 2$\sqrt{ab}

$$\sigma_x^2=\left\langle(x-\langle x\rangle)^2\right\rangle=\langle x^2\rangle-\langle x\rangle^2$$

$$\begin{aligned}\langle x^2\rangle=&\sqrt{\frac{a}{\pi}}\int e^{-a(x-x_0)^2}x^2dx=\sqrt{\frac{a}{\pi}}\int e^{-ax^2}\left(x^2+2xx_0+x_0^2\right)dx=\\ =&x_0^2-\sqrt{\frac{a}{\pi}}\frac{d}{da}\int e^{-ax^2}dx=x_0^2-\sqrt{\frac{a}{\pi}}\frac{d}{da}\sqrt{\frac{\pi}{a}}=x_0^2+\frac{1}{2a}\end{aligned}$$

$$\sigma_x = \sqrt{\langle x^2 \rangle - x_0^2} = \sqrt{\frac{1}{2a}}$$

In the same way $\sigma_p = \sqrt{\frac{1}{2b}}$

$$\rightarrow N = 2\sqrt{ab} = \frac{1}{\sigma_x \sigma_p}$$

$$\begin{aligned} E = \langle \mathcal{H}(x,p) \rangle &= 2\sqrt{ab} \int \int e^{-a(x-x_0)^2 - b(p-p_0)^2} \frac{p^2}{2m} \frac{dxdp}{2\pi} \\ &= \frac{1}{2m}\sqrt{\frac{b}{\pi}} \int e^{-b(p-p_0)^2} p^2 d = \frac{1}{2m}\left(p_0^2 + \frac{1}{2b}\right) = \frac{p_0^2}{2m} + \frac{\sigma_p^2}{2m} \end{aligned}$$

3. The equations of motion are

$$\begin{aligned} \dot{x} &= \frac{\partial \mathcal{H}}{\partial p} = \frac{p}{m} \\ \dot{p} &= -\frac{\partial \mathcal{H}}{\partial x} = 0 \end{aligned}$$

$$\begin{aligned} x &= x_0 + \frac{p}{m} t \\ p &= p_0 \end{aligned}$$

So

$$\begin{aligned} \hat{x_t} &= \hat{x}_{t=0} + \frac{\hat{p}_{t=0}}{m} t \\ \hat{p}_t &= \hat{p}_{t=0} \end{aligned}$$

4. we change the variables from Hizenberg picture to Schrodinger picture

$$\rho_t(x,p) \frac{dxdp}{2\pi} = \rho_{t=0}(x',p') \frac{dx'dp'}{2\pi} = \rho_{t=0}\left(x - \frac{p}{m}t, p\right) \left(\frac{dx'}{dx} \frac{dp'}{dp}\right) \frac{dxdp}{2\pi}$$

$$\rightarrow \rho_t(x,p) = \rho_{t=0}\left(x - \frac{p}{m}t, p\right)$$

5. We can calculate directly with $\rho_t(x,p)$

$$\begin{aligned} \langle x \rangle_t =& 2\sqrt{ab} \int \int e^{-a\left(x - \left(x_0 + \frac{p_0}{m}t\right)\right)^2 - b(p-p_0)^2} x \frac{dxdp}{2\pi} \\ =& \sqrt{\frac{a}{\pi}} \int e^{-a\left(x - \left(x_0 + \frac{p_0}{m}t\right)\right)^2} x dx = \sqrt{\frac{a}{\pi}} \int e^{-ax^2} \left(x + \left(x_0 + \frac{p_0}{m}t\right)\right) dx \\ =& \left(x_0 + \frac{p_0}{m}t\right) \sqrt{\frac{a}{\pi}} \int e^{-ax^2} dx + \sqrt{\frac{a}{\pi}} \int e^{-ax^2} x dx = x_0 + \frac{p_0}{m}t \end{aligned}$$

Or we can use the the characteristics of random variables

$$\langle x \rangle_t = \langle x_t \rangle = \left\langle x_{t=0} + \frac{p_{t=0}}{m} t \right\rangle = x_0 + \frac{p_0}{m} t$$

In the same way $\langle p\rangle_t = p_0$

$$\sigma_x^2(t) = \left\langle (x - \langle x\rangle)^2 \right\rangle_t = \langle x_t^2\rangle - \langle x_t\rangle^2$$

$$=\left\langle x_{t=0}^2 + 2x_{t=0}\frac{p_{t=0}}{m}t + \left(\frac{p_{t=0}}{m}t\right)^2 \right\rangle - \left(x_0 + \frac{p_0}{m}t\right)^2$$
$$=\langle x_{t=0}^2\rangle + 2\langle x_{t=0}\rangle \frac{\langle p_{t=0}\rangle}{m}t + \left(\frac{t}{m}\right)^2 \langle p_{t=0}^2\rangle - \left(x_0 + \frac{p_0}{m}t\right)^2$$
$$=x_0^2 + \frac{1}{2a} + 2x_0\frac{p_0}{m}t + \left(\frac{t}{m}\right)^2\left(p_0^2 + \frac{1}{2b}\right) - \left(x_0^2 + 2x_0\frac{p_0}{m}t + \left(\frac{t}{m}\right)^2 p_0^2\right) = \frac{1}{2a} + \left(\frac{t}{m}\right)^2 \frac{1}{2b}$$

$$\sigma_x(t) = \sqrt{\frac{1}{2a} + \left(\frac{t}{m}\right)^2 \frac{1}{2b}} = \sqrt{\sigma_x^2(0) + \left(\frac{t}{m}\right)^2 \sigma_p^2(0)}$$

σ_p stay $\sigma_p = \sqrt{\frac{1}{2b}}$

$$E(t) = \left\langle \frac{p_t^2}{2m} \right\rangle = \frac{1}{2m}\left(p_0^2 + \sigma_p^2\right)$$

micro-canonical state and spectral functions

For the Hamiltonian $H(x,p)$ the distribution function

$$\rho(x,p)\frac{dxdp}{2\pi}$$

is the probability to the system to be in $x < \hat{x} < x + dx, p < \hat{p} < p + dp$
In equilibrium the distribution function is a function of the energy and it constant in time

$$\rho(x,p) = F(H(x,p))$$

For micro-canonical state, the energy is given and the distribution function

$$\rho(x,p) = C\delta(E - H(x,p)) = \frac{1}{g(E)}\delta(E - H(x,p))$$

where $g(E)$ is the density of states.
For canonical state, the temperature is given and the distribution function

$$\rho(x,p) = \frac{1}{Z}e^{-\beta H(x,p)}$$

or, for discrete state

$$\rho(r) = \frac{1}{Z}e^{-\beta E_r}$$

where Z is the partition function

$$Z(\beta) = \int e^{-\beta H(x,p)}\frac{dxdp}{2\pi}$$

or

$$Z(\beta) = \sum_r e^{-\beta E_r} = \int g(E)\, e^{-\beta E} dE$$

Also, we can see that

$$E = \langle H \rangle = \sum_r \rho(r) E_r = \sum_r \frac{1}{Z} e^{-\beta E_r} E_r = -\sum_r \frac{1}{Z} \frac{\partial}{\partial \beta} e^{-\beta E_r} = -\frac{1}{Z} \frac{\partial}{\partial \beta} \sum_r e^{-\beta E_r}$$

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

Exercise 0060 - Oscillator in a micro-canonical state

Assume that a harmonic oscillator with frequency Ω and mass m is prepared in a micro-canonical state with energy E.

1. Write the probability distribution $\rho(x,p)$
2. Find the projected probability distribution $\rho(x)$

Answer

1.

$$H = \frac{p^2}{2m} + \frac{m\Omega^2}{2} x^2$$

so the probability distribution is

$$\rho(x,p) = \frac{1}{g(E)} \delta\left(\frac{p^2}{2m} + \frac{m\Omega^2}{2} x^2 - E\right)$$

2. to find $\rho(x)$ we calculate

$$\rho(x) = \int \rho(x,p) \frac{dp}{2\pi} = \frac{1}{g(E)} \int_{-\infty}^{\infty} \delta\left(\frac{p^2}{2m} + \frac{m\Omega^2}{2} x^2 - E\right) \frac{dp}{2\pi} =$$

we use $\delta(g(x)) = \sum_i \frac{\delta(x - x_i)}{|g'(x_i)|}$

$$= \frac{1}{g(E)} \int_{-\infty}^{\infty} \frac{1}{\left|\frac{p}{m}\right|} \left[\delta\left(p + \sqrt{2mE - m^2\Omega^2 x^2}\right) + \delta\left(p - \sqrt{2mE - m^2\Omega^2 x^2}\right)\right] \frac{dp}{2\pi} = \frac{1}{\pi\Omega g(E)} \frac{1}{\sqrt{\frac{2E}{m\Omega^2} - x^2}}$$

$$\rho(x) = \begin{cases} \frac{1}{\pi\Omega g(E)} \frac{1}{\sqrt{\frac{2E}{m\Omega^2} - x^2}} & x^2 < \frac{2E}{m\Omega^2} \\ 0 & \text{else} \end{cases}$$

To find $g(E)$ we calculate

$$\int \rho(x)\, dx = 1$$

$$\frac{1}{\pi\Omega g(E)} \int_{-\sqrt{\frac{2E}{m\Omega^2}}}^{\sqrt{\frac{2E}{m\Omega^2}}} \frac{1}{\sqrt{\frac{2E}{m\Omega^2} - x^2}} dx = \frac{1}{\pi\Omega g(E)} \int_{-1}^{1} \frac{1}{\sqrt{1 - u^2}} du$$

$$= \frac{1}{\pi\Omega g(E)} \arcsin(u)\,|_{-1}^{1} = \frac{1}{\Omega g(E)} = 1$$

$$g(E) = \frac{1}{\Omega}$$

$$\rho(x) = \begin{cases} \frac{1}{\pi\sqrt{\frac{2E}{m\Omega^2} - x^2}} & x^2 < \frac{2E}{m\Omega^2} \\ 0 & \text{else} \end{cases}$$

$$\rho(x,p) = \Omega\delta\left(\frac{p^2}{2m} + \frac{m\Omega^2}{2}x^2 - E\right)$$

Exercise 0150 - Spectral functions for N spins

Consider an N spin system:

$$\hat{H} = \sum_{\alpha=1}^{N} \frac{\varepsilon}{2}\hat{\sigma}_z^{(\alpha)}$$

Calculate $Z_N(\beta)$ in two different ways:

1. The short way - Calculate $Z_N(\beta)$ by factoring the sum.
2. The long way - Write the energy levels E_n of the system. Mark with $n = 0$ the ground level, and with $n = 1, 2, 3, ...$ the excited levels. Find the degeneracy g_n of each level. Use these results to express $Z_N(\beta)$, and show the that the same result is obtained.

Answer

1. The short way

$$\hat{H}_1 = \frac{\varepsilon}{2}\hat{\sigma}_z$$

$$Z_1(\beta) = e^{-\beta\left(\frac{\varepsilon}{2}\right)} + e^{-\beta\left(-\frac{\varepsilon}{2}\right)} = 2\cosh\left(\frac{\beta\varepsilon}{2}\right)$$

$$Z_N(\beta) = \sum_{\sigma^1=\pm1} \cdots \sum_{\sigma^N=\pm1} e^{-\beta\sum_{\alpha=1}^{N}\frac{\varepsilon}{2}\sigma^\alpha} = \prod_{\alpha=1}^{N}\sum_{\sigma^\alpha=\pm1} e^{-\beta\frac{\varepsilon}{2}\sigma^\alpha} = (Z_1(\beta))^N = 2^N\cosh^N\left(\frac{\beta\varepsilon}{2}\right)$$

2. The long way
n is the number of spin "up"

$$E_n = \frac{\varepsilon}{2}n - \frac{\varepsilon}{2}(N-n)$$

the degeneracy of n "up" and $N-n$ "down"

$$g_n = \frac{N!}{(N-n)!n!}$$

$$Z_N(\beta) = \sum_{n=0}^{N} g_n e^{-\beta E_n} = \sum_{n=0}^{N}\frac{N!}{(N-n)!n!}e^{-\beta\left[\frac{\varepsilon}{2}n - \frac{\varepsilon}{2}(N-n)\right]} =$$

$$= \sum_{n=0}^{N} \frac{N!}{(N-n)!n!} \left(e^{-\beta\frac{\varepsilon}{2}}\right)^{n} \left(e^{\beta\frac{\varepsilon}{2}}\right)^{(N-n)}$$

from the binomial theorem $(a+b)^N = \sum_{n=0}^{N} \frac{N!}{(N-n)!n!} a^n b^{N-n}$ we get

$$Z_N(\beta) = \left(e^{-\beta\frac{\varepsilon}{2}} + e^{\beta\frac{\varepsilon}{2}}\right)^N = 2^N \cosh^N\left(\frac{\beta\varepsilon}{2}\right)$$

Statistical Mechanics - Class Exercise 2

Free energy and entropy

The partition function

$$Z(\beta, X) = \sum_r e^{-\beta E_r}$$

We can define a function

$$Z(\beta, X) = e^{-\beta F(\beta, X)}$$

so

$$F(\beta, X) = -\frac{1}{\beta} \ln Z$$

We can define the entropy

$$S = -\sum_r p_r \ln p_r = -\sum_r p_r (-\beta E_r - \ln Z) = \beta \sum_r p_r E_r + \sum_r p_r \ln Z = \beta E + \ln Z$$

$$\to F = E - TS$$

Exercise 1817 - Adiabatic cooling of spins

Consider an ideal gas whose N atoms have mass m, spin 1/2 and a magnetic moment γ. The kinetic energy of a particle is $p^2/(2m)$ and the interaction with the magnetic field B is $\pm\gamma B$ for up/down spins.

1. Calculate the entropy as $S(T, B) = S_{kinetic} + S_{spin}$.
2. Consider an adiabatic process in which the magnetic field is varied from B to zero. Show that the initial and final temperatures T_i and T_f are related by the equation:

$$\ln \frac{T_f}{T_i} = \frac{2}{3N} [S_{spin}(T_i, B) - S_{spin}(T_f, 0)]$$

3. Find the solution for $\frac{T_f}{T_i}$ in the large B limit.
4. Extend (3) to the case of space dimensionality d and general spin S.

Answer

1. The Hamiltonian is

$$H = \sum_{n=1}^{N} \frac{p_n^2}{2m} + \sum_{n=1}^{N} \gamma B \sigma_z^n$$

We can define a thermal wavelength

$$\lambda_T = \sqrt{\frac{2\pi}{mT}}$$

$$
\begin{aligned}
Z =& \sum_r e^{-\beta E_r} = \sum_r e^{-\beta \sum_{n=1}^N \frac{p_n^2}{2m}} e^{-\beta \sum_{n=1}^N \gamma B \sigma_z^n} \\
=& \left(\prod_{n=1}^N \int \int \frac{d\vec{x}_n d\vec{p}_n}{2\pi} e^{-\beta \frac{p_n^2}{2m}} \right) \left(\prod_{n=1}^N \left(e^{\beta\gamma B} + e^{-\beta\gamma B} \right) \right) = \frac{1}{N!} \left(\frac{V}{\lambda_T^3} \right)^N 2^N \cosh^N(\beta\gamma B) \\
=& Z_{kinetic} Z_{spin}
\end{aligned}
$$

We use Stirling's approximation

$$\ln N! \approx N \ln N - N$$

$$F = -\frac{1}{\beta} \ln Z = -NT \ln \left(\frac{V}{N\lambda_T^3} \right) - NT - NT \ln \left(2\cosh\left(\frac{\gamma B}{T} \right) \right) = F_{kinetic} + F_{spin}$$

$$S = -\frac{\partial F}{\partial T} = N \ln \left(\frac{V}{N\lambda_T^3} \right) + \frac{5}{2} N + N \ln 2\cosh\left(\frac{\gamma B}{T} \right) - \frac{N\gamma B}{T} \tanh\left(\frac{\gamma B}{T} \right)$$

$$S_{kinetic} = \frac{5}{2} N + N \ln \left(\frac{V}{N\lambda_T^3} \right)$$

$$S_{spin} = N \ln \left(2\cosh\left(\frac{\gamma B}{T} \right) \right) - \frac{N\gamma B}{T} \tanh\left(\frac{\gamma B}{T} \right)$$

2. For adiabatic process the entropy stay constant

$$S(T_i, B) = S_{kinetic}(T_i) + S_{spin}(T_i, B) = S_{kinetic}(T_f) + S_{spin}(T_f, 0) = S(T_f, 0)$$

$$S_{kinetic}(T_f) - S_{kinetic}(T_i) = \frac{5}{2} N + N \ln \left(\frac{V T_f^{\frac{3}{2}}}{N \left(\frac{2\pi}{m} \right)^{\frac{3}{2}}} \right) - \frac{5}{2} N - N \ln \left(\frac{V T_i^{\frac{3}{2}}}{N \left(\frac{2\pi}{m} \right)^{\frac{3}{2}}} \right) = \frac{3}{2} N \ln \frac{T_f}{T_i}$$

$$\rightarrow \ln \frac{T_f}{T_i} = \frac{2}{3N} [S_{spin}(T_i, B) - S_{spin}(T_f, 0)]$$

3. In the large B limit:

$$\lim_{B\to\infty} S_{spin}(T_i, B) = \lim_{B\to\infty} N \ln \left(e^{\frac{\gamma B}{T_i}} + e^{-\frac{\gamma B}{T_i}} \right) - \frac{N\gamma B}{T_i} \tanh\left(\frac{\gamma B}{T_i} \right) = \frac{N\gamma B}{T_i} - \frac{N\gamma B}{T_i} = 0$$

in the other hand

$$\lim_{B\to 0} S_{spin}(T, B) = \lim_{B\to 0} N \ln \left(2\cosh\left(\frac{\gamma B}{T} \right) \right) - \frac{N\gamma B}{T} \tanh\left(\frac{\gamma B}{T} \right) = N \ln 2$$

$$\rightarrow \ln \frac{T_f}{T_i} = \frac{2}{3N} [S_{spin}(T_i, B) - S_{spin}(T_f, 0)] = -\frac{2}{3} \ln 2$$

$$\frac{T_f}{T_i} = 2^{-\frac{2}{3}}$$

4. For the case of space dimensionality d and general spin S:

$$Z_{kinetic} = \frac{1}{N!} \left(\frac{L}{\lambda_T} \right)^{dN}$$

$$\rightarrow S_{kinetic}(T_f) - S_{kinetic}(T_i) = \frac{d}{2} N \ln \frac{T_f}{T_i}$$

$$
\begin{aligned}
Z_{spin} = & \left(e^{\beta\gamma BS} + e^{\beta\gamma B(S-1)} \cdots + e^{-\beta\gamma B(S-1)} + e^{-\beta\gamma BS}\right)^N \\
\rightarrow & S_{spin} = \ln Z_{spin} + T\frac{\partial}{\partial T}\ln Z_{spin}
\end{aligned}
$$

$$
\begin{aligned}
S_{spin} = & N\ln\left(e^{\beta\gamma BS} + e^{\beta\gamma B(S-1)} \cdots + e^{-\beta\gamma BS}\right) \\
& - \frac{N\gamma B}{T}\frac{\left(Se^{\beta\gamma BS} + (S-1)\, e^{\beta\gamma B(S-1)} \cdots - Se^{-\beta\gamma BS}\right)}{\left(e^{\beta\gamma BS} + e^{\beta\gamma B(S-1)} \cdots + e^{-\beta\gamma BS}\right)}
\end{aligned}
$$

$$
\begin{aligned}
\lim_{B\to\infty} S_{spin}(T_i, B) = & \lim_{B\to\infty} N\ln\left[e^{\beta\gamma BS}\left(1 + e^{-\beta\gamma B} \cdots + e^{-2\beta\gamma BS}\right)\right] \\
& - \frac{N\gamma B}{T}\frac{\left(S + (S-1)\, e^{-\beta\gamma B} \cdots - Se^{-2\beta\gamma BS}\right)}{\left(1 + e^{-\beta\gamma B} \cdots + e^{-2\beta\gamma BS}\right)} \\
= & \frac{N\gamma BS}{T} - \frac{N\gamma BS}{T} = 0 \\
\lim_{B\to 0} & S_{spin}(T, B) = N\ln(2S+1) \\
& \rightarrow \frac{T_f}{T_i} = (2S+1)^{-\frac{2}{d}}
\end{aligned}
$$

Exercise 2311 - Imperfect lattice with defects

A perfect lattice is composed of N atoms on N sites. If n of these atoms are shifted to interstitial sites (i.e. between regular positions) we have an imperfect lattice with n defects. The number of available interstitial sites is M and is of order N. Every atom can be shifted from lattice to any defect site. The energy needed to create a defect is ω. The temperature is T. Define $x \equiv e^{-\omega/T}$.

1. Write the expression for the partition function $Z(x)$ as a sum over n.
2. Using Stirling approximation (see note) determine what is the most probable n, and write for it the simplest approximation assuming $x \ll 1$.
3. Explain why your result for $\bar{n}$ merely reproduces the law of mass action.
4. Evaluate $Z(x)$ using a Gaussian integral.
5. Derive the expressions for the entropy and for the specific heat.
6. What would be the result if instead of Gaussian integration one were taking only the largest term in the sum?

Note: Regarding n as a continuous variable the derivative of $\ln(n!)$ is approximately $\ln(n)$.

Answer

1. If n is the number of the atoms that shifted the energy is $E = n\omega$, for the degeneracy we known that from N site and M interstitial sites we have $N - n$ occupied sites and n unoccupied sites and n occupied interstitial sites and $M - n$ unoccupied interstitial sites:

$$Z(x) = \sum_{n=0}^{N} \frac{M!}{n!\,(M-n)!} \frac{N!}{n!\,(N-n)!} x^n = \sum_{n=0}^{N} Z_n(x)$$

where $Z_n(x)$ is the partition function for n shifted atoms

2. The probability of n shifted atoms is $p_n = \frac{Z_n(x)}{Z(x)} = \frac{e^{-\beta F_n(x)}}{Z(x)}$, so if we want to find the most probable n we need to derivative $F_n(x)$ for n and found the minima of $F_n(x)$

$$F_n(x) = -\frac{1}{\beta} \ln Z_n(x) = -\frac{1}{\beta} \left(\ln M! + \ln N! - 2\ln n! - \ln(N-n)! - \ln(M-n)! + \ln x^n \right)$$

from the Stirling approximation we get

$$F_n(x) \approx -\frac{1}{\beta} \left(M \ln M + N \ln N - 2n \ln n - (N-n)\ln(N-n) - (M-n)\ln(M-n) + n \ln x \right)$$

$$\frac{\partial}{\partial n} F_n(x) = -\frac{1}{\beta} \left(-2\ln n + \ln(N-n) + \ln(M-n) + \ln x \right) = 0$$

$$\frac{n^2}{(N-n)(M-n)} = x$$

in the limit $x \ll 1$ and when N, M are the same order we get that $n \ll N, M$ so we can neglect n in the denominator and get

$$\bar{n} = \sqrt{NMx} = \sqrt{NM} e^{-\frac{\omega}{2T}}$$

3. We can look on the system like four type of particles, full site, empty site, full shifted site and empty shifted site. In this view our result is exactly the law of mass action

4. In our case the most probable state is for $n = \bar{n}$, where $F_n'(x)|_{n=\bar{n}} = 0$, so we can develop $F_n(x)$ around $\bar{n}$

$$F_n(x) = F_n(\bar{n}) + \frac{F_n''(\bar{n})}{2} (n - \bar{n})^2$$

$$Z(x) = \sum_{n=0}^{N} e^{-\beta F_n(x)}$$

$$\sum_{n=0}^{N} \to \int_0^{\infty} = \frac{1}{2} \int_{-\infty}^{\infty}$$

$$Z(x) \approx \frac{1}{2} e^{-\beta F_n(\bar{n})} \int_{-\infty}^{\infty} e^{-\frac{\beta F_n''(\bar{n})}{2}(n-\bar{n})^2} = \sqrt{\frac{\pi}{2\beta F_n''(\bar{n})}} e^{-\beta F_n(\bar{n})}$$

$$
\begin{aligned}
e^{-\beta F_n(\bar{n})} =& e^{\left(M\ln M+N\ln N-2\bar{n}\ln\bar{n}-(N-\bar{n})\ln(N-\bar{n})-(M-\bar{n})\ln(M-\bar{n})+\bar{n}\ln\left(\frac{\bar{n}^2}{NM}\right)\right)} \\
=& e^{-\left((N-\bar{n})\ln\left(1-\frac{\bar{n}}{N}\right)+(M-\bar{n})\ln\left(1-\frac{\bar{n}}{M}\right)\right)} \approx e^{2\bar{n}}
\end{aligned}
$$

$$
F_n''(x) = \frac{1}{\beta}\left(\frac{2}{n}+\frac{1}{(N-n)}+\frac{1}{(M-n)}\right) \approx \frac{2}{\beta n}
$$

$$
Z(x) = \sqrt{\frac{\pi\bar{n}}{4}}e^{2\bar{n}} = \sqrt{\frac{\pi\sqrt{MN}}{4}}e^{2\bar{n}}e^{-\frac{\omega}{4T}}
$$

5. For the entropy

$$
S = -\frac{\partial F}{\partial T} = \frac{\partial}{\partial T}(T\ln Z) = \frac{\partial}{\partial T}T\left(\frac{1}{2}\ln\frac{\pi}{4}+\frac{1}{2}\ln\bar{n}+2\bar{n}\right) = \left(\frac{1}{2}\ln\frac{\pi}{4}+\frac{1}{2}\ln\bar{n}+\frac{T}{2\bar{n}}\frac{\partial\bar{n}}{\partial T}+2\bar{n}+T2\frac{\partial\bar{n}}{\partial T}\right)
$$

$$
= \left(\frac{1}{2}\ln\frac{\pi}{4}+\frac{1}{2}\ln\sqrt{NM}-\frac{\omega}{4T}+\frac{\omega}{4T}+2\bar{n}+\frac{\omega\bar{n}}{T}\right) = \frac{1}{2}\ln\left(\frac{\pi\sqrt{MN}}{4}\right)+\left(2+\frac{\omega}{T}\right)\bar{n}
$$

When we use

$$
\frac{\partial\bar{n}}{\partial T} = \frac{\omega}{2T^2}\sqrt{NM}e^{-\frac{\omega}{2T}} = \frac{\omega\bar{n}}{2T^2}
$$

and for the specific heat.

$$
C = T\frac{\partial S}{\partial T} = T\left[-\frac{\omega}{T^2}\bar{n}+\left(2+\frac{\omega}{T}\right)\frac{\omega}{2T^2}\bar{n}\right] = \frac{\bar{n}}{2}\left(\frac{\omega}{T}\right)^2
$$

6. If instead of Gaussian integration one were taking only the largest term in the sum

$$
Z(x) \approx e^{-\beta F_n(\bar{n})}
$$

we will get the same equation without a prefactor, so

$$
S = \left(2+\frac{\omega}{T}\right)\bar{n}
$$

$$
C = \frac{\bar{n}}{2}\left(\frac{\omega}{T}\right)^2
$$

Gibbs Hamiltonian

For the Hamiltonian

$$
H(\cdots,x)
$$

where x is parameter of the system, we can apply force f and change x to be a dynamical variable ,the new Hamiltonian

$$
H_G(\cdots,f) = H(\cdots,x)+fx
$$

The partition function of H_G is a Laplace transform of the partition function of H

$$
Z_G(\beta,f) = \sum_{r,x}e^{-\beta(E_{r,x}+fx)} = \sum_x\sum_r e^{-\beta E_{r,x}}e^{-\beta fx} = \sum_x Z(\beta,x)e^{-\beta fx}
$$

Exercise 2351 - Tension of a rubber band

The elasticity of a rubber band can be described by a one dimensional model of a polymer. The polymer consists of N monomers that are arranged along a straight line, hence forming a chain. Each unit can be either in a state of length a with energy E_a, or in a state of length b with energy E_b. We define f as the tension, i.e. the force that is applied while holding the polymer in equilibrium.

1. Write expressions for the partition function $Z_G(\beta, f)$.
2. For very high temperatures $F_G(T, f) \approx F_G^{(\infty)}(T, f)$, where $F_G^{(\infty)}(T, f)$ is a linear function of T. Write the explicit expression for $F_G^{(\infty)}(T, f)$.
3. Write the expression for $F_G(T, f) - F_G^{(\infty)}(T, f)$. Hint: this expression is quite simple - within this expression f should appear only once in a linear combination with other parameters.
4. Derive an expression for the length L of the polymer at thermal equilibrium, given the tension f. Write two separate expressions: one for the infinite temperature result $L(\infty, f)$ and one for the difference $L(T, f) - L(\infty, f)$.
5. Assuming $E_a = E_b$, write a linear approximation for the function $L(T, f)$ in the limit of weak tension.
6. Treating L as a continuous variable, find the probability distribution $P(L)$, assuming $E_a = E_b$ and $f = 0$.
7. Write an expression that relates the function $f(L)$ to the probability distribution $P(L)$. Write also the result that you get from this expression.
8. Find what would be the results for $Z_G(\beta, f)$ if the monomer could have any length $\in [a, b]$. Assume that the energy of the monomer is independent of its length.
9. Find what would be the results for $L(T, f)$ in the latter case.

Note: Above a "linear function" means $y = Ax + B$.
Please express all results using $(N, a, b, E_a, E_b, f, T, L)$.

Answer

1. For the partition function $Z_G(\beta, f)$.

$$H = nE_a + (N-n)\,E_b$$

$$H_G = nE_a + (N-n)\,E_b + f\,(na + (N-n)\,b)$$

$$\begin{aligned} Z_G\,(\beta, f) &= \sum_{n=0}^{N} \frac{N!}{n!\,(N-n)!} e^{-\beta[nE_a + (N-n)E_b + f(na + (N-n)b)]} \\ &= \sum_{n=0}^{N} \frac{N!}{n!\,(N-n)!} e^{-\beta n(E_a + fa)} e^{-\beta(N-n)(E_b + fb)} \end{aligned}$$

from the binomial theorem $(a+b)^N = \sum_{n=0}^{N} \frac{N!}{(N-n)!n!} a^n b^{N-n}$ we get

$$Z_G(\beta, f) = \left(e^{-\beta(E_a+fa)} + e^{-\beta(E_b+fb)}\right)^N$$

Another way

$$H_G^1 = E_x + fx$$

$$Z^1 = \sum_{x=a,b} e^{-\beta(E_x+fx)} = e^{-\beta(E_a+fa)} + e^{-\beta(E_b+fb)}$$

$$Z_G = \left(Z^1\right)^N = \left(e^{-\beta(E_a+fa)} + e^{-\beta(E_b+fb)}\right)^N$$

2. We define

$$\begin{aligned}
\frac{F_G(T,f)}{N} &= -\frac{T}{N}\ln\left(Z_G\right) = -T\ln\left(e^{-\frac{1}{T}(E_a+fa)} + e^{-\frac{1}{T}(E_b+fb)}\right) \\
&= -T\ln\left(e^{-\frac{1}{2T}(E_a+E_b+fa+fb)}\left(e^{\frac{1}{2T}(E_b-E_a-fa+fb)} + e^{-\frac{1}{2T}(E_b-E_a-fa+fb)}\right)\right) \\
&= \frac{E_a+E_b}{2} + \frac{b+a}{2}f - T\ln\left(2\cosh\left(\frac{1}{T}\left(\frac{E_a-E_b}{2} + f\frac{a-b}{2}\right)\right)\right)
\end{aligned}$$

For $T \to \infty$

$$\frac{F_G(\infty, f)}{N} \approx \frac{E_a+E_b}{2} + \frac{b+a}{2}f - T\ln\left(2\right)$$

3. We get

$$\begin{aligned}
\frac{F_G(T,f) - F_G^{(\infty)}(T,f)}{N} &= \left(\frac{E_a+E_b}{2} + f\frac{b+a}{2}\right) - T\ln\left(2\cosh\left(\frac{1}{T}\left(\frac{E_a-E_b}{2} + f\frac{a-b}{2}\right)\right)\right) + T\ln\left(2\right) - \left(\right. \\
&= -T\ln\left(\cosh\left(\frac{1}{T}\left(\frac{E_a-E_b}{2} + f\frac{a-b}{2}\right)\right)\right)
\end{aligned}$$

4. For the infinite temperature result $L(\infty, f)$

$$\frac{L(\infty, f)}{N} = \frac{1}{N}\frac{\partial F_G(\infty, f)}{\partial f} = \frac{b+a}{2}$$

$$\frac{L(T,f) - L(\infty,f)}{N} = \frac{\partial}{\partial f}\left(\frac{F_G(T,f) - F_G^{(\infty)}(T,f)}{N}\right) = -\frac{a-b}{2}\tanh\left(\frac{1}{T}\left(\frac{E_a-E_b}{2} + f\frac{a-b}{2}\right)\right)$$

5. For $E_a = E_b$

$$\frac{L(T,f) - L(\infty,f)}{N} = -\frac{a-b}{2}\tanh\left(\frac{f}{T}\frac{a-b}{2}\right)$$

For $f \to 0$

$$\frac{L(T,f) - L(\infty,f)}{N} \approx -\frac{\left(a-b\right)^2}{4T}f$$

We get Hook's law

$$f = -\frac{4T}{N\left(a-b\right)^2}\left(L - \langle L\rangle\right)$$

6. For $E_a = E_b$ the probability for configuration of a single monomer is $\frac{1}{2}$

$$\langle L\rangle = \sum_i \langle x_i\rangle = N\langle x_i\rangle = N\left(\frac{a+b}{2}\right)$$

$$\sigma^2 = \left\langle L^2\right\rangle - \langle L\rangle^2 = N\left[\left(\frac{a^2+b^2}{2}\right) - \left(\frac{a+b}{2}\right)^2\right] = N\left(\frac{a-b}{2}\right)^2$$

For a long monomer ($N \gg 1$) we can now use the central limit theorem, (Gaussian disterbution)

$$P(L) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{1}{2}\left(\frac{L-\langle L\rangle}{\sigma}\right)^2}$$

7. We can define $L = na + (N-n)b \to \frac{L-Nb}{a-b} = n$

$$Z_G(\beta, f) = \sum_{n=0}^{N} \frac{N!}{n!\,(N-n)!} e^{-\beta[nE_a + (N-n)E_b + f(na + (N-n)b)]}$$

$$= \sum_L \frac{N!}{\left(\frac{L-Nb}{a-b}\right)!\left(\frac{L-Na}{b-a}\right)!} e^{-\beta\left[\frac{L(E_a-E_b)-N(bE_a-aE_b)}{a-b}+fL\right]} = \sum_L Z(L)$$

By definition

$$P(L) = \frac{Z(L)}{Z}$$

And by definition

$$f(L) = \frac{\partial F}{\partial L} = \frac{1}{\beta}\frac{\partial \ln(Z(L))}{\partial L} = \frac{1}{\beta}\frac{\partial \ln(P(L))}{\partial L} = -T\left(\frac{L-\langle L\rangle}{\sigma^2}\right) = -\frac{4T}{N(a-b)^2}(L-\langle L\rangle)$$

8. For $E_x = E$ and $x \in [a,b]$

$$H^1 = E + fx$$

$$Z^1 = \int_a^b dx e^{-\beta(E+fx)} = e^{-\beta E}\int_a^b dx e^{-\beta f x} = \frac{1}{\beta f}\left(e^{-\beta(E+fa)} - e^{-\beta(E+fb)}\right)$$

$$Z_G = \left(Z^1\right)^N = \left[\frac{1}{\beta f}\left(e^{-\beta(E+fa)} - e^{-\beta(E+fb)}\right)\right]^N$$

We can take $E = 0$

$$Z_G = \left(Z^1\right)^N = \left[\frac{1}{\beta f}\left(e^{-\beta f a} - e^{-\beta f b}\right)\right]^N$$

9.

$$\frac{F_G(T,f)}{N} = -\frac{T}{N}\ln(Z_G) = T\ln\left(\frac{f}{T}\right) - T\ln\left(e^{-\beta f\left(\frac{a+b}{2}\right)} 2\sinh\left(\beta f\left(\frac{a-b}{2}\right)\right)\right)$$

$$= T\ln\left(\frac{f}{T}\right) + f\left(\frac{a+b}{2}\right) - T\ln\left(2\sinh\left(\frac{f}{T}\left(\frac{a-b}{2}\right)\right)\right)$$

$$L = \frac{\partial F_G}{\partial f}$$

$$\frac{L(T,f)}{N} = \frac{T}{f} + \left(\frac{a+b}{2}\right) - \left(\frac{a-b}{2}\right)\coth\left(\frac{f}{T}\left(\frac{a-b}{2}\right)\right)$$

Thw expention of $\coth(x) \approx \frac{1}{x} + \frac{x}{3}$, so for $f \to 0$

$$\to \frac{L(T,f) - L(\infty,f)}{N} = \frac{T}{f} + \left(\frac{a+b}{2}\right) - \left[\frac{T}{f} + \frac{\frac{f}{T}\left(\frac{a-b}{2}\right)^2}{3}\right] - \left(\frac{a+b}{2}\right) = -\frac{(a-b)^2}{12T}f$$

$$f = -\frac{12T}{N\left(a-b\right)^2}\left(L - \langle L\rangle\right)$$

Statistical Mechanics - Class Exercise 3

The basic integrals for ideal gas

$$N = \sum_r f(\epsilon_r - \mu) = \int_0^\infty g(\epsilon) f(\epsilon - \mu)\, d\epsilon$$

$$E = \sum_r \epsilon_r f(\epsilon_r - \mu) = \int_0^\infty g(\epsilon) \epsilon f(\epsilon - \mu)\, d\epsilon$$

$$\boldsymbol{Z} = \prod_r \mathcal{Z}^{(r)}, \quad \mathcal{Z}^{(r)} = \sum_n e^{-\beta(\epsilon_r - \mu) n_r} = \left(1 \pm e^{-\beta(\epsilon_r - \mu)}\right)^{\pm 1}$$

$$\ln(\boldsymbol{Z}) = \pm \sum_r \ln\left(1 \pm e^{-\beta(\epsilon_r - \mu)}\right) = \{\text{Integration by parts}\} = \beta \int_0^\infty \mathcal{N}(\epsilon) f(\epsilon - \mu)\, d\epsilon$$

$$P = \frac{1}{\beta}\frac{\partial \ln(\boldsymbol{Z})}{\partial V} = \frac{1}{\beta}\frac{\ln(\boldsymbol{Z})}{V} = \frac{1}{V}\int_0^\infty \mathcal{N}(\epsilon) f(\epsilon - \mu)\, d\epsilon$$

Exercise 3336 - Condensation for general dispersion

An ideal Bose gas consists of particles that have the dispersion relation $\epsilon = c|p|^s$ with $s > 0$. The gas is contained in a box that has volume V in d dimensions. The gas is maintained in a uniform temperature T.

1. Calculate the single particle density of states.
2. Find a condition involving s and d for the existence of Bose-Einstein condensation. In particular relate to relativistic ($s = 1$) and nonrelativistic ($s = 2$) particles in two dimensions.
3. Find the dependence of the number of particles N on the chemical potential μ.
4. Find the dependence of the total energy E on the chemical potential, and show how the pressure P is obtained from this result.
5. Find an expression for the heat capacity C_v. Show how this result can be expressed using N in the limit of infinite temperature.
6. Repeat item 1 for relativistic gas whose particles have finite mass such that their dispersion relation is $\epsilon = \sqrt{m^2c^4 + c^2p^2}$.
7. Consider a relativistic gas in $2D$. Find expressions for N and E and P. Should one expect Bose-Einstein condensation?

Answer

1. We have the dispersion relation $\epsilon = c|p|^s$

$$\rightarrow |p| = \left(\frac{\epsilon}{c}\right)^{\frac{1}{s}}$$

$$\mathcal{N}(\epsilon) = \int_{H<\epsilon} \frac{d^d x d^d p}{(2\pi)^d} = \frac{V}{(2\pi)^d} \int \cdots \int_{\sqrt{p_1^2 + \cdots + p_d^2} \le \left(\frac{\epsilon}{c}\right)^{\frac{1}{s}}} d^d p = \frac{V}{(2\pi)^d}\Omega_d \int_0^{\left(\frac{\epsilon}{c}\right)^{\frac{1}{s}}} p^{d-1} dp = \frac{V}{(2\pi)^d}\frac{\Omega_d}{d}\left(\frac{\epsilon}{c}\right)^{\frac{d}{s}}$$

$$\mathcal{N}(\epsilon) = \frac{1}{d}\frac{V}{(2\pi)^d}\frac{\Omega_d}{c^{\frac{d}{s}}}\epsilon^{\frac{d}{s}}$$

$$g(\epsilon) = \frac{\partial \mathcal{N}(\epsilon)}{\partial \epsilon} = \frac{1}{s}\frac{V}{(2\pi)^d}\frac{\Omega_d}{c^{\frac{d}{s}}}\epsilon^{\frac{d}{s}-1}$$

$$\rightarrow \mathcal{N}(\epsilon) = \frac{s}{d}g(\epsilon)\,\epsilon$$

2. We define $\alpha = \frac{d}{s}, c = \frac{1}{(2\pi)^d}\frac{\Omega_d}{sc^{\frac{d}{s}}}$
In general

$$N = \int_0^\infty g(\epsilon) f(\epsilon - \mu) d\epsilon = cV \int_0^\infty \frac{\epsilon^{\alpha-1}}{e^{\beta(\epsilon-\mu)} - 1} d\epsilon$$

For Bose-Einstein condensation we need that the integral will converge, and this happen for $\alpha > 1 \rightarrow d > s$.
For nonrelativistic ($s = 2$) particles in 2D $d = s$, so the system will not exhibit BEC.
For relativistic ($s = 1$) particles in 2D $d > s$, so the system can exhibit BEC.
3. Define $z = e^{\beta\mu}$

$$N = cV \int_0^\infty \frac{\epsilon^{\alpha-1}}{e^{\beta(\epsilon-\mu)} - 1} d\epsilon = \left\{ \begin{array}{c} x = \beta\epsilon \\ Tdx = d\epsilon \end{array} \right\} = cVT^\alpha \int_0^\infty \frac{x^{\alpha-1}}{\frac{1}{z}e^x - 1} dx = cVT^\alpha F_\alpha(\beta\mu)$$

Where

$$F_\alpha(\beta\mu) = \Gamma(\alpha)\, Li_\alpha(z)\,, \quad Li_\alpha(z) = \sum_{\ell=1}^{\infty} \frac{z^\ell}{\ell^\alpha}$$

4. To calculate the total energy E:

$$E = \int_0^\infty g(\epsilon)\,\epsilon f(\epsilon - \mu) d\epsilon = cV \int_0^\infty \frac{\epsilon^\alpha}{e^{\beta(\epsilon-\mu)} - 1} d\epsilon = cVT^{\alpha+1} F_{\alpha+1}(\beta\mu)$$

In the other side

$$\ln(Z) = \beta \int_0^\infty \mathcal{N}(\epsilon) f(\epsilon - \mu) d\epsilon = \frac{\beta}{\alpha} \int_0^\infty g(\epsilon)\,\epsilon f(\epsilon - \mu) d\epsilon = \frac{\beta}{\alpha} cVT^{\alpha+1} F_{\alpha+1}(\beta\mu) = \frac{\beta}{\alpha} E$$

We know that

$$P = \frac{1}{\beta}\frac{\partial \ln(Z)}{\partial V} = \frac{1}{\beta}\frac{\ln(Z)}{V} = \frac{1}{\alpha}\frac{E}{V}$$

5. The heat capacity C_v.

$$C_v = \left.\frac{\partial E}{\partial T}\right|_{V,N}$$

In the limit of infinite temperature can use Boltzmann approximation; in this limit $f(\epsilon - \mu) = e^{-\beta(\epsilon-\mu)}$

$$N = cV \int_0^\infty \epsilon^{\alpha-1} e^{-\beta(\epsilon-\mu)} d\epsilon = cVe^{\beta\mu}T^\alpha \int_0^\infty x^{\alpha-1}e^{-x} dx = cVe^{\beta\mu}T^\alpha \Gamma(\alpha)$$

$$E = cV \int_0^\infty \epsilon^\alpha e^{-\beta(\epsilon-\mu)} d\epsilon = cVe^{\beta\mu}T^{\alpha+1}\Gamma(\alpha+1) = cVe^{\beta\mu}T^{\alpha+1}\alpha\Gamma(\alpha) = \alpha NT$$

$$\rightarrow C_v = \left.\frac{\partial E}{\partial T}\right|_{V,N} = \alpha N$$

6. For relativistic gas with dispersion relation is $\epsilon = \sqrt{m^2c^4 + c^2p^2}$.

$$\rightarrow |p| = \sqrt{\left(\frac{\epsilon}{c}\right)^2 - m^2c^2}$$

$$\mathcal{N}(\epsilon) = \int_{H<\epsilon} \frac{d^dx d^dp}{(2\pi)^d} = \frac{V}{(2\pi)^d} \int \cdots \int_{\sqrt{p_1^2+\cdots+p_d^2} \le \sqrt{\left(\frac{\epsilon}{c}\right)^2 - m^2c^2}} d^dp = \frac{V}{(2\pi)^d}\Omega_d \int_0^{\sqrt{\left(\frac{\epsilon}{c}\right)^2 - m^2c^2}} p^{d-1}dp$$

$$= \frac{V}{(2\pi)^d}\frac{\Omega_d}{d}\left(\left(\frac{\epsilon}{c}\right)^2 - m^2c^2\right)^{\frac{d}{2}}$$

$$g(\epsilon) = \frac{\partial \mathcal{N}(\epsilon)}{\partial \epsilon} = \frac{V}{(2\pi)^d}\Omega_d \left(\left(\frac{\epsilon}{c}\right)^2 - m^2c^2\right)^{\frac{d}{2}-1} \frac{\epsilon}{c^2}$$

7. For relativistic gas in $2D$ the momentum $|p| \sim \epsilon \rightarrow \alpha = \frac{d}{s} = 2$

$$\mathcal{N}(\epsilon) = \frac{1}{2}\frac{V}{2\pi c^2}\left(\epsilon^2 - m^2c^4\right)$$

$$g(\epsilon) = \frac{\partial \mathcal{N}(\epsilon)}{\partial \epsilon} = \frac{V}{2\pi c^2}\epsilon$$

$$N = \frac{V}{2\pi c^2}\int_{mc^2}^{\infty} \frac{\epsilon}{e^{\beta(\epsilon-\mu)} - 1} d\epsilon = \left\{\epsilon' = \epsilon - mc^2\right\} = \frac{V}{2\pi c^2}\int_0^{\infty} \frac{\epsilon' + mc^2}{e^{\beta(\epsilon' + mc^2 - \mu)} - 1} d\epsilon' =$$

$$= \frac{V}{2\pi c^2} T^2 F_2\left(\frac{\mu - mc^2}{T}\right) + \frac{Vmc^2}{2\pi c^2} T F_1\left(\frac{\mu - mc^2}{T}\right)$$

$$N = \frac{V}{2\pi c^2}\left[T^2 F_2\left(\frac{\mu - mc^2}{T}\right) + mc^2 T F_1\left(\frac{\mu - mc^2}{T}\right)\right]$$

In the same way

$$E = \frac{V}{2\pi c^2}\int_{mc^2}^{\infty} \frac{\epsilon^2}{e^{\beta(\epsilon-\mu)} - 1} d\epsilon = \frac{V}{2\pi c^2}\int_0^{\infty} \frac{\epsilon'^2 + 2\epsilon' mc^2 + m^2c^4}{e^{\beta(\epsilon' + mc^2 - \mu)} - 1} d\epsilon'$$

$$E = \frac{V}{2\pi c^2}\left[T^3 F_3\left(\frac{\mu - mc^2}{T}\right) + 2mc^2T^2 F_2\left(\frac{\mu - mc^2}{T}\right) + m^2c^4 T F_1\left(\frac{\mu - mc^2}{T}\right)\right]$$

For P we need to calculate $\ln(Z)$

$$\ln(Z) = \beta \int_0^{\infty} \mathcal{N}(\epsilon) f(\epsilon - \mu) d\epsilon = \beta \frac{V}{4\pi c^2}\int_{mc^2}^{\infty} \frac{\left(\epsilon^2 - m^2c^4\right)}{e^{\beta(\epsilon-\mu)} - 1} d\epsilon$$

$$= \beta \frac{V}{4\pi c^2}\int_0^{\infty} \frac{\epsilon'^2 + 2\epsilon' mc^2}{e^{\beta(\epsilon' + mc^2 - \mu)} - 1} d\epsilon' = \beta \frac{V}{4\pi c^2}\left[T^3 F_3\left(\frac{\mu - mc^2}{T}\right) + 2mc^2 T^2 F_2\left(\frac{\mu - mc^2}{T}\right)\right]$$

$$P = \frac{1}{\beta}\frac{\ln(Z)}{V} = \frac{1}{4\pi c^2}\left[T^3 F_3\left(\frac{\mu - mc^2}{T}\right) + 2mc^2 T^2 F_2\left(\frac{\mu - mc^2}{T}\right)\right]$$

for get BEC we need that $N = \int_0^\infty g(\epsilon) f(\epsilon - \mu) d\epsilon$ will be finite for $\mu \to 0$

$$N = \frac{V}{2\pi c^2}\int_0^\infty \frac{\epsilon' + mc^2}{e^{\beta(\epsilon' + mc^2 - \mu)} - 1} d\epsilon' = \frac{V}{2\pi c^2}\int_0^\infty \frac{\epsilon' + mc^2}{e^{\beta(\epsilon' - \mu')} - 1} d\epsilon'$$

For $\mu \to mc^2 \Leftrightarrow \mu' \to 0$ we get that $\int_0^\infty \frac{mc^2}{e^{\beta(\epsilon'-\mu')}-1} d\epsilon'$ does not converge and so we can't expect to get BEC.
In another way we can see that for $\frac{p}{m} \ll c$

$$\epsilon = \sqrt{m^2c^4 + c^2p^2} \approx mc^2 + \frac{p^2}{2m} \to \alpha = 1$$

Exercise 3021 - Spin 1 bosons in 3D box with Zeeman interaction

N Bosons that have mass m and spin 1 are placed in a box that has volume V. A magnetic field B is applied, such that the interaction is $-\gamma B S_z$, where $S_z = 1, 0, -1$, and γ is the gyromagnetic ratio. In items (3-6) assume the Boltzmann approximation for the occupation of the $S_z \neq 1$ states.

1. Find an equation for the condensation temperature T_c.
2. Find the condensation temperature $T_c(B)$ for $B = 0$ and for $B \to \infty$.
3. Find the critical B for condensation if T is set in the range of temperatures that has been defined in item (2).
4. Describe how $T_c(B)$ depends of B in a qualitatively manner. Find approximate expressions for moderate and large fields.
5. Find the condensate fraction as a function of T and B.
6. Find the heat capacity of the gas assuming large but finite field.

Answer

1. The Hamiltonian for one particle:

$$H = \frac{p^2}{2m} - \gamma B S_z$$

For $\alpha = \frac{d}{s} = \frac{3}{2}, c = \frac{1}{(2\pi)^d}\frac{\Omega_d}{s c^{\frac{d}{s}}} = \frac{(2m)^{\frac{3}{2}}}{(2\pi)^2}$ For spinless particles we get

$$N = cVT^{\frac{3}{2}} F_{\frac{3}{2}}(\beta\mu) = V\frac{2^{\frac{3}{2}}\left(\frac{mT}{2\pi}\right)^{\frac{3}{2}}}{(2\pi)^{\frac{1}{2}}}\Gamma\left(\frac{3}{2}\right) Li_{\frac{3}{2}}\left(e^{\beta\mu}\right) = \frac{V}{\lambda_T^3} Li_{\frac{3}{2}}\left(e^{\beta\mu}\right)$$

we can treat the particles of the system like three different spinless gasses with different S_z.

$$N = \sum f(\epsilon - \mu) = \sum f\left(\frac{p^2}{2m} - \gamma B - \mu\right) + \sum f\left(\frac{p^2}{2m} - \mu\right) + \sum f\left(\frac{p^2}{2m} + \gamma B - \mu\right)$$

We can define $\mu' = \mu + \gamma B S_z$ and get

$$\frac{N}{V} = \frac{1}{\lambda_T^3}\left(\mathrm{Li}_{3/2}\left(e^{\beta(\mu+\gamma B)}\right) + \mathrm{Li}_{3/2}\left(e^{\beta\mu}\right) + \mathrm{Li}_{3/2}\left(e^{\beta(\mu-\gamma B)}\right)\right)$$

The condition to condensation is that μ goes to the lowest energy, here this mean $\mu \to -\gamma B$ $(S_z = 1)$

$$\frac{N}{V} = n = n_0 + \frac{1}{\lambda_T^3}\left(\mathrm{Li}_{3/2}(1) + \mathrm{Li}_{3/2}\left(e^{-\beta\gamma B}\right) + \mathrm{Li}_{3/2}\left(e^{-2\beta\gamma B}\right)\right)$$

For $T = T_c$

$$n \approx \frac{1}{\lambda_T^3}\left(\zeta\left(\frac{3}{2}\right) + e^{-\beta\gamma B} + e^{-2\beta\gamma B}\right), \quad \zeta\left(\frac{3}{2}\right) \approx 2.612$$

2. For $B = 0$\frac{3}{2}\left(\frac{m}{2\pi}\right)^{\frac{3}{2}}

$$n = \frac{1}{\lambda_T^3}\left(\mathrm{Li}_{3/2}(1) + \mathrm{Li}_{3/2}(1) + \mathrm{Li}_{3/2}(1)\right) = \frac{3}{\lambda_T^3}\zeta\left(\frac{3}{2}\right) = 3\left(\frac{m}{2\pi}\right)^{\frac{3}{2}}\zeta\left(\frac{3}{2}\right)T_c^{\frac{3}{2}}$$

$$\to T_c(B=0) = \frac{2\pi}{m}\left(\frac{n}{3\cdot 2.612}\right)^{\frac{2}{3}}$$

For $B \to \infty$ the occupation states are just $S_z = 1$, we get $\mathrm{Li}_{3/2}\left(e^{-\beta\gamma B}\right) \to 0$

$$n = \left(\frac{m}{2\pi}\right)^{\frac{3}{2}}\zeta\left(\frac{3}{2}\right)T_c^{\frac{3}{2}}$$

$$\to T_c(B=\infty) = \frac{2\pi}{m}\left(\frac{n}{2.612}\right)^{\frac{2}{3}}$$

$$\frac{T_c(B=\infty)}{T_c(B=0)} = 3^{\frac{2}{3}} \approx 2$$

3. Now we assume $B \neq 0$, $\gamma B \gg T$, so for $S_z \neq 1$ we can use the Boltzmann approximation.

$$n \approx \frac{1}{\lambda_T^3}\left(\mathrm{Li}_{3/2}(1) + e^{-\beta\gamma B} + e^{-2\beta\gamma B}\right) \approx \frac{1}{\lambda_T^3}\left(\zeta\left(\frac{3}{2}\right) + e^{-\beta\gamma B}\right)$$

$$\to B_c = -\frac{T}{\gamma}\ln\left(\lambda_T^3 n - \zeta\left(\frac{3}{2}\right)\right)$$

4. As B is increased, T_c rises until B_c is reached. At $B = B_c, T = T_c$ and the condensation occurs

$$n = \left(\frac{m}{2\pi}\right)^{\frac{3}{2}}T_c^{\frac{3}{2}}\left(\zeta\left(\frac{3}{2}\right) + e^{-\beta\gamma B}\right)$$

5. We get

$$n_0 = n - \frac{1}{\lambda_T^3}\left(\zeta\left(\frac{3}{2}\right) + e^{-\beta\gamma B}\right)$$

So

$$\frac{n_0}{n} = 1 - \frac{\left(\zeta\left(\frac{3}{2}\right) + e^{-\beta\gamma B}\right)}{n\lambda_T^3} = 1 - \frac{n(T,B)}{n}$$

6. For large but finite field $\gamma B \gg T$

$$\frac{E}{V} = \frac{3}{2}\frac{T}{\lambda_T^3}\left(\mathrm{Li}_{5/2}\left(1\right) + e^{-\beta\gamma B} + e^{-2\beta\gamma B}\right) \approx \frac{3}{2}\left(\frac{m}{2\pi}\right)^{\frac{3}{2}} T^{\frac{5}{2}}\left(\zeta\left(\frac{5}{2}\right) + e^{-\frac{\gamma B}{T}}\right)$$

$$\frac{C_V}{V} = \frac{\partial}{\partial T}\left(\frac{E}{V}\right) = \frac{3}{2}\frac{1}{\lambda_T^3}\left[\frac{5}{2}\zeta\left(\frac{5}{2}\right) + \left(\frac{5}{2} + \beta\gamma B\right)e^{-\beta\gamma B}\right] \approx \frac{3}{2}\frac{1}{\lambda_T^3}\left[\frac{5}{2}\zeta\left(\frac{5}{2}\right) + \beta\gamma B e^{-\beta\gamma B}\right]$$

Exercise 3745 - Fermions in a uniform gravitational field

Consider fermions of mass M and spin $1/2$ in a gravitational field with constant acceleration g and at uniform temperature T. The density of the Fermions at zero height is $n(0) = n_0$. In item (3) assume that at zero height the fermions form a degenerate gas with Fermi energy ϵ_F^0 that is much larger compared with T.

1. Assume that the fermions behave as classical particles and find their density $n(h)$ as function of the height.
2. Assume $T = 0$. Find the local Fermi momentum $p_F(h)$ and the density $n(h)$ as function of the height.
3. Assume low temperatures. Estimate the height h_c such that for $h \gg h_c$ the fermions are non-degenerate.
4. In the latter case find $n(h)$ for $h \gg h_c$, given as before n_0 at zero height.

Answer

1. We look on a layer of gas in the high $z \in [h, h + \delta h]$ in a virtual box with size $L \times L \times \delta h$.
The partition function for one classical particles

$$\mathcal{Z}_1\left(\beta, h\right) = \underbrace{2}_{spin}\int_0^L\int_0^L\int_h^{h+\delta h} e^{-\beta\left(\frac{p^2}{2m} + mgz\right)}\frac{dxdydzd^3p}{\left(2\pi\right)^3} = \frac{2L^2}{\beta mg\lambda_T^3}\left(e^{-\beta mgh} - e^{-\beta mg(h+\delta h)}\right)$$

$$= \frac{2L^2}{\beta mg\lambda_T^3}e^{-\beta mgh}\left(1 - e^{-\beta mg\delta h}\right) \approx \frac{2L^2\delta h}{\lambda_T^3}e^{-\beta mgh}$$

The partition function with $L^2\delta h = V$:

$$\mathcal{Z}_N\left(\beta, h\right) = \frac{1}{N\left(h\right)!}\left(\frac{2V}{\lambda_T^3}e^{-\beta mgh}\right)^{N(h)}$$

The Free energy:

$$F\left(\beta, h\right) = -T\ln\mathcal{Z}_N = T\ln\left(N\left(h\right)!\right) - TN\left(h\right)\ln\left(\frac{2V}{\lambda_T^3}\right) + N\left(h\right)mgh$$

with Stirling's approximation

$$F\left(\beta, h\right) \approx -TN\left(h\right) - TN\left(h\right)\ln\left(\frac{2V}{N\left(h\right)\lambda_T^3}\right) + N\left(h\right)mgh$$

The chemical potential:

$$\mu(\beta,h)=\frac{\partial F(\beta,h)}{\partial N(h)}=-T\ln\left(\frac{2V}{N(h)\lambda_T^3}\right)+mgh=-T\ln\left(\frac{2}{n(h)\lambda_T^3}\right)+mgh$$

at zero height

$$\mu(0)=-T\ln\left(\frac{2}{n(0)\lambda_T^3}\right)$$

From chemical equilibrium $\mu(h)=\mu(0)$

$$-T\ln\left(\frac{2}{n(h)\lambda_T^3}\right)+mgh=-T\ln\left(\frac{2}{n_0\lambda_T^3}\right)$$

$$\beta mgh=\ln\left(\frac{n_0}{n(h)}\right)$$

$$n(h)=n_0e^{-\beta mgh}$$

2. At $T=0$ we have a degenerate gas when all the energy state up to ϵ_F are occupied.
The number of states:

$$N(\beta,h,\mu)=\int_0^\infty g(\epsilon_p)\,f(\epsilon_p+mgh-\mu)\,d\epsilon_p$$

where for fermions of mass M and spin 1/2

$$g(\epsilon)=2\frac{V(2m)^{\frac{3}{2}}}{(2\pi)^2}\epsilon^{\frac{1}{2}}$$

In $T=0$ the occupation function is a step function with $\mu'(h)=\epsilon_F-mgh$, so we get

$$n(h)=\frac{(2m)^{\frac{3}{2}}}{3\pi^2}(\epsilon_F-mgh)^{\frac{3}{2}}$$

At zero hight

$$n(0)=n_0=\frac{(2m)^{\frac{3}{2}}}{3\pi^2}(\epsilon_F)^{\frac{3}{2}}$$

$$\epsilon_F=\frac{(3\pi^2n_0)^{\frac{2}{3}}}{2m}$$

$$\rightarrow n(h)=\frac{(2m)^{\frac{3}{2}}}{3\pi^2}\left(\frac{(3\pi^2n_0)^{\frac{2}{3}}}{2m}-mgh\right)^{\frac{3}{2}}$$

For the Fermi momentum

$$\epsilon_F=\frac{p_F^2(h)}{2m}+mgh$$

$$\rightarrow p_F(h)=\sqrt{2m\epsilon_F-2m^2gh}=\sqrt{(3\pi^2n_0)^{\frac{2}{3}}-2m^2gh}$$

3. We assume that at zero height the fermions form a degenerate gas with Fermi energy ϵ_F^0, for $h > 0$ the energy form the momentum is

$$\epsilon_p = \epsilon_F^0 - mgh$$

The limit for non-degenerate fermions is $\epsilon_p(h_c) = T$

$$\epsilon_F^0 - mgh_c = T$$

$$\rightarrow h_c = \frac{\epsilon_F^0 - T}{mg} \approx \frac{\epsilon_F^0}{mg}$$

4. For $h \gg h_c$ the gas behave as classical gas, we have the same chemical equilibrium $\mu(h) = \mu(0)$, but now $\mu(0) = \epsilon_F^0 \approx mgh_c$

$$-T \ln\left(\frac{2}{n(h)\lambda_T^3}\right) + mgh = mgh_c$$

$$n(h) = \frac{2}{\lambda_T^3} e^{-\beta mg(h-h_c)}$$

For $h = 0$

$$n(0) = \frac{2}{\lambda_T^3} e^{\beta mgh_c}$$

$$\rightarrow n(h) = n_0 e^{-\beta mgh}$$

Statistical Mechanics - Class Exercise 4

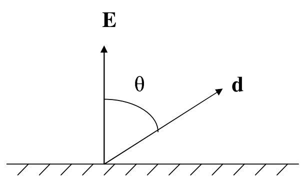
Exercise 4016 - Polar adsorption of particles to a surface

Consider an M site system in an equilibrium with gas of particles that have mass m. The chemical potential of the gas is μ and its temperature is T. A particle can bind to a site. Each site can absorb at most one atom. The binding energy is ε, and the length of the bonds is a. In such state it behaves as a rotor that has moment of inertia $I = ma^2$, and a dipole moment qa. The polarization can be in any direction away from the surface (2π steradians).
Tip: The kinetic part in a rotor Hamiltonian is

$$\frac{1}{2I}\left[p_\theta^2 + \frac{p_\varphi^2}{\sin^2(\theta)}\right]$$

1. Calculate the partition function $Z_\perp(\beta, f)$ for an occupied site, assuming electric field f perpendicular to the surface.
2. Calculate the partition function $Z_{||}(\beta, f)$ for an occupied site, assuming electric field f parallel to the surface.
3. Express the M site grand partition function $\mathcal{Z}(\beta, \mu, f)$ in terms of Z. Additionally, write an explicit expression for zero field.
4. Express the average number N of adsorbed particles in terms of Z. Additionally, write an explicit expression for zero field.
5. Find a leading order expression for the average polarization D/N for weak perpendicular f.
6. Find a leading order expression for the average polarization D/N for weak parallel f.

(*) Tip: one can use a shortcut in the calculation of Z, bypassing the integration over the momentum variables.



Answer

1. The Hamiltonian for one absorb atom in perpendicular electric field:

$$H = \frac{1}{2I}\left[p_\theta^2 + \frac{p_\varphi^2}{\sin^2(\theta)}\right] - f \cdot qa\cos(\theta)$$

Were the $\hat{z}$ direction is perpendicular to the surface.

The partition function $Z_\perp(\beta, f)$

$$Z_\perp(\beta, f) = \int \frac{d\theta d\varphi dp_\theta dp_\varphi}{(2\pi)^2} e^{-\beta H} = \int_0^{\frac{\pi}{2}} d\theta \int_0^{2\pi} d\varphi \sqrt{\frac{I}{2\pi\beta}} \sqrt{\frac{I \sin^2(\theta)}{2\pi\beta}} e^{\beta fqa\cos(\theta)}$$
$$= \frac{I}{\beta} \int_0^{\frac{\pi}{2}} d\theta \sin(\theta) e^{\beta fqa\cos(\theta)} = \frac{I}{\beta} \int_0^1 du e^{\beta fqau} = \frac{I}{\beta} \frac{\left(e^{\beta fqa} - 1\right)}{\beta fqa}$$

2. The Hamiltonian for one absorb atom in parallel electric field is the same Hamiltonian, but now we take the $\hat{z}$ direction to be parallel to the surface.
The partition function $Z_\parallel(\beta, f)$

$$Z_\parallel(\beta, f) = \int \frac{d\theta d\varphi dp_\theta dp_\varphi}{(2\pi)^2} e^{-\beta H} = \frac{I}{2\pi\beta} \int_0^{\pi} d\theta \int_0^{\pi} d\varphi \sin(\theta) e^{\beta fqa\cos(\theta)}$$
$$= \frac{I}{2\beta} \int_{-1}^1 du e^{\beta fqau} = \frac{I}{2\beta} \frac{\left(e^{\beta fqa} - e^{-\beta fqa}\right)}{\beta fqa} = \frac{I}{\beta} \frac{\sinh(\beta fqa)}{\beta fqa}$$

We can see that for $f \to 0$

$$Z_\perp(\beta, 0) = Z_\parallel(\beta, 0) = \frac{I}{\beta} = \frac{Tm2\pi a^2}{2\pi} = \frac{2\pi a^2}{\lambda_T^2}$$

3. In the grand canonical formalism

$$\mathcal{Z}(\beta, \mu) = \sum_R e^{-\beta(E_R - \mu N_R)}$$

in our case the "particles" is the sites and this are "Fermionic sites", so for site that absorb atom $E = H + \epsilon,\ N = 1$ and for empty site $E = 0,\ N = 0$.
For M sites we get

$$\mathcal{Z}(\beta, \mu, f) = \left(1 + Z(\beta, f) e^{-\beta(\epsilon - \mu)}\right)^M$$

For zero field

$$\mathcal{Z}(\beta, \mu, 0) = \left(1 + \frac{I}{\beta} e^{-\beta(\epsilon - \mu)}\right)^M$$

4. We can obtained the number N of adsorbed particles by derivative of the grand partition function

$$N(f) = \frac{1}{\beta} \frac{\partial \ln \mathcal{Z}}{\partial \mu} = M \frac{Z(\beta, f) e^{-\beta(\epsilon - \mu)}}{1 + Z(\beta, f) e^{-\beta(\epsilon - \mu)}} = \frac{M}{1 + Z^{-1}(\beta, f) e^{\beta(\epsilon - \mu)}}$$

For zero field

$$N(0) = \frac{M}{1 + \frac{\beta}{I} e^{\beta(\epsilon - \mu)}}$$

5. The average polarization D/N is the polarization of one absorb site, we can calculate this from the partition function. for weak perpendicular f

$$Z_\perp(\beta, f) = \frac{I}{\beta} \frac{\left(e^{\beta fqa} - 1\right)}{\beta fqa} \approx \frac{I}{\beta} \frac{\left(1 + \beta fqa + \frac{1}{2}(\beta fqa)^2 - 1\right)}{\beta fqa} = \frac{I}{\beta}\left(1 + \frac{1}{2}\beta fqa\right)$$

$$\frac{D}{N} = \frac{1}{\beta}\frac{\partial \ln Z_{\perp}(\beta, f)}{\partial f} = \frac{\frac{1}{2}qa}{\left(1+\frac{1}{2}\beta f qa\right)} \approx \frac{1}{2}qa$$

6. In the same way

$$Z_{\parallel}(\beta, f) = \frac{I}{\beta}\frac{\sinh\left(\beta f qa\right)}{\beta f qa} \approx \frac{I}{\beta}\frac{\beta f qa + \frac{1}{3!}\left(\beta f qa\right)^3}{\beta f qa} = \frac{I}{\beta}\left(1+\frac{1}{6}\left(\beta f qa\right)^2\right)$$

$$\frac{D}{N} = \frac{1}{\beta}\frac{\partial \ln Z_{\parallel}(\beta, f)}{\partial f} = \frac{1}{\beta}\frac{\frac{1}{3}\left(\beta qa\right)^2 f}{\left(1+\frac{1}{6}\left(\beta f qa\right)^2\right)} \approx \frac{1}{3}\beta\left(qa\right)^2 f$$

Exercise 4211 - The law of mass action for diatomic molecules

Consider a diatomic AB molecule, where A and B are different spin 0 atoms, each having a 1-unit atomic mass m_0. The length of the molecule is a, the binding energy is $-\epsilon_0$, and the vibration frequency of the bond is ω_0. The vibration amplitude is much smaller compared with a. The temperatures are not low, namely $T \gg 1/(m_0 a^2)$, such that the rotation-spectrum can be treated as a continuum. For higher temperatures ($T \gg \omega_0$) also the vibration-spectrum can be treated using a classical approximation.
In item (3) below we consider Hydrogen H_2, Deuterium D_2, and HD molecules. The respective masses of the atoms are m_H, m_D. Note that the Deuterium nucleus has spin 1. Assume that neither the energy nor the "spring constant" of the binding are affected by the $H \mapsto D$ replacement.

1. Find the one molecule partition function Z^{AB} for an AB molecule that is held in a container that has volume L^3. Assume that the temperature is not low, but not necessarily high.
2. Write the law of mass action for the reaction $A{+}B \leftrightarrow AB$. Find an explicit expression for the equilibrium constant $K(T)$ in the high temperature regime.
3. Write the law of mass action for the reaction $H_2 + D_2 \leftrightarrow 2HD$. Express the equilibrium constant $K(T)$ in terms of one-particle partition functions Z^C, were C stands for H_2, and D_2, and HD.
4. Find expressions for the ratio Z^C/Z^{AB} in the high temperature regime, where A and B are distinct spinless atoms that have the same masses as that of the C constituents. Explain why the high temperature assumpation is essential in order to get a simple result.
5. What is the explicit result for $K(T)$ of item (3) in the high temperature regime?

Tip: The Hamiltonian of a diatomic molecule consist of center of mass degrees of freedom, and of a relative motion degrees of freedom. The latter involves the reduced mass $m_A m_B/(m_A + m_B)$. For intermediate calculations you can use the notation α for spring constant.

Answer

1. To find the one molecule partition function Z^{AB} we need to separate the motion to the center of mass motion, and of a relative motion

$$H = -\epsilon_0 + \frac{P^2}{2M} + \frac{1}{2}m\omega_0^2 x^2 + \frac{\ell^2}{2I}$$

When

$$M = m_A + m_B = 2m_0, m = \frac{m_A m_B}{(m_A + m_B)} = \frac{m_0}{2}$$

$$I = 2m_0 \left(\frac{a}{2}\right)^2, \omega_0 = \sqrt{\frac{\alpha}{m}} = \sqrt{\frac{2\alpha}{m_0}}$$

$$E = -\epsilon_0 + \frac{P^2}{2M} + \omega_0\left(n + \frac{1}{2}\right) + \frac{l\,(l+1)}{2I}$$

In the continuum limit for the rotation

$$Z_l = \sum_l (2l+1)\, e^{-\beta\frac{l(l+1)}{2I}} \approx \int_0^\infty 2le^{-\beta\frac{l^2}{2I}}\,dl = \frac{2I}{\beta}$$

so we get

$$Z^{AB} = \left(\frac{L}{\lambda_M}\right)^3 e^{\beta\epsilon_0}\frac{1}{2\sinh\left(\frac{1}{2}\beta\omega_0\right)}\frac{m_0 a^2}{\beta}$$

$$\lambda_M = \sqrt{\frac{2\pi}{MT}} = \frac{1}{\sqrt{2}}\sqrt{\frac{2\pi}{m_0 T}} = \frac{1}{\sqrt{2}}\lambda_T$$

$$Z^{AB} = \left(\frac{\sqrt{2}L}{\lambda_T}\right)^3 e^{\beta\epsilon_0}\frac{1}{2\sinh\left(\frac{1}{2}\beta\omega_0\right)}\frac{m_0 a^2}{\beta}$$

2. The partition functions for the atoms A and B are

$$Z^A = \left(\frac{L}{\lambda_T}\right)^3 = Z^B$$

for the reaction $A + B \leftrightarrow AB$

$$Z = \sum_n Z^{AB}_{N_{AB}-n} Z^A_{N_A+n} Z^B_{N_B+n} = \sum_n e^{-\beta F(n)}$$

to find the Chemical equilibrium we need to find most probable value for n

$$\frac{\partial F}{\partial n} = -\mu_{AB}\,(N_{AB} - n) + \mu_A\,(N_A + n) + \mu_B\,(N_B + n) = 0$$

we remember that

$$\mu = \frac{\partial F}{\partial N} = \frac{\partial}{\partial N}\left(-T\ln\left(\frac{Z_1^N}{N!}\right)\right) = T\ln\left(\frac{N}{Z_1}\right)$$

$$\frac{(N_{AB} - n)}{(N_A + n)\,(N_B + n)} = \frac{Z^{AB}}{Z^A Z^B}$$

$$\frac{\frac{(N_{AB}-n)}{V}}{\frac{(N_A+n)}{V}\frac{(N_B+n)}{V}} = K(T) = \left(\sqrt{2}\lambda_T\right)^3 e^{\beta\epsilon_0}\frac{1}{2\sinh\left(\frac{1}{2}\beta\omega_0\right)}m_0 a^2 T$$

in the high temperature regime for vibration $T \gg \omega_0$

$$K(T) \approx \left(\sqrt{2}\lambda_T\right)^3 e^{\beta\epsilon_0}\frac{m_0}{\omega_0}a^2T^2$$

3. We have three molecule partition functions that differ from one another by the mass and the spin

$$Z^{H_2} = \left(\frac{1}{2}\right)_{\text{Gibs}}(2\cdot 2)_{\text{spin}}\left(\frac{L}{\lambda_{M_{H_2}}}\right)^3 e^{\beta\epsilon_0}\frac{1}{2\sinh\left(\frac{1}{2}\beta\sqrt{\frac{\alpha}{m_{H_2}}}\right)}\frac{2m_{H_2}a^2}{\beta}$$

$$Z^{D_2} = \left(\frac{1}{2}\right)_{\text{Gibs}}(3\cdot 3)_{\text{spin}}\left(\frac{L}{\lambda_{M_{D_2}}}\right)^3 e^{\beta\epsilon_0}\frac{1}{2\sinh\left(\frac{1}{2}\beta\sqrt{\frac{\alpha}{m_{D_2}}}\right)}\frac{2m_{D_2}a^2}{\beta}$$

$$Z^{HD} = (2\cdot 3)_{\text{spin}}\left(\frac{L}{\lambda_{M_{HD}}}\right)^3 e^{\beta\epsilon_0}\frac{1}{2\sinh\left(\frac{1}{2}\beta\sqrt{\frac{\alpha}{m_{HD}}}\right)}\frac{2m_{HD}a^2}{\beta}$$

the law of mass action for the reaction $H_2 + D_2 \leftrightarrow 2HD$

$$\frac{(N_{HD}-2n)^2}{(N_{H_2}+n)(N_{D_2}+n)} = \frac{\left(Z^{HD}\right)^2}{Z^{H_2}Z^{D_2}} = K(T)$$

4. in the high temperature regime

$$Z^{H_2} = \left(\frac{1}{2}\right)_{\text{Gibs}}(2\cdot 2)_{\text{spin}}\left(\frac{L}{\lambda_{M_{H_2}}}\right)^3 e^{\beta\epsilon_0}\frac{1}{2\sinh\left(\frac{1}{2}\beta\sqrt{\frac{\alpha}{m_{H_2}}}\right)}\frac{2m_{H_2}a^2}{\beta}$$

$$\approx \left(\frac{1}{2}\right)_{\text{Gibs}}(2\cdot 2)_{\text{spin}}\left(\frac{L}{\sqrt{\frac{2\pi}{T}}}\right)^3 M_{H_2}^{\frac{3}{2}}e^{\beta\epsilon_0}\frac{1}{\sqrt{\alpha}}\frac{2m_{H_2}^{\frac{3}{2}}a^2}{\beta^2} = \left(\frac{1}{2}\right)_{\text{Gibs}}(2\cdot 2)_{\text{spin}}\left(\frac{L}{\sqrt{\frac{2\pi}{T}}}\right)^3 e^{\beta\epsilon_0}\frac{1}{\sqrt{\alpha}}\frac{2a^2}{\beta^2}(m_H m$$

The ratio

$$\frac{Z^{H_2}}{Z^{AB}} \approx \left(\frac{1}{2}\right)_{\text{Gibs}}(2\cdot 2)_{\text{spin}}\left(\frac{m_H m_H}{m_A m_B}\right)^{\frac{3}{2}} = 2$$

in the same way

$$\frac{Z^{D_2}}{Z^{AB}} \approx \frac{9}{2}$$

$$\frac{Z^{HD}}{Z^{AB}} \approx 6$$

5. In the high temperature regime

$$K(T) = \frac{\left(Z^{HD}\right)^2}{Z^{H_2}Z^{D_2}} \approx \frac{6^2(m_H m_D)^3}{2(m_H m_H)^{\frac{3}{2}}\frac{9}{2}(m_D m_D)^{\frac{3}{2}}} = 4$$

Statistical Mechanics - Class Exercise 5

The Boltzmann distribution function

If we want to calculate the flux of particles with velocity v

$$J_v = \iint_{\theta<\frac{\pi}{2}} \frac{d\Omega}{4\pi}\frac{N}{V} v\cos(\theta) = \frac{1}{2}\int_\theta^{\frac{\pi}{2}} d\theta \sin(\theta)\frac{N}{V} v\cos(\theta) = \frac{1}{4}\left(\frac{N}{V}\right) v$$

The number of particles

$$\begin{aligned} N = &\iint d\boldsymbol{r}\frac{d\boldsymbol{p}}{(2\pi)^3} f(\epsilon_{\boldsymbol{p}} - \mu) \\ =&V\left(\frac{m}{2\pi}\right)^3 \int d\boldsymbol{v} f\left(\frac{mv^2}{2} - \mu\right) \\ =&V\left(\frac{m}{2\pi}\right)^3 \int 4\pi v^2 dv f\left(\frac{mv^2}{2} - \mu\right) = \int F(v)\, dv \end{aligned}$$

$$F(v) = V\left(\frac{m}{2\pi}\right)^3 4\pi v^2 f\left(\frac{mv^2}{2} - \mu\right)$$

So the total flux is

$$J = \int_0^\infty \frac{1}{4}\left(\frac{F(v)\, dv}{V}\right) v$$

Exercise 6030 - Thermionic emission of electrons from a metal

A spherical piece of metal ("cathode"), that has radius R and temperature T, is placed inside a vacuum tube. A second metallic piece ("anode") is used to collect the electrons that are emitted from the cathode. The effective temperature of the anode is zero. The cathode has a work function W, while the anode has work function W'. The depth of the potential that holds the electrons inside the cathode, aka the potential floor, is V_0.

1. Write an integral expression for the saturation current I_s that would be measured if the bias voltage is very large.
   (a) Show that V_0 does not appear in the final result: the outcome of the calculation is the same for sections that are close to the surface or deep in the metal.
   (b) Calculate the integral using the Boltzmann approximation. Specify the range of temperatures for which the approximation is valid.
2. Using the result of the previous item write an estimate for the current if a reverse (stopping) voltage V_{battery} is applied. Explain whether W or W' is relevant.

(a) Explain the relation to the analysis of the stopping voltage in the photoelectric effect.

3. Assume that the cathode is detached and left alone in free space. Calculate the charge $Q(t)$ of the cathode as a function of time assuming that $Q(0) = 0$.

   (a) Explain the limitations of the result that you have obtained.

Answer

1. The energy of electron on the surface of the cathode is

$$E = \frac{mv^2}{2} - eV_0$$

The velocity $v^2 = v_{\parallel}^2 + v_{\perp}^2$, Where $v_{\parallel}$ and $v_{\perp}$ are the electron velocities in the direction parallel and perpendicular to the surface respectively.
The minimum energy for electron to escape from the cathode is when $v_{\parallel} = 0, v_{\perp} = \sqrt{\frac{2eV_0}{m}}$. For a large (repelling) bias voltage, all escaping electrons reach the anode and contribute to the current. We want to calculate he total flux, but because the different in the minimum of the velocity in the different directions let's define $F(\boldsymbol{v})$such that

$$\int F(\boldsymbol{v})\, d\boldsymbol{v} = \int F(v)\, dv$$

So $F(\boldsymbol{v}) = 2 \times V \times \left(\frac{m}{2\pi}\right)^3 f\left(\frac{mv^2}{2} - \mu\right)$,

$$J = \int \left(\frac{F(\boldsymbol{v})\, d\boldsymbol{v}}{V}\right) v_{\perp}$$

$$J = 2\left(\frac{m}{2\pi}\right)^3 \iint d^2 v_{\parallel} \int_{\sqrt{\frac{2eV_0}{m}}}^{\infty} dv_{\perp} f\left(\frac{mv^2}{2} - \mu\right) v_{\perp}$$

Where $\mu = eV_0 - W$

$$J = \left(\frac{m}{2\pi}\right)^3 \iint_{-\infty}^{\infty} d^2 v_{\parallel} \int_{\frac{2eV_0}{m}}^{\infty} dv_{\perp}^2 f\left(\frac{mv_{\parallel}^2}{2} + \frac{mv_{\perp}^2}{2} - eV_0 + W\right)$$

1(a). take $v^2 = v^2 - \frac{2eV_0}{m}$

$$J = \left(\frac{m}{2\pi}\right)^3 \iint_{-\infty}^{\infty} d^2 v_{\parallel} \int_0^{\infty} f\left(\frac{mv_{\parallel}^2}{2} + \frac{mv_{\perp}^2}{2} + W\right) dv_{\perp}^2$$

The saturation current

$$I_s = 4\pi R^2 J = \frac{m^3 R^2}{2\pi^2} \iint_{-\infty}^{\infty} d^2 v_{\parallel} \int_0^{\infty} f\left(\frac{mv_{\parallel}^2}{2} + \frac{mv_{\perp}^2}{2} + W\right) dv_{\perp}^2$$

1(b). In the Boltzmann approximation

$$f\left(\frac{mv^2}{2}+W\right)\approx e^{-\beta\left(\frac{mv^2}{2}+W\right)}$$

$$J=\left(\frac{m}{2\pi}\right)^3\iint_{-\infty}^{\infty}e^{-\beta\left(\frac{mv_\parallel^2}{2}\right)}d^2v_\parallel\int_0^\infty e^{-\beta\left(\frac{mv_\perp^2}{2}+W\right)}dv_\perp^2=\frac{m^2}{2^2\pi^2}T\int_0^\infty e^{-\beta\left(\frac{mv_\perp^2}{2}+W\right)}dv_\perp^2=\frac{m}{2\pi^2}T^2e^{-\frac{W}{T}}$$

$$I_s=4\pi R^2J=\frac{2mR^2}{\pi}T^2e^{-\frac{W}{T}}$$

2. In this situation the electron need energy that

$$\mu_{\text{anode}}+W'-\mu_{\text{cathode}}=W'+eV_{\text{battery}},$$

so we expect that the expression for the current will be:

$$I\propto T^2e^{-\beta\left(W'+eV_{\text{battery}}\right)}$$

2(a). In the photoelectric effect the cathode isn't heated so one assumes zero temperature Fermi occupation for the cathode also. That means there is no thermionic emission. The electrons are excited out of the cathode by photons with a fixed energy. These photons need to be with enough energy for the electrons to pass the energetic barrier, which is again $W'+eV_{\text{battery}}$. So if we measure the voltage needed to stop the current for a given photons energy, we know that at that voltage we have:

$$E_{\text{photon}}=W'+eV_{\text{battery}}\implies W'=E_{\text{photon}}-eV_{\text{battery}}$$

So we can calculate the anode work function.

3. We can treat the cathode as a capacitor. The charge will be $Q=VC$, and the current: $I=C\frac{d}{dt}V$. Here $C=\frac{1}{R}$, and V are the capacitance and voltage of a charged sphere in vacuum with respect to infinity. On the other hand we know from item (2) that when there is a voltage difference the current is $\sim I_0e^{-\beta eV}$, where I_0 is independent of V. So we need to solve:

$$\frac{d}{dt}V=\frac{I_0}{C}e^{-\beta eV}$$

given that $Q\left(t=0\right)=0$:

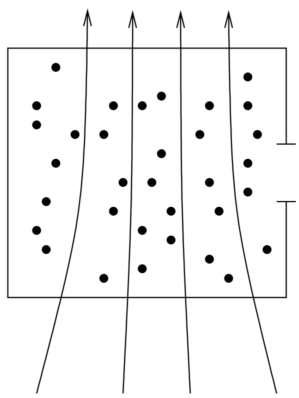
$$e^{\beta eV}dV=\frac{I_0}{C}dt\implies\frac{T}{e}e^{\beta eV}=\frac{I_0}{C}t+\frac{T}{e}$$

$$V=\frac{T}{e}\ln\left(\frac{e}{T}\frac{I_0}{C}t+1\right)\implies Q\left(t\right)=\frac{CT}{e}\ln\left(\frac{e}{T}\frac{I_0}{C}t+1\right)$$

3(a). The result is limited because it is valid only when the Boltzmann approximation is valid, and it does not take into consideration finite number of electrons.

Exercise 6040 - Effusion of electrons from a box in magnetic field

A box with electrons of mass m is subjected to a magnetic field B. The single particle interaction is described by $-\gamma B\sigma_z$. The chemical potential of the electrons inside the box is μ. A hole through one of the walls is drilled. The electrons that are emitted from the hole with a velocity in the range $v < v' < v+dv$ are filtered, and subsequently their spin is measured. The measured current is defined as $I = I_\uparrow + I_\downarrow$.



1. Find the ratio $\alpha(B;\mu) = (I_\uparrow - I_\downarrow)/I$.
2. Find a linear approximation for $\alpha(B;\mu)$ regarded as a function of the magnetic field.
3. What is the maximal value of $\alpha(B;\mu)/B$, and what is the range for which the result is valid.

Answer

1. The flux for N electrons in volume V with velocity v is :

$$J = \iint_{|\theta|<\frac{\pi}{2}} \frac{d\Omega}{4\pi}\frac{N}{V} v\cos\theta = \frac{1}{4}\left(\frac{N}{V}\right) v$$

The number of the particles N:

$$N = \int g(E) f(E-\mu)\, dE = \int F(v)\, dv$$

The number of spin up electrons in the velocity range $v < v' < v + dv$ is given by :

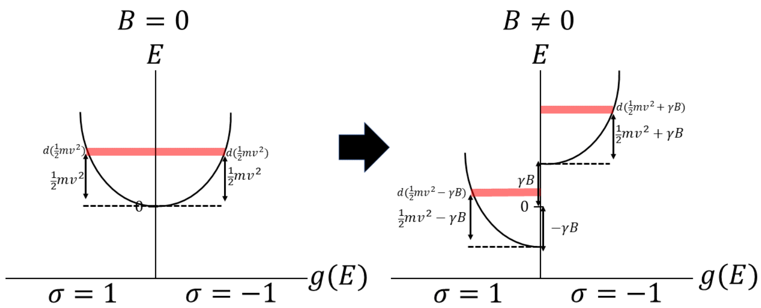
$$N_\uparrow(v < v' < v{+}dv) = dN_\uparrow = g\left(\frac{1}{2}mv^2 - \gamma B\right) f\left(\frac{1}{2}mv^2 - \gamma B - \mu\right) d\left(\frac{1}{2}mv^2 - \gamma B\right)$$

So

$$I_\uparrow = J_\uparrow dAdt = \frac{1}{4}\frac{g\left(\frac{1}{2}mv^2 - \gamma B\right) f\left(\frac{1}{2}mv^2 - \gamma B - \mu\right) d\left(\frac{1}{2}mv^2 - \gamma B\right)}{V} vdAdt$$

$$I_{\downarrow} = J_{\downarrow} dAdt = \frac{1}{4} \frac{g\left(\frac{1}{2}mv^2 + \gamma B\right) f\left(\frac{1}{2}mv^2 + \gamma B - \mu\right) d\left(\frac{1}{2}mv^2 + \gamma B\right)}{V} v dAdt$$

But we can see that $g\left(\frac{1}{2}mv^2 - \gamma B\right) = g\left(\frac{1}{2}mv^2 + \gamma B\right) = g\left(\frac{1}{2}mv^2\right)$ and $d\left(\frac{1}{2}mv^2 - \gamma B\right) = d\left(\frac{1}{2}mv^2 + \gamma B\right) = d\left(\frac{1}{2}mv^2\right)$



So we get

$$\alpha(B;\mu) = \frac{I_{\uparrow} - I_{\downarrow}}{I_{\uparrow} + I_{\downarrow}} = \frac{f\left(\frac{1}{2}mv^2 - \gamma B - \mu\right) - f\left(\frac{1}{2}mv^2 + \gamma B - \mu\right)}{f\left(\frac{1}{2}mv^2 - \gamma B - \mu\right) + f\left(\frac{1}{2}mv^2 + \gamma B - \mu\right)}$$

2. The linear approximation for $\alpha(B;\mu)$ regarded as a function of the magnetic field:

$$f\left(\frac{1}{2}mv^2 \pm \gamma B - \mu\right) \approx f\left(\frac{1}{2}mv^2 - \mu\right) \pm f'\left(\frac{1}{2}mv^2 - \mu\right)\gamma B$$

$$\alpha(B;\mu) \approx \frac{-f'\left(\frac{1}{2}mv^2 - \mu\right)}{f\left(\frac{1}{2}mv^2 - \mu\right)}\gamma B$$

$$f'\left(\frac{1}{2}mv^2 - \mu\right) = \left(\frac{1}{e^{\beta\left(\frac{1}{2}mv^2 - \mu\right)} + 1}\right)' = -\frac{\beta e^{\beta\left(\frac{1}{2}mv^2 - \mu\right)}}{\left(e^{\beta\left(\frac{1}{2}mv^2 - \mu\right)} + 1\right)^2} = -f\left(\frac{1}{2}mv^2 - \mu\right)^2 \beta e^{\beta\left(\frac{1}{2}mv^2 - \mu\right)}$$

$$\alpha(B;\mu) \approx f\left(\frac{1}{2}mv^2 - \mu\right) e^{\beta\left(\frac{1}{2}mv^2 - \mu\right)} \beta\gamma B = \frac{1}{1 + e^{-\beta\left(\frac{1}{2}mv^2 - \mu\right)}}\beta\gamma B$$

3. For

$$\beta\left(\frac{1}{2}mv^2 - \mu\right) \gg 1$$

$$\frac{mv^2}{2} \gg (T + \mu)$$

$$\alpha(B;\mu)/B \to \frac{\gamma}{T}$$

Statistical Mechanics - Class Exercise 6

Exercise 5024 - Pressure of Lenard Jones gas

A gas of N particles is confined in a box of volume V at temprature of T. The two-body interaction between the particles is given by the Lenard Jones expression:

$$u(r) \quad = \quad \frac{a}{r^{12}} - \frac{b}{r^6}$$

Note that this interaction is characterized by a length scale r_0 and an energy scale ϵ_0 that correspond to the position and the depth of the potential.

1. Find an expression for the pressure via the Virial theorem, assuming that the moments $\langle r^n \rangle_T$ are known.

2. Using the Virial expansion, find an explicit expression for the pressure assuming low temperatures.

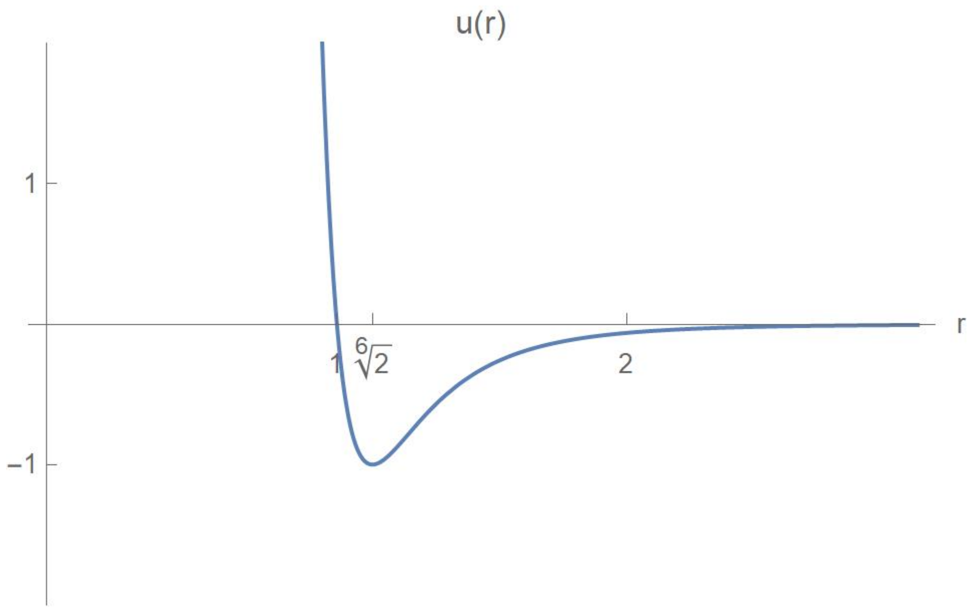
3. Using the Virial expansion, find an explicit expression for the pressure assuming high temperatures.

4. Comparing your answers to items (1) and (3) deduce explicit expressions for the $n = -6$ and for the $n = -12$ moments. Express your result in terms of (V, r_0, ϵ_0, T).

Answer

The Lenard Jones potential is:

$$u(r) = \frac{a}{r^{12}} - \frac{b}{r^6}$$



The length scale is r_0, so

$$u(r_0) = \frac{a}{r_0^{12}} - \frac{b}{r_0^6} = 0$$

$$\rightarrow r_0 = \left(\frac{a}{b}\right)^{\frac{1}{6}}$$

the minimum is

$$u'(r) = -12\frac{a}{r^{13}} + 6\frac{b}{r^7} = 0$$

$$\rightarrow r_m = \left(\frac{2a}{b}\right)^{\frac{1}{6}} = 2^{\frac{1}{6}} r_0$$

In this point

$$u(r_m) = \frac{a}{r_m^{12}} - \frac{b}{r_m^6} = \frac{b^2}{4a} - \frac{b^2}{2a} = -\frac{b^2}{4a} = -\epsilon_0$$

so we get

$$u(r) = \left(\frac{b^2}{a}\frac{r_0^{12}}{r^{12}} - \frac{b^2}{a}\frac{r_0^6}{r^6}\right) = 4\epsilon_0\left(\frac{r_0^{12}}{r^{12}} - \frac{r_0^6}{r^6}\right)$$

$$u''(r_m) = 4\epsilon_0\left(12\cdot 13\frac{r_0^{12}}{r_m^{14}} - 6\cdot 7\frac{r_0^6}{r_m^8}\right) = 4\epsilon_0\left(12\cdot 13\frac{1}{2^{\frac{14}{6}}r_0^2} - 6\cdot 7\frac{1}{2^{\frac{8}{6}}r_0^2}\right) = 72\frac{\epsilon_0}{2^{\frac{1}{3}}r_0^2} = 72\frac{\epsilon_0}{r_m^2}$$

1. The pressure is given by the Virial theorem:

$$P = \frac{1}{V}\left[NT - \frac{1}{3}\langle r\cdot\frac{\partial U}{\partial r}\rangle\right]$$

Where

$$U = \sum_{\langle i,j\rangle} u\left(|\vec{r}_i - \vec{r}_j|\right)$$

$$r\cdot\frac{\partial u}{\partial r} = -24\epsilon_0\left(2\frac{r_0^{12}}{r^{12}} - \frac{r_0^6}{r^6}\right)$$

The sum is over all the interaction $\frac{N(N-1)}{2} \approx \frac{N^2}{2}$, so we get

$$P = \frac{NT}{V}\left[1 + 4\frac{\epsilon_0}{T}Nr_0^6\left(2r_0^6\left\langle r^{-12}\right\rangle - \left\langle r^{-6}\right\rangle\right)\right]$$

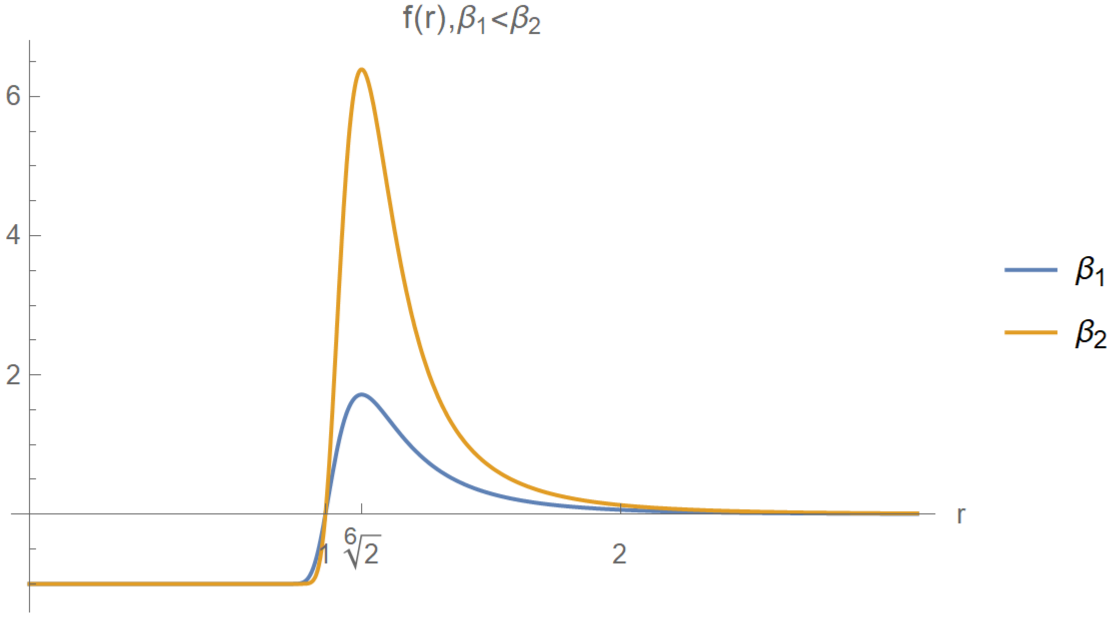
2. The Virial expansion for the pressure is:

$$P = \frac{NT}{V}\left[1 + a_2\left(\frac{N}{V}\right) + a_3\left(\frac{N}{V}\right)^2 + ...\right]$$

The second Virial coefficient is:

$$a_2 = -\frac{1}{2}\int\left(e^{-\beta u(r)} - 1\right)d^3r = -\frac{1}{2}\int f\left(r\right)d^3r$$

For low temperatures ($\beta\epsilon_0 \gg 1$) we can take the saddle point approximation around the minimum point of $u(r)$



$$a_2 \approx -\frac{1}{2}\int e^{-\beta\left[u(r_m)+\frac{1}{2}u''(r_m)(r-r_m)^2\right]}d^3r = -2\pi e^{-\beta u(r_m)}\int_0^\infty e^{-\frac{1}{2}\beta u''(r_m)(r-r_m)^2}r^2dr$$

We need to solve

$$\int_0^\infty e^{-\frac{1}{2}\beta u''(r_m)(r-r_m)^2}r^2dr = \int_{-r_m}^\infty e^{-\frac{1}{2}\beta u'' r^2}\left(r^2+2rr_m+r_m^2\right)dr =$$

For the the first integral we use $\left(e^{-\frac{1}{2}\beta u'' r^2}\right)' = -\beta u'' r e^{-\frac{1}{2}\beta u'' r^2}$, so with integration by parts we get

$$\begin{aligned}\frac{1}{-\beta u''}\int_{-r_m}^\infty\left(-\beta u'' e^{-\frac{1}{2}\beta u'' r^2}r\right)rdr =&\frac{1}{-\beta u''}e^{-\frac{1}{2}\beta u'' r^2}r|_{-r_m}^\infty - \frac{1}{-\beta u''}\int_{-r_m}^\infty e^{-\frac{1}{2}\beta u'' r^2}dr\\ =&-\frac{1}{72\beta\epsilon_0}e^{-36\beta\epsilon_0}r_m^3 + \frac{1}{\beta u''}\int_{-r_m}^\infty e^{-\frac{1}{2}\beta u'' r^2}dr\end{aligned}$$

The second part

$$\begin{aligned}\int_{-r_m}^\infty e^{-\frac{1}{2}\beta u'' r^2}(2rr_m)\,dr =&2r_m\left(\int_0^\infty e^{-\frac{1}{2}\beta u'' r^2}rdr - \int_0^{r_m} e^{-\frac{1}{2}\beta u'' r^2}rdr\right)\\ =&r_m\left(\int_0^\infty e^{-\frac{1}{2}\beta u'' z}dz - \int_0^{r_m^2} e^{-\frac{1}{2}\beta u'' z}dz\right) = r_m\left(\frac{1}{\frac{1}{2}\beta u''} - \frac{e^{-\frac{1}{2}\beta u'' r_m^2}-1}{-\frac{1}{2}\beta u''}\right)\\ =&2r_m^3\frac{e^{-36\beta\epsilon_0}}{72\beta\epsilon_0}\end{aligned}$$

we stay with

$$\left(r_m^2+\frac{1}{\beta u''}\right)\int_{-r_m}^{\infty}e^{-\frac{1}{2}\beta u'' r^2}dr=\left(r_m^2+\frac{1}{\beta u''}\right)\left(\int_0^{\infty}e^{-\frac{1}{2}\beta u'' r^2}dr+\int_0^{r_m}e^{-\frac{1}{2}\beta u'' r^2}dr\right)$$
$$=\left(r_m^2+\frac{1}{\beta u''}\right)\left(\sqrt{\frac{\pi}{\beta u''}}+\frac{1}{\sqrt{\frac{1}{2}\beta u''}}\int_0^{\sqrt{\frac{1}{2}\beta u''}r_m}e^{-t^2}dt\right)$$
$$=r_m^3\left(1+\frac{1}{72\beta\epsilon_0}\right)\frac{\sqrt{\pi}}{12}\frac{1}{\sqrt{\beta\epsilon_0}}\left(1+\mathrm{erf}\left(6\sqrt{\beta\epsilon_0}\right)\right)$$

$\left(\mathrm{erf}\left(x\right)=\frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}dt\right)$
All together we get

$$a_2\approx-2\pi e^{-\beta u(r_m)}\int_0^{\infty}e^{-\frac{1}{2}\beta u''(r_m)(r-r_m)^2}r^2dr$$
$$=-2\pi e^{\frac{\epsilon_0}{T}}r_m^3\left[\frac{\sqrt{\pi}}{12}\left(\frac{1}{72}\left(\frac{T}{\epsilon_0}\right)^{\frac{3}{2}}+\left(\frac{T}{\epsilon_0}\right)^{\frac{1}{2}}\right)\left(\mathrm{erf}\left(6\sqrt{\frac{\epsilon_0}{T}}\right)+1\right)+\frac{T}{\epsilon_0}\frac{e^{-\frac{36\epsilon_0}{T}}}{72}\right]$$
$$\approx-\frac{\pi^{\frac{3}{2}}}{6}e^{\frac{\epsilon_0}{T}}r_m^3\left[\frac{1}{72}\left(\frac{T}{\epsilon_0}\right)^{\frac{3}{2}}+\left(\frac{T}{\epsilon_0}\right)^{\frac{1}{2}}\right]\left(\mathrm{erf}\left(6\sqrt{\frac{\epsilon_0}{T}}\right)+1\right)$$

For $\frac{\epsilon_0}{T}\gg 1$

$$\mathrm{erf}\left(6\sqrt{\frac{\epsilon_0}{T}}\right)\approx 1$$

$$a_2\approx-e^{\frac{\epsilon_0}{T}}\frac{r_0^3}{3}\left(2\pi^3\right)^{\frac{1}{2}}\left(\frac{T}{\epsilon_0}\right)^{\frac{1}{2}}$$

$$P=\frac{NT}{V}\left[1-e^{\frac{\epsilon_0}{T}}\frac{r_0^3}{3}\left(2\pi^3\right)^{\frac{1}{2}}\left(\frac{T}{\epsilon_0}\right)^{\frac{1}{2}}\left(\frac{N}{V}\right)\right]$$

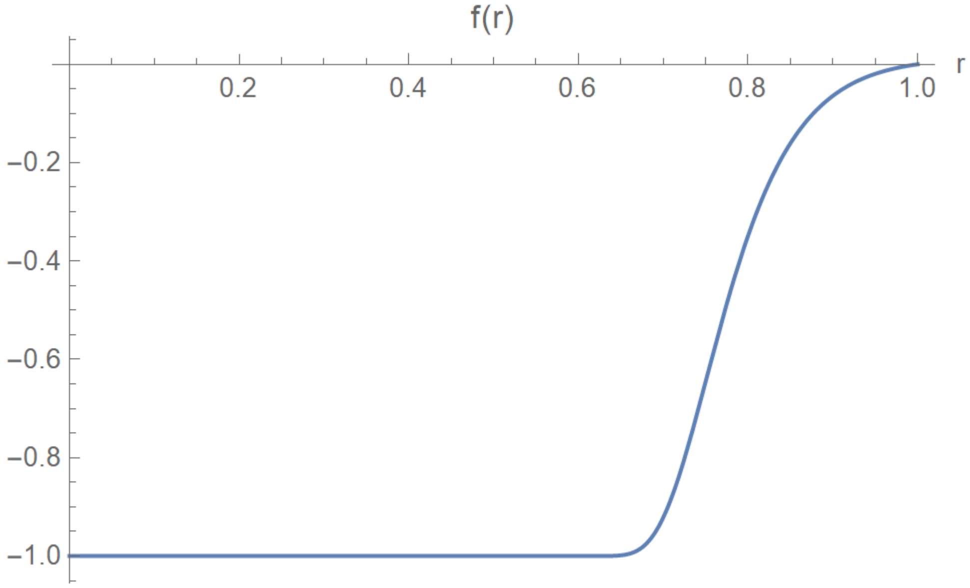
3. For $(\beta\epsilon_0\ll 1)$

$$f\left(r\right)=e^{-\beta u(r)}-1\approx-\beta u\left(r\right)$$
$$a_2=\frac{\beta}{2}\int u\left(r\right)d^3r=8\pi\beta\epsilon_0\int_0^{\infty}\left[\left(\frac{r_0}{r}\right)^{12}-\left(\frac{r_0}{r}\right)^{6}\right]r^2dr$$

But this integral does not converge for $r\to 0$, so we divide it to two parts $0<r<r_0,\ \ r_0<r<\infty$

$$a_{2>}=8\pi\beta\epsilon_0\int_{r_0}^{\infty}\left[\left(\frac{r_0}{r}\right)^{12}-\left(\frac{r_0}{r}\right)^{6}\right]r^2dr=-\frac{16\pi}{9}\frac{\epsilon_0}{T}r_0^3$$

For the second range we can see that in this range $f\left(0\right)=-1$ and $f\left(r_0\right)=0$,So we can approximate $f(r)$ as a step function with the width $\tilde{r}$, when for $\tilde{r}$, $e^{-\beta u(\tilde{r})}=e^{-1}$



$$\beta u(\tilde{r}) = 4\frac{\epsilon_0}{T}\left[\left(\frac{r_0}{\tilde{r}}\right)^{12} - \left(\frac{r_0}{\tilde{r}}\right)^{6}\right] = 1$$

$$\tilde{r}^{12} + 4\frac{\epsilon_0}{T}r_0^6\tilde{r}^6 - 4\frac{\epsilon_0}{T}r_0^{12} = 0$$

$$\tilde{r}^6 = -2\frac{\epsilon_0}{T}r_0^6 \pm 2\sqrt{\frac{\epsilon_0}{T}}r_0^6\sqrt{\left(\frac{\epsilon_0}{T}\right)+1} = -2\frac{\epsilon_0}{T}r_0^6 \pm 2r_0^6\sqrt{\frac{\epsilon_0}{T}}\sqrt{1+\left(\frac{\epsilon_0}{T}\right)} \approx 2r_0^6\sqrt{\frac{\epsilon_0}{T}}$$

$$\tilde{r} \approx \left(\frac{4\epsilon_0}{T}\right)^{\frac{1}{12}} r_0$$

$$a_{2<} = -2\pi\int_0^{\tilde{r}} (-1)\, r^2 dr = \frac{2\pi}{3}\left(\frac{4\epsilon_0}{T}\right)^{\frac{1}{4}} r_0^3$$

So

$$a_2 = \frac{2\pi}{3}\left[\left(\frac{4\epsilon_0}{T}\right)^{\frac{1}{4}} - \frac{2}{3}\frac{4\epsilon_0}{T}\right] r_0^3$$

$$P = \frac{NT}{V}\left[1 + \frac{2\pi}{3}\left[\left(\frac{4\epsilon_0}{T}\right)^{\frac{1}{4}} - \frac{2}{3}\frac{4\epsilon_0}{T}\right] r_0^3\left(\frac{N}{V}\right)\right]$$

4. We comperes

$$P = \frac{NT}{V}\left[1 + 4\frac{\epsilon_0}{T}Nr_0^6\left(2r_0^6\left\langle r^{-12}\right\rangle - \left\langle r^{-6}\right\rangle\right)\right] = \frac{NT}{V}\left[1 + \frac{2\pi}{3}\left[\left(\frac{4\epsilon_0}{T}\right)^{\frac{1}{4}} - \frac{2}{3}\frac{4\epsilon_0}{T}\right] r_0^3\left(\frac{N}{V}\right)\right]$$

$$8\frac{\epsilon_0}{T}Nr_0^{12}\left\langle r^{-12}\right\rangle = \frac{2\pi}{3}\left(\frac{4\epsilon_0}{T}\right)^{\frac{1}{4}} r_0^3\left(\frac{N}{V}\right)$$

$$\left\langle r^{-12}\right\rangle = \frac{\pi}{3Vr_0^9}\left(\frac{4\epsilon_0}{T}\right)^{-\frac{3}{4}}$$

$$\langle r^{-6} \rangle = \frac{4\pi}{9Vr_0^3}$$

Exercise 5963 - Stoner ferromagnetism

Consider Fermi gas of N spin 1/2 electrons, at temperature $T = 0$. Define N_+ and N_- as the number of "up" and "down" electrons respectively, such that $N = N_+ + N_-$. Due to the antisymmetry of the total wave function the energy of the system is $U = \alpha N_+ N_- / \mathsf{V}$, where V is the volume. Note that this interaction favors parallel spin states. Define the magnetization as $M = (N_+ - N_-)/\mathsf{V}$.

1. Write the total energy $E(M)$, including both the kinetic energy and the interaction, and expand up to 4th order in M.
2. Find the critical value α_c, such that for $\alpha > \alpha_c$ the electron gas can lower its total energy by spontaneously developing magnetization. This is known as the Stoner instability.
3. Explain the instability qualitatively, and sketch the behavior of the spontaneous magnetization versus α.
4. Repeat (1) at finite but low temperatures T, and find $\alpha_c(T)$ to second order in T.

Guidance: In the last item explain why the energy $E(M)$ should be replaced by the M-constrained "free energy" $F(M)$. Use know results [Patria] for the free energy of electrons at finite temperature.

Answer

1. the total energy

$$E_T = E_K + U$$

for E_k we need to find k_F

$$N_\pm = V \int_{k<k_F} \frac{d^3k}{(2\pi)^3} = \frac{V}{2\pi^2} \int_0^{k_F} k^2 dk = \frac{V k_{F\pm}^3}{6\pi^2} \Rightarrow k_{F\pm} = \left(6\pi^2 n_\pm\right)^{1/3}$$

$$E_{K\pm} = V \int_{k_{F\pm}} \epsilon(k) \frac{d^3k}{(2\pi)^3} = V \int_0^{k_{F\pm}} \frac{k^2}{2m} 4\pi k^2 \frac{dk}{(2\pi)^3} = \frac{V}{2m} \frac{k_{F\pm}^5}{10\pi^2}$$

So for $T = 0$ the kinetic energy is

$$E_K = \frac{V}{2m} \frac{3}{5} \left(6\pi^2\right)^{2/3} \left(n_+^{5/3} + n_-^{5/3}\right)$$

For $n_+ = n_- = \frac{n}{2}$

$$E_0 = \frac{V}{2m} \frac{6}{5} \left(6\pi^2\right)^{2/3} \left(\frac{n}{2}\right)^{5/3}$$

Now we evaluate $n_+ = \frac{n}{2} + \delta, n_- = \frac{n}{2} - \delta$ so $M = n_+ - n_- = 2\delta$ and expand up to 4th order in M

$$n_\pm^{5/3} = \left(\frac{n}{2}\right)^{\frac{5}{3}} \left(1 \pm \frac{M}{n}\right)^{\frac{5}{3}} \approx \left(\frac{n}{2}\right)^{\frac{5}{3}} \left[1 \pm \frac{5}{3}\frac{M}{n} + \frac{5}{9}\left(\frac{M}{n}\right)^2 \mp \frac{5}{81}\left(\frac{M}{n}\right)^3 + \frac{5}{243}\left(\frac{M}{n}\right)^4\right]$$

so

$$\left(n_+^{5/3}+n_-^{5/3}\right)=2\left(\frac{n}{2}\right)^{\frac{5}{3}}\left[1+\frac{5}{9}\left(\frac{M}{n}\right)^2+\frac{5}{243}\left(\frac{M}{n}\right)^4\right]$$

$$E_K=E_0\left[1+\frac{5}{9}\left(\frac{M}{n}\right)^2+\frac{5}{243}\left(\frac{M}{n}\right)^4\right]$$

In the same way the interaction:

$$U=\alpha\frac{N_+N_-}{V}=\alpha Vn_+n_-=\alpha V\left(\frac{n}{2}+\frac{M}{2}\right)\left(\frac{n}{2}-\frac{M}{2}\right)=\alpha V\left(\frac{n}{2}\right)^2\left(1+\frac{M}{n}\right)\left(1-\frac{M}{n}\right)$$

$$=\alpha V\left(\frac{n}{2}\right)^2\left(1-\left(\frac{M}{n}\right)^2\right)$$

notice that $0\leq\left(\frac{M}{n}\right)^2\leq 1$,we are in the limit $\frac{M}{n}\ll 1$.
And we get

$$\frac{E_T}{V}=\frac{E_0}{V}+\alpha\left(\frac{n}{2}\right)^2+\left[\frac{5}{9}\frac{E_0}{V}-\alpha\left(\frac{n}{2}\right)^2\right]\left(\frac{M}{n}\right)^2+\frac{5}{243}\frac{E_0}{V}\left(\frac{M}{n}\right)^4$$

2. To find the critical value α_c, we can see that the coefficient of M^4 is always positive but on the other hand for different values of α the coefficient of M^2 can change its sign. The critical value α_c is defined when the coefficient equals zero

$$\alpha_c=\frac{5}{9}\frac{E_0}{V}\left(\frac{n}{2}\right)^{-2}=\frac{1}{2m}\frac{2}{3}\left(6\pi^2\right)^{2/3}\left(\frac{n}{2}\right)^{-\frac{1}{3}}$$

we can see that for:

$$n_+=n_-=\frac{n}{2}=\frac{k_F^3}{6\pi^2}=\frac{\left(2m\epsilon_F\right)^{\frac{3}{2}}}{6\pi^2}$$

$$\alpha_c=\frac{\left(2\pi\right)^2}{\left(2m\right)^{\frac{3}{2}}}\left(\epsilon_F\right)^{-\frac{1}{2}}=\frac{V}{g\left(\epsilon_F\right)}$$

3. To find the magnetization for minimum energy we need to derive the energy:

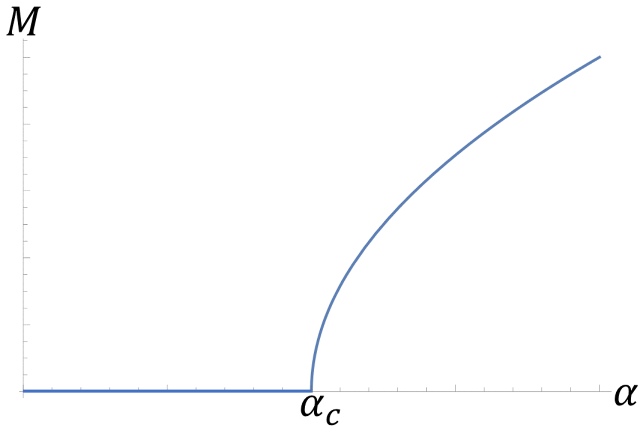
$$\frac{E_T}{V}=const+\frac{1}{4}\left[\alpha_c-\alpha\right]M^2+C_4M^4$$

$$\frac{\partial}{\partial M}\left(\frac{E_T}{V}\right)=\frac{1}{2}\left[\alpha_c-\alpha\right]M+4C_4M^3=0$$

we get

$$M=0\ \mathrm{OR} M=\pm\sqrt{\frac{1}{8C_4}\left[\alpha-\alpha_c\right]}$$

so we can see that when $\alpha<\alpha_c$ we have not spontaneous magnetization and when $\alpha>\alpha_c$ the spontaneous magnetization grow as a sours function



4.At finite but low temperatures T, The the energy $E(M)$ should be replaced by the M-constrained "free energy" $F(M)$, we can use the Sommerfeld expansion (equation 6.43 in the lecture notes):

$$F = \frac{3}{5}N\epsilon_F \left[1 - \frac{5\pi^2}{12}\left(\frac{T}{\epsilon_F}\right)^2 + O\left(\frac{T}{\epsilon_F}\right)^4\right]$$

we see that

$$k_{F\pm} = \left(6\pi^2 n_\pm\right)^{1/3} \to \epsilon_{F\pm} = \frac{\left(6\pi^2 n_\pm\right)^{\frac{2}{3}}}{2m}$$

$$F_\pm = \frac{3}{5}\frac{V}{2m}\left(6\pi^2\right)^{\frac{2}{3}}\left(n_\pm\right)^{\frac{5}{3}}\left[1 - \frac{5\pi^2}{12}\left(\frac{T}{\epsilon_F}\right)^2\right] = E_{K\pm} - 2mV\left(n_\pm\right)^{\frac{1}{3}}\frac{\pi^2}{4\left(6\pi^2\right)^{\frac{2}{3}}}T^2$$

$$n_\pm^{1/3} = \left(\frac{n}{2}\right)^{\frac{1}{3}}\left(1 \pm \frac{M}{n}\right)^{\frac{1}{3}} \approx \left(\frac{n}{2}\right)^{\frac{1}{3}}\left[1 \pm \frac{1}{3}\frac{M}{n} - \frac{1}{9}\left(\frac{M}{n}\right)^2 \pm \frac{5}{81}\left(\frac{M}{n}\right)^3 - \frac{40}{243}\left(\frac{M}{n}\right)^4\right]$$

$$\left(\left(n_+\right)^{\frac{1}{3}} + \left(n_-\right)^{\frac{1}{3}}\right) = 2\left(\frac{n}{2}\right)^{\frac{1}{3}}\left[1 - \frac{1}{9}\left(\frac{M}{n}\right)^2 - \frac{40}{243}\left(\frac{M}{n}\right)^4\right]$$

we need to add the interactions:

$$\to \frac{F}{V} = \frac{E_0}{V}\left[1 + \frac{5}{9}\left(\frac{M}{n}\right)^2 + \frac{5}{243}\left(\frac{M}{n}\right)^4\right] + \alpha\left(\frac{n}{2}\right)^2 - \alpha\left(\frac{n}{2}\right)^2\left(\frac{M}{n}\right)^2 - 2m\frac{\pi^2}{4\left(6\pi^2\right)^{\frac{2}{3}}}T^2 2\left(\frac{n}{2}\right)^{\frac{1}{3}}\left[1 - \frac{1}{9}\left(\frac{M}{n}\right)^2\right.$$

$$\to \frac{F}{V} = const + \left(\frac{n}{2}\right)^2\left[\alpha_c\left(0\right) - \alpha + \Delta\alpha T^2\right]\left(\frac{M}{n}\right)^2 + \left[\frac{5}{243}\frac{E_0}{V} + 2m\frac{\pi^2}{2\left(6\pi^2\right)^{\frac{2}{3}}}T^2\frac{40}{243}\left(\frac{n}{2}\right)^{\frac{1}{3}}\right]\left(\frac{M}{n}\right)^4$$

where

$$\Delta\alpha = 2m\frac{\pi^2}{18\left(6\pi^2\right)^{\frac{2}{3}}}\left(\frac{n}{2}\right)^{-\frac{5}{3}}$$

So we find

$$\alpha_c(T) = \alpha_c\left(0\right) + \Delta\alpha T^2$$

Statistical Mechanics - Class Exercise 7

Exercise 5651 - Ising spins with interaction that is mediated by atoms

Consider a one dimensional Ising model of spins $\sigma_i = \pm 1$ labeled $i = 1, 2, 3, ..., M$, with periodic boundary condition. Between each two spins there is a site $n_i = 0, 1$ that can be occupied by an atom. If the atom is present the fero-magnetic coupling is decreased from J to $(1-\lambda)J$.

1. Evaluate the partition sum assuming that there are N atoms in the M sites. Allow all configurations of spins and of atoms. Calculate the free energy F.

2. If the atoms are stationary impurities one needs to evaluate the free energy F for some random configuration of the atoms. What is the entropy difference between the results?

Answer

1. The partition function is:

$$Z = \sum_{\{n\}} \sum_{\{\sigma\}} e^{-\beta\left(-J\sum_{i=1}^{M}(1-\lambda n_i)\sigma_i\sigma_{i+1}\right)}$$

If we have open chain We can define

$$s_i = \sigma_i \sigma_{i+1} = \pm 1$$

So the partition function can be written as:

$$Z = \sum_{\sigma_1=\pm1} \sum_{\{n\}} \sum_{\{s\}} e^{\beta J \sum_{i=1}^{M-1}(1-\lambda n_i)s_i} = 2\sum_{\{n\}} \prod_{i=1}^{M-1} \sum_{\{s\}} e^{\beta J(1-\lambda n_i)s_i} = 2\sum_{\{n\}} \prod_{i=1}^{M-1} 2\cosh\left(\beta J\left(1-\lambda n_i\right)\right)$$

We know that we have N atoms in the M sites, so

$$Z = \frac{M!}{N!\,(M-N)!} 2^M \cosh^{M-1-N}\left(\beta J\right) \cosh^{N}\left(\beta J\left(1-\lambda\right)\right)$$

The free energy is therefore ($M-1 \approx M$):

$$F = -T\ln Z = -T\ln\left(M!\right) + T\ln\left(N!\right) + T\ln\left((M-N)!\right) - T\left(M-N\right)\ln\left(2\cosh\left(\beta J\right)\right) - TN\ln\left(2\cosh\left(\beta J\left(1-\right.\right.\right.$$

If we have closed chain we need to use Transfer matrices formalism:

$$T_{\sigma_i\sigma_{i+1}} = \begin{pmatrix} e^{\beta J(1-\lambda n_i)} & e^{-\beta J(1-\lambda n_i)} \\ e^{-\beta J(1-\lambda n_i)} & e^{\beta J(1-\lambda n_i)} \end{pmatrix}$$

where

$$e^{\beta J(1-\lambda n_i)\sigma_i\sigma_{i+1}} = \left\langle \sigma_i \left| T_{\sigma_i\sigma_{i+1}} \right| \sigma_{i+1} \right\rangle, \quad \sigma_i = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$Z = \sum_{\sigma_1=\pm1} \sum_{\sigma_2=\pm1} ... \sum_{\sigma_n=\pm1} \langle \sigma_1 | T_{\sigma_1\sigma_2} | \sigma_2 \rangle \langle \sigma_2 | T_{\sigma_2\sigma_3} | \sigma_3 \rangle ... \langle \sigma_M | T_{\sigma_M\sigma_1} | \sigma_1 \rangle =$$
$$= \sum_{\{\sigma\}} T_{\sigma_1\sigma_2} T_{\sigma_2\sigma_3} ... T_{\sigma_M\sigma_1} = \text{trace}\left(T_{\sigma_1\sigma_2} T_{\sigma_2\sigma_3} ... T_{\sigma_M\sigma_1} \right)$$

We have two kinds of matrices

$$T = \begin{pmatrix} e^{\beta J} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J} \end{pmatrix}, \; T^{'} = \begin{pmatrix} e^{\beta J(1-\lambda)} & e^{-\beta J(1-\lambda)} \\ e^{-\beta J(1-\lambda)} & e^{\beta J(1-\lambda)} \end{pmatrix}$$

But both matrices commute So the multiplication order does not matter:

$$\left[T, T^{'} \right] = 0$$

So

$$Z = \frac{M!}{N!\,(M-N)!} \text{trace}\left(T^{M-N} T^{'N} \right)$$
$$= \frac{M!}{N!\,(M-N)!} \text{trace}\left(\left(\begin{array}{cc} 2^{M-N}\cosh^{M-N}(\beta J) & 0 \\ 0 & 2^{M-N}\sinh^{M-N}(\beta J) \end{array} \right) \left(\begin{array}{cc} 2^{N}\cosh^{N}(\beta J(1-\lambda)) & \\ 0 & 2^{N}\sin \end{array} \right. \right.$$
$$= \frac{M!}{N!\,(M-N)!} 2^M \cosh^{M-N}(\beta J) \cosh^N(\beta J(1-\lambda)) \left(1 + \tanh^{M-N}(\beta J) \tanh^N(\beta J(1-\lambda)) \right)$$

For $M \to \infty$ because $-1 \le \tanh(x) \le 1$

$$Z = \frac{M!}{N!\,(M-N)!} 2^M \cosh^{M-N}(\beta J) \cosh^N(\beta J(1-\lambda))$$

2. For any configuration with exactly M impurities, the partition function is:

$$Z = 2^M \cosh^{M-N}(\beta J) \cosh^N(\beta J(1-\lambda))$$

As the number of impurities is fixed, the combinatorial factor is not needed.
The free energy for any configuration with M impurities is:

$$F = -T \ln Z = -T(M-N)\ln(2\cosh(\beta J)) - TN\ln(2\cosh(\beta J(1-\lambda)))$$

The average free energy for a given M is:

$$\langle F \rangle = \frac{\sum_{configurations} F}{\sum_{configurations}} = \frac{\frac{M!}{N!(M-N)!}\left(-T(M-N)\ln(2\cosh(\beta J)) - TN\ln(2\cosh(\beta J(1-\lambda))) \right)}{\frac{M!}{N!(M-N)!}}$$

$$\langle F \rangle = -T(M-N)\ln(2\cosh(\beta J)) - TN\ln(2\cosh(\beta J(1-\lambda)))$$

The entropy difference between the two calculations:

$$\triangle S = -\frac{\partial F}{\partial T} + \frac{\partial \langle F \rangle}{\partial T} = \ln\left(\frac{M!}{N!\,(M-N)!} \right)$$

Statistical Mechanics - Class Exercise 8

Exercise 5713 - Mean field approximation for a classical Heisenberg model

Apply the mean field approximation to the classical spin vector model

$$\mathcal{H} = -\epsilon \sum_{\langle i,j \rangle} \boldsymbol{s}_i \cdot \boldsymbol{s}_j - \boldsymbol{h} \cdot \sum_i \boldsymbol{s}_i$$

where $\boldsymbol{s}_i$ is a unit vector and $\langle i,j \rangle$ are neighboring sites on a lattice with coordination number c. The lattice has N sites and each site has c neighbors.

1. Assume that $\boldsymbol{h} = (0,0,h)$, define a mean field $\boldsymbol{h}_{eff}$, and evaluate the partition function Z in terms of $\boldsymbol{h}_{eff}$.
2. Define θ_i as the inclination angle of $\boldsymbol{s}_i$ with respect to $\boldsymbol{h}$. Assume that at equilibrium $\boldsymbol{s}_i = (0,0,M)$, where $M = \langle \cos\theta \rangle$. Find the equation for M, and find the transition temperature T_c.
3. Write an expression for the mean field energy of the system assuming that $M(T)$ is known.
4. Identify exponents γ and β that describe the susceptibility $\chi \sim (T - T_c)^{-\gamma}$ above T_c, and the magnetization $M \sim (T_c - T)^{\beta}$ below T_c.
5. Find the jump in the heat capacity C_V at T_c.

Answer

1. In the mean field approximation

$$\mathcal{H} = -\epsilon \sum_{\langle i,j \rangle} \boldsymbol{s}_i \cdot \langle \boldsymbol{s}_j \rangle - \boldsymbol{h} \cdot \sum_i \boldsymbol{s}_i = -\left(\epsilon c \langle \boldsymbol{s} \rangle + \boldsymbol{h}\right) \cdot \sum_i \boldsymbol{s}_i = -\boldsymbol{h}_{eff} \cdot \sum_i \boldsymbol{s}_i$$

so

$$\boldsymbol{h}_{eff} = \left(\epsilon c \langle \boldsymbol{s} \rangle + \boldsymbol{h}\right)$$

Because $\boldsymbol{h} = (0,0,h)$ we can assume $\langle \boldsymbol{s} \rangle = s\hat{z}$, so $\boldsymbol{h}_{eff} = h_{eff}\hat{z}$ and $\boldsymbol{h}_{eff} \cdot \boldsymbol{s}_i = h_{eff}\cos\theta_i$, and because the mean field approximation the problem became a sum over single spins, so the partition function

$$Z_1 = \frac{1}{4\pi}\int_0^{2\pi} d\varphi \int_{-1}^{1} d(\cos\theta)\, e^{\beta h_{eff}\cos\theta} = \frac{1}{2\beta h_{eff}}\left(e^{\beta h_{eff}} - e^{-\beta h_{eff}}\right) = \frac{\sinh(\beta h_{eff})}{\beta h_{eff}}$$

$$Z_N = Z_1^N = \left(\frac{\sinh(\beta h_{eff})}{\beta h_{eff}}\right)^N$$

2. For $M = \langle \cos\theta \rangle$

$$M = \langle \cos\theta \rangle = \frac{1}{Z_1}\frac{1}{4\pi}\int_0^{2\pi} d\varphi \int_{-1}^{1} d(\cos\theta)\cos\theta e^{\beta h_{eff}\cos\theta} = \frac{1}{\beta}\frac{1}{Z_1}\frac{\partial Z_1}{\partial h_{eff}} = \frac{1}{\beta}\frac{\partial \ln Z_1}{\partial h_{eff}}$$

$$= \frac{1}{\beta}\frac{\partial}{\partial h_{eff}}\left(\ln(\sinh(\beta h_{eff})) - \ln(\beta h_{eff})\right) = \left(\coth(\beta h_{eff}) - \frac{1}{\beta h_{eff}}\right)$$

$$M = \left(\coth\left(\beta\left(\epsilon c M + h\right)\right) - \frac{1}{\beta\left(\epsilon c M + h\right)} \right)$$

For $h \to 0, M \to 0$, and with $\coth(x) \approx \frac{1}{x} + \frac{x}{3} - \frac{x^3}{15}$

$$M \approx \left(\frac{1}{\beta\epsilon c M} + \frac{\beta\epsilon c M}{3} - \frac{1}{\beta\epsilon c M} \right) = \frac{\beta\epsilon c M}{3}$$

$$T_c = \frac{\epsilon c}{3}$$

3. For the mean field approximation in $h \to 0$

$$E = \langle \mathcal{H} \rangle = \left\langle -\epsilon \sum_{\langle i,j \rangle} \boldsymbol{s}_i \cdot \langle \boldsymbol{s}_j \rangle \right\rangle = -\epsilon \sum_{\langle i,j \rangle} \langle \boldsymbol{s}_i \rangle \langle \boldsymbol{s}_j \rangle = -\frac{1}{2}\epsilon c N M^2$$

4. We see

$$\begin{aligned} M &= \left(\coth\left(\beta\left(\epsilon c M + h\right)\right) - \frac{1}{\beta\left(\epsilon c M + h\right)} \right) \\ &\approx \left(\frac{1}{\beta\left(\epsilon c M + h\right)} + \frac{\beta\left(\epsilon c M + h\right)}{3} - \frac{\left(\beta\left(\epsilon c M + h\right)\right)^3}{15} - \frac{1}{\beta\left(\epsilon c M + h\right)} \right) = \left(\frac{\left(T_c M + \frac{h}{3}\right)}{T} - \frac{9\left(T_c M + \frac{h}{3}\right)^3}{5T^3} \right) \end{aligned}$$

Above T_c

$$M \approx \frac{\left(T_c M + \frac{h}{3}\right)}{T}$$

$$M = \frac{1}{3\left(T - T_c\right)} h = \chi h$$

So $\gamma = 1$
below T_c for $h \to 0$ and $T \approx T_c$

$$M = \frac{T_c M}{T} - \frac{9 T_c^3 M^3}{5 T^3}$$

$$\left(T - T_c\right) M = -\frac{9 T_c M^3}{5}$$

$$M = \frac{\sqrt{5}}{3} \left(\frac{T_c - T}{T_c} \right)^{\frac{1}{2}}$$

So $\beta = \frac{1}{2}$
5. We calculate the mean field energy in $h = 0$

$$E = -\frac{1}{2}\epsilon c N M^2$$

$$C_V = \frac{\partial E}{\partial T} = -\epsilon c N \frac{\partial M}{\partial T}$$

Above T_c

$$M = \chi h = 0$$

$$\to C_V = 0$$

below T_c

$$M = \frac{\sqrt{5}}{3}\left(\frac{T_c - T}{T_c}\right)^{\frac{1}{2}}$$

using that $T_c = \frac{\epsilon c}{3}$

$$\rightarrow C_V = -\frac{3}{2}NT_c\frac{\partial M^2}{\partial T} = \frac{5}{6}N$$

Exercise 5825 - Ising model 1D, domain walls

Consider the one dimensional Ising model with the Hamiltonian $\mathcal{H} = -\sum_{n,n'} J(n-n')\sigma(n)\sigma(n')$ with $\sigma(n) = \pm 1$ at each site n, and long range interaction $J(n) = b/n^\gamma$ with $b > 0$. Find the energy of a domain wall at $n = 0$, i.e. all the $n < 0$ spins are "down" and the others are "up". Show that the standard argument for the absence of spontaneous magnetization at finite temperatures fails if $\gamma < 2$.

Answer

In the case of short range interaction (nearest neighbors) the energy gain a domain wall is $2J$, and the domain wall can be in N different site, so the change in the free energy is

$$\Delta F = 2J - T\ln(N)$$

so for huge N this is negative for any finite temperature, making this transition favorable.
In our case all the spins are interact with each other, so the the energy gain is (for Nspins)

$$\Delta E = 2\sum_{n=0}^{\frac{N}{2}}\sum_{n'=-1}^{-\frac{N}{2}}\frac{b}{(n-n')^\gamma} = 2\sum_{n=0}^{\frac{N}{2}}\sum_{n'=1}^{\frac{N}{2}}\frac{b}{(n+n')^\gamma}$$

For $N \gg 1$ we can go to the continuum limit, define $x = n, y = n', dx = dy = 1$

$$\Delta E = 2b\int_0^{\frac{N}{2}} dx \int_1^{\frac{N}{2}} dy \frac{1}{(x+y)^\gamma}$$

For $\gamma > 2$

$$\begin{aligned}\Delta E =& 2b\int_0^{\frac{N}{2}} dx \frac{1}{(\gamma-1)}\left((x+1)^{-\gamma+1} - \left(x + \frac{N}{2}\right)^{-\gamma+1}\right)\\ =& 2b\frac{1}{(\gamma-1)(\gamma-2)}\left[1 - \left(\frac{N}{2}+1\right)^{-\gamma+2} - \left(\frac{N}{2}\right)^{-\gamma+2} + N^{-\gamma+2}\right]\end{aligned}$$

For $N \rightarrow \infty$

$$\Delta E = \frac{2b}{(\gamma-1)(\gamma-2)}$$

This is finite value so

$$\Delta F = \frac{2b}{(\gamma-1)(\gamma-2)} - T\ln(N)$$

is negative for any finite temperature.
But for $\gamma = 2$

$$\Delta E = 2b \int_0^{\frac{N}{2}} dx \int_1^{\frac{N}{2}} dy \frac{1}{(x+y)^2} = 2b \int_0^{\frac{N}{2}} dx \left[\frac{1}{(x+1)} - \frac{1}{(x+\frac{N}{2})} \right]$$
$$= 2b \left[\ln\left(\frac{N}{2}+1\right) - \ln(N) + \ln\left(\frac{N}{2}\right) \right]$$

$$\Delta E = 2b \ln\left(\frac{N+2}{4}\right) \approx 2b\ln(N) - 2b\ln(4)$$

So

$$\Delta F = 2b\ln(N) - T\ln(N)$$

so for $T = 2b$ the energy cost is large of the entropy gain.
For $1 < \gamma < 2$

$$\Delta E = 2b\frac{1}{(\gamma-1)(\gamma-2)} \left[1 - \left(\frac{N}{2}+1\right)^{-\gamma+2} - \left(\frac{N}{2}\right)^{-\gamma+2} + N^{-\gamma+2} \right] \approx [2-2^{\gamma}]\, b\frac{N^{2-\gamma}}{(\gamma-1)(\gamma-2)}$$

$$\Delta F = [2-2^{\gamma}]\, b\frac{N^{2-\gamma}}{(\gamma-1)(\gamma-2)} - T\ln(N)$$

So we never get domain wall

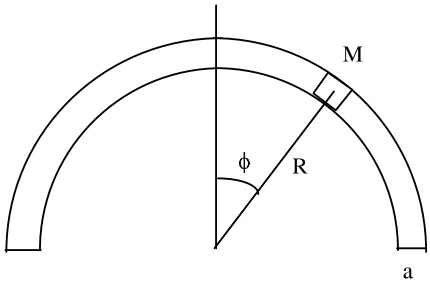
Statistical Mechanics - Class Exercise 9

Exercise 5811 - Mechanical model for symmetry breaking

An airtight piston of mass M is free to move inside a cylindrical tube of cross sectional area a. The tube is bent into a semicircular shape of radius R. On each side of the piston there is an ideal gas of N atoms at a temperature T. The angular position of the piston is φ (see figure). The gravitation field of Earth exerts a force Mg on the piston, while its effect on the gas particles can be neglected.
The partition function of the system can be written as $d\varphi$ integral over $\exp[-A(\varphi)]$. The variable φ is regarded as the "order parameter" of the system. A small difference ΔN in the occupation of the two sides is regarded as the conjugate field. The susceptibility is defined via the relation $\langle\varphi\rangle \approx \chi\Delta N$.

1. Write an explicit expression for $A(\varphi)$.
2. Find the coefficients in the expansion $A(\varphi) = (a/2)\varphi^2 + (u/4)\varphi^4 - h\varphi$.
3. Deduce what is the critical temperature T_c.
4. Using Gaussian approximation find what is χ for $T > T_c$.
5. Using Gaussian approximation find what is χ for $T < T_c$.
6. Sketch a plot of χ versus T indicating by dashed lines the Gaussian approximations and by solid line the expected exact result. Write what is the range ΔT around T_c where the Gaussian approximation fails.
7. What is the way to take the "thermodynamic limit" such as to have a phase transition at finite temperature?
8. In reality, as the temperature is lowered, droplets condense on the walls of the left (larger) chamber. What do you expect to find in the right chamber (gas? liquid? both?).

Guidelines: In items (4) and (5) simplify the result assuming $T \sim T_c$ and express it in terms of T_c and $T - T_c$. The final answer should include one term only. Care about numerical prefactors - their correctness indicates that the algebra is done properly. In item (7) you are requested to identify the parameter that should be taken to infinity in order to get a "phase transition". Please specify what are the other parameters that should be kept constant while taking this limit.



Answer

1. The partition function of the system can be written as integral over φ

$$Z = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} e^{-A(\varphi)}$$

For specific φ we have two gases and the piston

$$Z_{\varphi} = Z_L e^{-\beta MgR\cos(\varphi)} Z_R = e^{-A(\varphi)}$$

For the ideal gas in the two sides

$$Z_{L/R} = \frac{1}{N_{L/R}!}\left(\frac{aR\left(\frac{\pi}{2}\pm\varphi\right)}{\lambda_T^3}\right)^{N_{L/R}}$$

So we get

$$\begin{aligned} A(\varphi) = -\ln(Z_\varphi) &= \ln(N_L!) + \ln(N_R!) - N_L \ln\left(\frac{aR\left(\frac{\pi}{2}+\varphi\right)}{\lambda_T^3}\right) - N_R \ln\left(\frac{aR\left(\frac{\pi}{2}-\varphi\right)}{\lambda_T^3}\right) + \beta MgR\cos(\varphi) \\ &= \ln(N_L!) + \ln(N_R!) - (N_L + N_R)\ln\left(\frac{aR\frac{\pi}{2}}{\lambda_T^3}\right) - N_L \ln\left(1+\frac{2\varphi}{\pi}\right) - N_R \ln\left(1-\frac{2\varphi}{\pi}\right) + \beta MgR\cos(\varphi) \end{aligned}$$

2. We assume $\varphi \ll 1$ and a small difference ΔN in the occupation of the two sides

$$N_L = N + \frac{\Delta N}{2}, \quad N_R = N - \frac{\Delta N}{2}$$

So

$$A(\varphi) = \ln\left(\left(N+\frac{\Delta N}{2}\right)!\right) + \ln\left(\left(N-\frac{\Delta N}{2}\right)!\right) - 2N\ln\left(\frac{aR\frac{\pi}{2}}{\lambda_T^3}\right) - N\ln\left(1-\left(\frac{2\varphi}{\pi}\right)^2\right) - \frac{\Delta N}{2}\left[\ln\left(1+\frac{2\varphi}{\pi}\right)\right.$$

Now we use taylor expansion up to fourth order in φ, but for the part that multiple by ΔN ,that regarded as the external field, we take just first order

$$\begin{aligned} A(\varphi) \approx& const + N\left(\frac{2\varphi}{\pi}\right)^2 + \frac{N}{2}\left(\frac{2\varphi}{\pi}\right)^4 - \Delta N\frac{2\varphi}{\pi} + \frac{MgR}{T}\left(1-\frac{\varphi^2}{2}+\frac{\varphi^4}{24}\right) \\ =& const + \frac{1}{2}\left(\frac{8N}{\pi^2} - \frac{MgR}{T}\right)\varphi^2 + \frac{1}{4}\left(\frac{32N}{\pi^4} + \frac{MgR}{6T}\right)\varphi^4 - \frac{2\Delta N}{\pi}\varphi \end{aligned}$$

So

$$a = \left(\frac{8N}{\pi^2} - \frac{MgR}{T}\right), \quad u = \left(\frac{32N}{\pi^4} + \frac{MgR}{6T}\right), \quad h = \frac{2\Delta N}{\pi}$$

3. The T_c is the temperature when $a(T_c) = 0$,so

$$\frac{8N}{\pi^2} - \frac{MgR}{T_c} = 0$$

$$T_c = \frac{\pi^2 MgR}{8N}$$

$$a=\frac{8N}{\pi^2}\left(1-\frac{\pi^2 MgR}{8NT}\right)=\frac{8N}{\pi^2}\left(\frac{T-T_c}{T}\right)$$

4. We need to find the minimum of $A(\varphi)$

$$A'(\varphi)=a\varphi+u\varphi^3-h=0$$

For $T>T_c$ we get $a(T)>0$, so for $h=0$ we have one solution

$$a\varphi+u\varphi^3=0\to\bar{\varphi}=0$$

So close to the minima we can neglect the fourth order and get

$$a\varphi-h=0\to\bar{\varphi}=\frac{h}{a}$$

And

$$A(\bar{\varphi})\approx\frac{a}{2}\bar{\varphi}^2-h\bar{\varphi}=-\frac{h^2}{2a}$$

$$A(\varphi)\approx A(\bar{\varphi})+\frac{1}{2}A''(\bar{\varphi})(\varphi-\bar{\varphi})^2=-\frac{h^2}{2a}+\frac{1}{2}a(\varphi-\bar{\varphi})^2$$

So

$$Z=\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}e^{-A(\varphi)}\approx\int_{-\infty}^{\infty}e^{\frac{h^2}{2a}-\frac{1}{2}a(\varphi-\bar{\varphi})^2}=\sqrt{\frac{2\pi}{a}}e^{\frac{h^2}{2a}}$$

And

$$\langle\varphi\rangle=\frac{\partial\ln Z}{\partial h}=\frac{h}{a}=\frac{2}{a\pi}\Delta N$$

$$\chi=\frac{2}{a\pi}$$

For $T\approx T_c$

$$a=\frac{8N}{\pi^2}\left(\frac{T-T_c}{T}\right)\approx\frac{8}{\pi^2}N\left(\frac{T-T_c}{T_c}\right)$$

$$\chi=\frac{2}{a\pi}=\frac{\pi}{4N}\frac{T_c}{(T-T_c)}$$

5. For $T<T_c$ we get $a(T)<0$ and for $h=0$

$$a\varphi+u\varphi^3=0\to\bar{\varphi}=0,\pm\sqrt{\frac{|a|}{u}}$$

So for the two minima we get

$$A(\bar{\varphi}_\pm)=\frac{a}{2}\bar{\varphi}_\pm^2+\frac{u}{4}\bar{\varphi}_\pm^4-h\bar{\varphi}_\pm=-\frac{|a|^2}{2u}+\frac{|a|^2}{4u}\mp h\sqrt{\frac{|a|}{u}}=-\frac{|a|^2}{4u}\mp h\sqrt{\frac{|a|}{u}}$$

$$A''(\bar{\varphi}_\pm)=a+3u\bar{\varphi}_\pm^2=2|a|$$

$$A_\pm(\varphi)\approx A(\bar{\varphi}_\pm)+\frac{1}{2}A''(\bar{\varphi}_\pm)(\varphi-\bar{\varphi}_\pm)^2=-\frac{|a|^2}{4u}\mp h\sqrt{\frac{|a|}{u}}+|a|(\varphi-\bar{\varphi}_\pm)^2$$

We need to calculate around the two minima

$$Z = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} e^{-A(\varphi)} \approx \int_{-\infty}^{\infty} e^{\frac{|a|^2}{4u} + h\sqrt{\frac{|a|}{u}} - |a|(\varphi-\bar{\varphi})^2} + \int_{-\infty}^{\infty} e^{\frac{|a|^2}{4u} - h\sqrt{\frac{|a|}{u}} - |a|(\varphi-\bar{\varphi})^2}$$

$$= \sqrt{\frac{\pi}{|a|}} e^{\frac{|a|^2}{4u}} \left(e^{h\sqrt{\frac{|a|}{u}}} + e^{-h\sqrt{\frac{|a|}{u}}} \right) = \sqrt{\frac{\pi}{|a|}} e^{\frac{|a|^2}{4u}} 2\cosh\left(h\sqrt{\frac{|a|}{u}} \right)$$

$$\langle \varphi \rangle = \frac{\partial \ln Z}{\partial h} = \sqrt{\frac{|a|}{u}} \tanh\left(h\sqrt{\frac{|a|}{u}} \right) \approx \frac{|a|}{u} h = \frac{2}{\pi} \frac{|a|}{u} \Delta N$$

$$\chi = \frac{2}{\pi} \frac{|a|}{u}$$

For $T \approx T_c$

$$|a| = \frac{8}{\pi^2} N \left(\frac{T_c - T}{T_c} \right), \quad u = \left(\frac{32N}{\pi^4} + \frac{MgR}{6T} \right) = \frac{8N}{6\pi^2} \left(\frac{24}{\pi^2} + \frac{T_c}{T} \right) \approx \frac{4N}{3\pi^4} \left(24 + \pi^2 \right)$$

$$\chi = \frac{12\pi}{(24+\pi^2)} \left(\frac{T_c - T}{T_c} \right)$$

6. The condition for the Gaussian approximation is that the the quadratic term is dominant
For $T > T_c$we have $\bar{\varphi} = 0$ and the condition is

$$a\varphi^2 \gg u\varphi^4$$

$$\frac{a}{u} \gg \varphi^2$$

We can see that varφ = $\left\langle (\varphi - \bar{\varphi})^2 \right\rangle = \langle \varphi^2 \rangle$, and in the other hand in the Gaussian approximation var$\varphi = \sigma^2 = \frac{1}{a}$, so we get the condition

$$\frac{a}{u} \gg \frac{1}{a}$$

$$\frac{\left(\frac{8}{\pi^2} N \left(\frac{T - T_c}{T_c} \right) \right)^2}{\frac{4N}{3\pi^4} (24 + \pi^2)} \gg 1$$

$$\left(\frac{T - T_c}{T_c} \right) \gg \frac{1}{\sqrt{N}}$$

For $T < T_c$we have $\bar{\varphi} = \pm\sqrt{\frac{|a|}{u}}$ and the condition is

$$|a| (\varphi - \bar{\varphi})^2 \gg u (\varphi - \bar{\varphi})^4$$

$$\frac{|a|}{u} \gg (\varphi - \bar{\varphi})^2 = \text{var}\varphi$$

in This limit $\sigma^2 = \frac{1}{2|a|}$, so we get

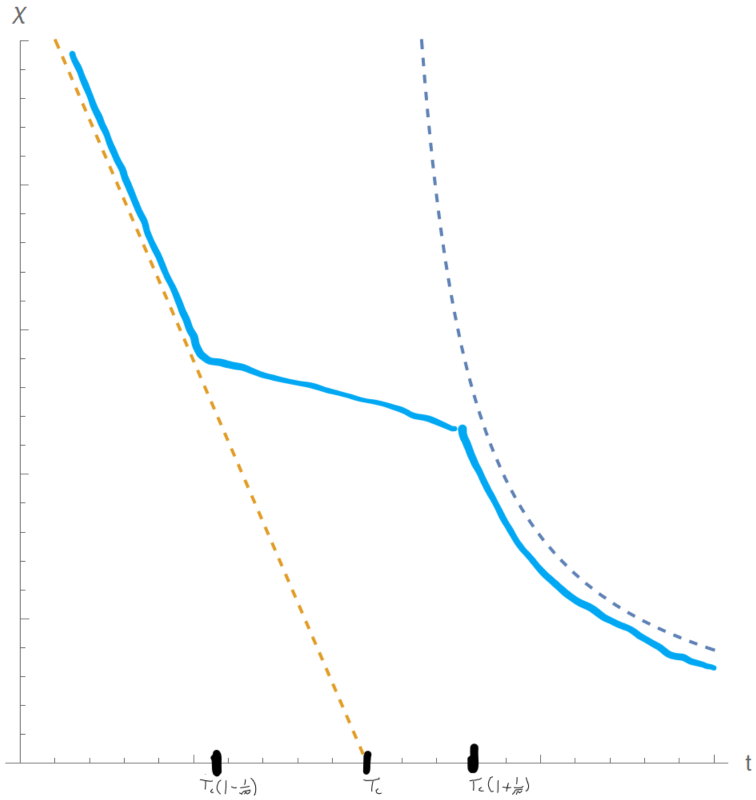
$$\frac{|a|}{u} \gg \frac{1}{2|a|}$$

$$\left(\frac{T_c - T}{T_c}\right) \gg \frac{1}{\sqrt{N}}$$

so we can conclude

$$\left|\frac{T - T_c}{T_c}\right| \gg \frac{1}{\sqrt{N}}$$

$$T \gg T_c\left(1 + \frac{1}{\sqrt{N}}\right) \text{ OR } T \ll T_c\left(1 - \frac{1}{\sqrt{N}}\right)$$



7. The "thermodynamic limit" is when $N \to \infty$, but the density $n = \frac{N}{a\pi R}$ stay constant. if we want to get a phase transition at finite temperature we need to keep $T_c = \frac{\pi^2 MgR}{8N}$ as a constant,so we need to keep $\frac{R}{N} = const$. in this condition we get a phase transition

$$\chi = \begin{cases} \frac{12\pi}{(24+\pi^2)}\left(\frac{T_c - T}{T_c}\right) & T < T_c \\ 0 & T > T_c \end{cases}$$

8. Assuming the system is in equilibrium we have $T_L = T_R$ and $P_R = P_L + \frac{Mg|sin(\varphi)|}{a}$. Remember that the state of coexistence of liquid and gas is a line $P(T)$, assuming the state of the side with the larger volume is on the line, since $P_R > P_L$ the state of the side with the smaller volume must be above the line thus contains liquid only.

Statistical Mechanics - Class Exercise 10

Exercise 7010 - Site occupation during a sweep process

Consider the occupation n of a site whose binding energy ϵ can be controlled, say by changing a gate voltage. The temperature of the environment is T and its chemical potential is μ. Consider separately 3 cases:
(a) The occupation n can be either 0 or 1.
(b) The occupation n can be any natural number $(0, 1, 2, 3, ...)$
(c) The occupation n can be any real positive number $\in [0, \infty]$
We define $\bar{n}$ as the average occupation at equilibrium. The fluctuations of $\delta n(t) = n(t) - \bar{n}$ are characterized by a correlation function $C(\tau)$. Assume that it has exponential relaxation with time constant τ_0. Later we define $\langle n \rangle$ as the average occupation during a sweep process, where the potential is varied with rate $\dot{\epsilon}$.

1. Calculate $\bar{n}$, express it using (T, ϵ, μ).
2. Calculate $\mathrm{Var}(n)$, express the result using $\bar{n}$.
3. Write an expression for the $\omega = 0$ intensity ν of the fluctuations.
4. Write an expression for $\langle n \rangle$ during a sweep process.

Irrespective of whether you have solved (1) and (2), in item (3) express the result using $\mathrm{Var}(n)$. In item (4) use the classical version of the fluctuation-dissipation relation, and express the result using $(T, \tau_0, \bar{n}, \dot{\epsilon})$, where $\bar{n}$ had been given by your answer to item (1). Note that the time dependence is implicit via $\bar{n}$.

Answer

1. The energy for n particles is $E_n = n\epsilon$.
The probability for n particles is $p_n = \frac{1}{Z} e^{-\beta(\epsilon-\mu)n}$
the average occupation

$$\bar{n} = \sum p_n n = \frac{1}{Z} \sum n e^{-\beta(\epsilon-\mu)n} = \frac{1}{Z\beta}\frac{\partial Z}{\partial \mu} = \frac{1}{\beta}\frac{\partial \ln(Z)}{\partial \mu}$$

(a) There are only two options $n = 0, 1$, then $Z = 1 + e^{-\beta(\epsilon-\mu)}$. And the average occupation:

$$\bar{n} = \frac{1}{\beta}\frac{\partial \ln(Z)}{\partial \mu} = \frac{e^{-\beta(\epsilon-\mu)}}{1 + e^{-\beta(\epsilon-\mu)}} = \frac{1}{e^{\beta(\epsilon-\mu)} + 1}$$

we get a Fermi-Dirac occupation.
(b) Now $n = 0, 1, 2....$ The partition function:

$$Z = \sum_{n=0}^{\infty} e^{-\beta(\epsilon-\mu)n} = \frac{1}{1 - e^{-\beta(\epsilon-\mu)}}$$

And the average occupation:

$$\bar{n} = \frac{1}{\beta}\frac{\partial \ln(Z)}{\partial \mu} = \frac{e^{-\beta(\epsilon-\mu)}}{1 - e^{-\beta(\epsilon-\mu)}} = \frac{1}{e^{\beta(\epsilon-\mu)} - 1}$$

we get a Bose–Einstein occupation.
(c) The partition function:

$$Z = \int_0^\infty e^{-\beta(\epsilon-\mu)n} dn = \frac{1}{\beta(\epsilon-\mu)}$$

And the average occupation:

$$\bar{n} = \frac{1}{\beta}\frac{\partial \ln(Z)}{\partial \mu} = \frac{1}{\beta(\epsilon-\mu)}$$

2. The variance is:

$$\mathrm{Var}(n) = \langle n^2\rangle - \langle n\rangle^2$$

$$\langle n^2\rangle = \sum p_n n^2 = \frac{1}{Z}\sum n^2 e^{-\beta(\epsilon-\mu)n} = \frac{1}{Z\beta^2}\frac{\partial^2 Z}{\partial\mu^2}$$

$$\langle n\rangle^2 = \bar{n}^2 = \frac{1}{Z^2\beta^2}\left(\frac{\partial Z}{\partial \mu}\right)^2$$

$$\mathrm{Var}(n) = \langle n^2\rangle - \langle n\rangle^2 = \frac{1}{\beta^2}\left[\frac{1}{Z}\frac{\partial^2 Z}{\partial\mu^2} - \frac{1}{Z^2}\left(\frac{\partial Z}{\partial\mu}\right)^2\right] = \frac{1}{\beta^2}\frac{\partial^2 \ln(Z)}{\partial\mu^2} = \frac{1}{\beta}\frac{\partial\bar{n}}{\partial\mu}$$

So we get
(a)

$$\mathrm{Var}(n) = \frac{1}{\beta}\frac{\partial\bar{n}}{\partial\mu} = \frac{e^{\beta(\epsilon-\mu)}}{\left(e^{\beta(\epsilon-\mu)}+1\right)^2} = \frac{e^{\beta(\epsilon-\mu)}+1-1}{\left(e^{\beta(\epsilon-\mu)}+1\right)^2} = \bar{n}\left(1-\bar{n}\right)$$

(b)

$$\mathrm{Var}(n) = \frac{1}{\beta}\frac{\partial\bar{n}}{\partial\mu} = \frac{e^{\beta(\epsilon-\mu)}}{\left(e^{\beta(\epsilon-\mu)}-1\right)^2} = \frac{e^{\beta(\epsilon-\mu)}-1+1}{\left(e^{\beta(\epsilon-\mu)}-1\right)^2} = \bar{n}\left(1+\bar{n}\right)$$

(c)

$$\mathrm{Var}(n) = \frac{1}{\beta}\frac{\partial\bar{n}}{\partial\mu} = \frac{1}{\beta^2(\epsilon-\mu)^2} = \bar{n}^2$$

3. The fluctuations of $\delta n(t) = n(t) - \bar{n}$ are characterized by a correlation function $C(\tau)$ assuming that it has exponential relaxation with time constant τ_0. Hence:

$$C(\tau) = \langle \delta n(\tau)\delta n(0)\rangle = Ae^{-\frac{|\tau|}{\tau_0}}$$

For $C(0) = \langle(\delta n(0))^2\rangle = \mathrm{Var}(n) = A$, so

$$C(\tau) = \mathrm{Var}(n)e^{-\frac{|\tau|}{\tau_0}}$$

The intensity

$$\nu = \tilde{C}(\omega=0) = \int_{-\infty}^{\infty} C(\tau)d\tau = \mathrm{Var}(n)\int_{-\infty}^{\infty} e^{-\frac{|\tau|}{\tau_0}}d\tau = 2\mathrm{Var}(n)\int_0^\infty e^{-\frac{\tau}{\tau_0}}d\tau = 2\mathrm{Var}(n)\tau_0$$

4. The conjugated variable to n is $-\epsilon$:

$$-\frac{\partial\mathcal{H}}{\partial n} = -\epsilon$$

From linear response we have:

$$\langle F\rangle_t = \langle F\rangle_X - \eta\dot{X}$$

where in our case the output signal $\langle F\rangle_t$ here is $\langle n\rangle_t$, and the input signal X is $-\epsilon$.
η is the imaginary part of the generalized susceptibility

$$\eta = \frac{\mathrm{Im}\left[\chi\left(\omega\right)\right]}{\omega} = \frac{1}{\hbar\omega}\tanh\left(\frac{\hbar\omega}{2T}\right)\tilde{C}\left(\omega\right)$$

In the classical version $\omega \to 0$ and we get the intensity of the fluctuations:

$$\eta = \frac{\nu}{2T} = \frac{\tau_0}{T}\mathrm{Var}(n)$$

$\langle n\rangle_t$ during a sweep process:

$$\langle n\rangle_t = \bar{n} + \dot{\epsilon}\eta = \bar{n} + \frac{\dot{\epsilon}\tau_0}{T}\mathrm{Var}(n)$$

Exercise 7040 - FDT for RL-circuit, Nyquist theory

Derive the Nyquist expression for the current-current correlation function in a closed ring, taking into account its inductance. Use the following procedure:

1. Cite an expression for the inductance L of a torus shaped ring given its radius R and its cross-section radius r.
2. Write the R-L circuit equation for the current I, where the flux $\Phi(t)$ through the ring is the driving parameter.
3. Identify the generalized susceptibility $\chi(\omega)$.
4. Calculate the current-current correlation function $\langle I(t)I(0)\rangle$, taking the classical / high temperature limit.
5. Verify that $\langle I^2\rangle$ agree with the canonical result.

Answer

1.

$$L = \mu_0 R\left[ln\left(\frac{8R}{r}\right) - 1.75\right]$$

(See https://en.wikipedia.org/wiki/Inductance)
2. For a closed ring with the flux $\Phi(t)$ through the ring, the electromotive force

$$\dot{\Phi} = RI - L\dot{I}$$

By taking Transform Fourier of the equation we get

$$i\omega\Phi_\omega = RI_\omega - i\omega LI_\omega$$

$$I_\omega = \frac{i\omega\Phi_\omega}{(R - i\omega L)}$$

3. From the last equation we get

$$I_\omega = \frac{i\omega}{(R - i\omega L)}\Phi_\omega$$

So, the generalized susceptibility

$$\chi(\omega) = \frac{i\omega}{(R - i\omega L)}$$

4. We get

$$\chi(\omega) = \frac{i\omega}{(R - i\omega L)} = -\frac{\omega^2 L}{(R^2 + \omega^2 L^2)} + i\frac{\omega R}{(R^2 + \omega^2 L^2)} = \mathrm{Re}\left[\chi(\omega)\right] + i\mathrm{Im}\ \left[\chi(\omega)\right]$$

from FDT we know that

$$\eta = \frac{\mathrm{Im}\left[\chi(\omega)\right]}{\omega} = \frac{1}{\hbar\omega}\tanh\left(\frac{\hbar\omega}{2T}\right)\tilde{C}^{II}(\omega)$$

taking the classical / high temperature limit we get

$$\frac{\mathrm{Im}\left[\chi(\omega)\right]}{\omega} = \frac{R}{(R^2 + \omega^2 L^2)} = \frac{1}{2T}\tilde{C}^{II}(\omega) \to \tilde{C}^{II}(\omega) = \frac{2TR}{(R^2 + \omega^2 L^2)}$$

The current-current correlation function in the classical limit $\langle I(t)I(0)\rangle = C^{II}(t)$ is the Transform Fourier of $\tilde{C}^{II}(\omega)$

$$C^{II}(t) = \int_{-\infty}^{\infty} e^{i\omega t}\tilde{C}^{II}(\omega)\frac{d\omega}{2\pi} = 2TR\int_{-\infty}^{\infty}\frac{e^{i\omega t}}{(R^2 + \omega^2 L^2)}\frac{d\omega}{2\pi} =$$
$$= \frac{2TR}{L^2}\int_{-\infty}^{\infty}\frac{e^{i\omega t}}{\left(\omega - i\frac{R}{L}\right)\left(\omega + i\frac{R}{L}\right)}\frac{d\omega}{2\pi} = \frac{T}{L}e^{-\frac{R}{L}t}$$

5. By taking $t \to 0$ we get

$$C^{II}(0) = \langle I(0)I(0)\rangle = \left\langle I^2\right\rangle = \frac{T}{L}$$

The Hamiltonian is $\mathcal{H} = \frac{1}{2}LI^2$ by using equal division rule for each quadratic term in the Hamiltonian we get the same result

$$\left\langle \frac{1}{2}LI^2\right\rangle = \frac{T}{2}$$

and therefore

$$\left\langle I^2\right\rangle = \frac{T}{L}$$

Statistical Mechanics - Class Exercise 11

Exercise 8481 - Mass on a spring

A balance for measuring weight consists of a sensitive spring which hangs from a fixed point. The spring constant is K. The balance is at temperature T and gravity acceleration is g in the x direction. A small mass m hangs at the end of the spring. There is an option to apply an external force $F(t)$, to which x is conjugate or apply an external vector potential $A(t)$.

1. Find the partition function Z.
2. Find $\langle x \rangle$ and $\langle x^2 \rangle$ and $\text{Var}(x)$.
3. Write a Langevin equation for $x(t)$, with friction η, and a random force $f(t)$.
4. Assuming $\langle f(t)f(0) \rangle = C\delta(t)$, find $\text{Var}(x)$, and deduce what is C by comparing with the canonical result.
5. Assuming x is measured in the lab by averaging over time period t_0, what is the minimal mass that can be meaningfully measured?
6. Describe the external force $F(t)$ by a scalar potential and demonstrate FDT.
7. Describe the external force $F(t)$ by a vector potential and demonstrate FDT.

Note: $\int \frac{d\omega}{(\omega^2-\omega_0^2)^2+\gamma^2\omega^2} = \frac{\pi}{\gamma\omega_0^2}$.

Answer

1. The Hamiltonian of the system is:

$$H = \frac{p^2}{2m} + \frac{1}{2}Kx^2 - mgx$$

We can rewrite the Hamiltonian in the following way

$$\begin{aligned} H =& \frac{p^2}{2m} + \frac{1}{2}K\left(x^2 - 2\frac{mg}{K}x + \left(\frac{mg}{K}\right)^2\right) - \frac{(mg)^2}{2K} \\ =& \frac{p^2}{2m} + \frac{1}{2}K(x-x_0)^2 - \frac{(mg)^2}{2K}, x_0 = \frac{mg}{K} \end{aligned}$$

So, the partition function

$$\frac{e^{\frac{\beta(mg)^2}{2K}}}{\lambda_T}\int_{-\infty}^{\infty} e^{-\beta\frac{K}{2}(x-x_0)^2}dx = \frac{e^{\frac{\beta(mg)^2}{2K}}}{\lambda_T}\sqrt{\frac{2\pi}{\beta K}}$$

2. The Gaussian in the partition function is centered around x_0, therefore we deduce that

$$\langle x \rangle = \frac{1}{Z_x}\int_{-\infty}^{\infty} xe^{-\beta\frac{K}{2}(x-x_0)^2}dx = \frac{1}{Z_x}\int_{-\infty}^{\infty}(x+x_0)\,e^{-\beta\frac{K}{2}x^2}dx = x_0$$

In order to find $\langle x^2 \rangle$ we use the equipartition and the Virial theorems

$$\langle x \cdot \frac{\partial U}{\partial x} \rangle = \langle p \cdot \frac{\partial \mathcal{K}}{\partial p} \rangle = \left\langle \frac{p^2}{m} \right\rangle = T$$

$$\langle xK(x - x_0) \rangle = T$$

$$\langle x^2 \rangle = \frac{T}{K} + x_0^2$$

And the variance of x is

$$\text{Var}(x) = \langle x^2 \rangle - \langle x \rangle^2 = \frac{T}{K}$$

3. The Langevin equation for this system is:

$$\dot{x} = \frac{\partial H}{\partial p}, \dot{p} = -\frac{\partial H}{\partial x}$$

$$m\ddot{x} + \eta\dot{x} + Kx - mg = f(t)$$

4. First we change the variable $x \to x - x_0$, that in equilibrium $\langle x \rangle = 0$,the Langevin equation became

$$m\ddot{x} + \eta\dot{x} + Kx = f(t)$$

After Fourier transform

$$(-m\omega^2 - i\eta\omega + K)x_\omega = f_\omega$$

Multiply by the conjugate the both sides and averege

$$\left(\left(K - m\omega^2\right)^2 + \eta^2\omega^2 \right) \left\langle |x_\omega|^2 \right\rangle = \left\langle |f_\omega|^2 \right\rangle$$

Using the Wiener-Khinchin theorem $\left\langle |f_\omega|^2 \right\rangle = \tilde{C}_{ff}(\omega) \times t$, we get

$$\tilde{C}_{xx}(\omega) = \frac{1}{m^2} \frac{\tilde{C}_{ff}(\omega)}{(\omega^2 - \frac{K}{m})^2 + (\gamma\omega)^2}, \gamma = \frac{\eta}{m}$$

The Fourier transform of $\delta(t)$ is 1, so the force-correlation is $\tilde{C}_{ff}(\omega) = C$. We get

$$\text{Var}(x) = C_{xx}(t = 0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{C}_{xx}(\omega) d\omega = \frac{1}{2\pi} \frac{C}{m^2} \int_{-\infty}^{\infty} \frac{d\omega}{(\omega^2 - \frac{K}{m})^2 + (\gamma\omega)^2} = \frac{C}{2\eta K}$$

when we use $\int \frac{d\omega}{(\omega^2 - \omega_0^2)^2 + \gamma^2\omega^2} = \frac{\pi}{\gamma\omega_0^2}$
so we get

$$\text{Var}(x) = \frac{C}{2\eta K} = \frac{T}{K}$$

$$C = 2\eta T = \nu$$

Finally we get

$$\tilde{C}_{xx}(\omega) = \frac{T}{m} \frac{2\gamma}{(\omega^2 - \frac{K}{m})^2 + (\gamma\omega)^2}$$

5. We measure $x(t)$ in the lab and average over time period t_0. This measurement introduces a new random variable X

$$X = \frac{1}{t_0} \int_0^{t_0} x(t) dt$$

This variable has a mean value $\langle X \rangle$ and variance $\mathrm{Var}(X)$. In order to get a meaningful measurement, it has to obey the condition - $\langle X \rangle \gg \sqrt{\mathrm{Var}(X)}$. From this condition, the minimal mass m_{min} will be found. The mean value of X is

$$\langle X \rangle = \frac{1}{t_0} \int_0^{t_0} \langle x(t) \rangle \, dt = x_0$$

The variance (after we change variables $x \to x - x_0$)

$$\mathrm{Var}(X) = \frac{1}{t_0^2} \int_0^{t_0} dt' \int_0^{t_0} dt'' \langle x(t') x(t'') \rangle = \frac{1}{t_0} \tilde{C}_{xx}(\omega = 0) = \frac{2\eta T}{t_0 K^2}$$

so, the minimal mass is given by

$$x_0 = \frac{mg}{K} \gg \sqrt{\frac{2\eta T}{t_0 K^2}}$$

$$m \gg \sqrt{\frac{2\eta T}{g^2 t_0}} = m_{\mathrm{min}}$$

6. The force $F(t)$ is described by a scalar potential U so the interaction term is $-\varepsilon(t) x$, so the conjugate variables are x and ε.
Averaging the Langevin formula

$$m \langle \ddot{x} \rangle + \eta \langle \dot{x} \rangle + K \langle x \rangle = \varepsilon$$

After Fourier transforming

$$x_\omega = \frac{1}{(-m\omega^2 + K) - i\omega\eta} \epsilon_\omega = \chi_\omega \varepsilon_\omega$$

Hence, we get the correlation function from FDT

$$\tilde{C}_{xx}(\omega) = \frac{2T}{\omega} \mathrm{Im} \chi_\omega = \frac{T}{m} \frac{2\gamma}{(\omega^2 - \frac{K}{m})^2 + (\gamma\omega)^2}$$

7. The force $F(t)$ is described by a vector potential $A(t)$, the interaction term is $v \cdot A$, so the conjugate variables are v and $-A$. The averaged Langevin formula becomes

$$m \langle \dot{v} \rangle + \eta \langle v \rangle + K \langle x \rangle = -\dot{A}$$

After Fourier transforming

$$v_\omega = \frac{1}{\frac{i}{\omega}(-m\omega^2 + K) + \eta} i\omega A_\omega$$

$$v_\omega = \frac{1}{m} \frac{\omega^2}{(-\omega^2 + \frac{K}{m}) - i\omega\gamma} A_\omega$$

We use that $F(t) = -\dot{A} \to F_\omega = i\omega A_\omega$
The correlation function is

$$v_\omega = \chi_\omega A_\omega$$

$$\tilde{C}_{vv}(\omega) = \frac{2T}{\omega}\text{Im}\chi_\omega = \frac{T}{m}\frac{2\gamma\omega^2}{(\omega^2 - \frac{K}{m})^2 + (\gamma\omega)^2} = \omega^2\tilde{C}_{xx}(\omega)$$

what we can get immediately from

$$\tilde{C}_{vv}(\omega) = \frac{1}{t}\left\langle |v_\omega|^2 \right\rangle = \frac{1}{t}\omega^2\left\langle |x_\omega|^2 \right\rangle = \omega^2\tilde{C}_{xx}(\omega)$$

Exercise 8483 - Millikan experiment

Consider a Millikan-type experiment whose purpose is to measure the charge e of a particle with mass m. The particle is located between plates of capacitor, where the electric field $\mathcal{E}$ is in the "up" direction, while the gravitation g is in the "down" direction. The distance between the plates is L, and the temperature of the system is T. Due to the poor vacuum the particle executes a Brownian motion that is described by a Langevin equation with friction force $-\eta v$. The charge of the electron is estimated via $\delta F = e\mathcal{E} - mg = 0$. In item (1) the system is prepared with a single particle in the middle. In item (3) assume a uniform gas of N particles. In both cases the current is integrated during a time interval t, and the charge $Q = \int I(t')dt'$ is inspected as "readout".

1. Assuming that $\delta F = 0$, determine the time t_d such that for $t \ll t_d$ it is not likely to get charge readout.
2. What is the δF for which the condition $t \ll t_d$ is no longer valid. We shall regard this value, call it δ_1, as the resolution of the measurement.
3. Assuming that $\delta F = 0$, determine the power spectrum $C(\omega)$ of the current $I(t)$.
4. Assume that the time of the measurement is t. What is the δF for which the condition $\langle Q \rangle \ll \sqrt{\text{var}(Q)}$ is no longer valid. We shall regard this value, call it δ_N, as the resolution of the measurement.
5. Express the ratio δ_N/δ_1 as a function of N and t/t_d.

Tips: In the absence of fluctuations $\delta F = 0$ is indicated by having zero readout. In item (3) the "readout" is a current versus voltage ("IV") measurement, and $\delta F = 0$ is indicated by zero current. Due to the fluctuations there is some blurring which determines the resolution δ_N. In order to calculate the fluctuations in item (3) define the one-particle current as the velocity (up to a prefactor).

Answer

1. The Langevin equation for the Brownian motion:

$$m\dot{v} + \eta v = f(t)$$

with $\langle f(t) \rangle = 0$ so for steady state $\langle v \rangle = 0$.

Solving this equation for the spreading of the particle yields $\left\langle (x(0)-x(t))^2\right\rangle = 2Dt$ where $D=\frac{T}{\eta}$. It follows, that it would be unlikely to get a charge readout for:

$$\frac{T}{\eta}\cdot t \ll L^2 \longrightarrow t_d = \frac{\eta L^2}{T}$$

2.When $e\mathcal{E}-mg\neq 0$ a "drift" term is to be added to the Langevin equation:

$$m\dot{v}+\eta v = f(t)+\delta F$$

So now the average velocity is $\langle v\rangle = \frac{\delta F}{\eta}$. In this case a minimum measurment time is $t=\frac{L}{\langle v\rangle}$. But we would also want this time to be shorter than the spreading time t_d we found in the previous item. This leads to the condition:

$$\frac{L}{\langle v\rangle} < t < \frac{\eta L^2}{T}$$

$$\delta F > \frac{T}{L} \equiv \delta_1$$

3. The current of a single particle is $I^1 = \frac{e}{L}v$. The power spectrum can be expressed as:

$$\left\langle |I^1_\omega|^2\right\rangle = \left(\frac{e}{L}\right)^2 \left\langle |v_\omega|^2\right\rangle$$

For Wiener-Khinchin theorem

$$C_{II}(\omega) = \left(\frac{e}{L}\right)^2 C_{vv}(\omega)$$

The Langevin equation:

$$(\eta - i\omega m)\, v_\omega = f_\omega$$

$$\left\langle |v_\omega|^2\right\rangle = \frac{1}{\eta^2+m^2\omega^2}\left\langle |f_\omega|^2\right\rangle$$

$$C_{vv}(\omega) = \frac{C_{ff}(\omega)}{\eta^2+m^2\omega^2}$$

when, for white noise $C_{ff}(\omega)=\nu=2\eta T$, so

$$C_{II}(\omega) = \left(\frac{e}{L}\right)^2 \frac{T}{m}\frac{2\gamma}{\gamma^2+\omega^2}, \gamma = \frac{\eta}{m}$$

The total current is a sum over single particle currents and so the power of the total current will be N times the power from a single particle:

$$C_{II}(\omega) = N\left(\frac{e}{L}\right)^2 \frac{T}{m}\frac{2\gamma}{\omega^2+\gamma^2}$$

4. The readout is the total charge $Q=\int_0^t I(t')dt'$. We can know that that the readout is not because the drift power only for $\sqrt{\mathrm{var}(Q)} \gg \langle Q\rangle$.

$$\langle Q\rangle = \langle I\rangle t = N\frac{e}{L}\langle v\rangle t = N\frac{e}{L}\frac{\delta F}{\eta}t$$

in the other side (that calculated assuming $\delta F = 0$):

$$\text{Var}(Q) = \langle Q^2 \rangle = \int_0^t \int_0^t dt'dt'' \langle I(t')I(t'') \rangle = C_{II}(\omega = 0)\, t = N \left(\frac{e}{L}\right)^2 \frac{2T}{\eta} t$$

The condition on δF is then:

$$\sqrt{N \left(\frac{e}{L}\right)^2 \frac{2T}{\eta} t} \gg N \frac{e}{L} \frac{\delta F}{\eta} t$$

and this break for

$$\delta F > \sqrt{\frac{T\eta}{Nt}} \equiv \delta_N$$

5. The ratio $\frac{\delta_N}{\delta_1}$ can be expressed as a function of N and t/t_d:

$$\frac{\delta_N}{\delta_1} = \frac{1}{\sqrt{N \frac{t}{t_d}}}$$

Exercise 8490 - Stochastic rate equation

Consider N classical particles in a two site system. The two sites are subjected to a potential difference ε. The temperature of the system is T. Define $n \in [-N, N]$ as the occupation difference. In items (3-6) assume that the thermalization process can be described by a stochastic rate equation

$$\frac{dn}{dt} = -\gamma n + A(t)$$

where $A(t)$ is a noisy term that reflects the fluctuations of the potential difference. Assuming that it has an average value A_0 and a power spectrum $\phi(\omega)$, it follows that n relaxes to an average value $\langle n \rangle$, with fluctuations that are characterized by a power spectrum $C(\omega)$.

1. Write what is the interaction energy H_{int} of n with the field ε. Later you will have to be careful with the identification of the conjugate variables.
2. Using the canonical formalism find what are $\langle n \rangle$ and $\text{Var}(n)$. Additionally provide approximations for small ε.
3. Determined what is A_0 such that $\langle n \rangle$ would be consistent with the canonical result. Assuming small ε deduce that $A_0 \propto \varepsilon$, and find the pre-factor.
4. What is the $\chi(\omega)$ that characterizes the response of n to the applied potential in the linear-response regime? Assume that the dynamics is described by the stochastic rate equation; care to identify correctly the conjugate variables; and take into account your answer to item (3).
5. Deduce from the fluctuation-dissipation relation what is the power spectrum $C(\omega)$. Care to use the appropriate definition for $\chi(\omega)$, else the result will come out wrong.

6. Deduce what is the power spectrum $\phi(\omega)$ that is required in order to reproduce $C(\omega)$ from the stochastic rate equation.

Advice: In item (5) verify that your result is consistent with the answer to item (2). Likewise you can debug the numerical pre-factor in your answer to item (6). Care about factors of "2" in your answers. Failure to provide strictly correct pre-factors will be regarded as an essential error.

Answer

1. We take the potential difference ε in That way, potential of $-\frac{\varepsilon}{2}$ in site 1and $\frac{\varepsilon}{2}$ in site 2

$$\mathcal{H}_{\text{int}} = -\frac{\varepsilon}{2}N_1 + \frac{\varepsilon}{2}N_2 = -\frac{\varepsilon}{2}n$$

2. The partition function is

$$Z_1 = e^{\beta\frac{\varepsilon}{2}} + e^{-\beta\frac{\varepsilon}{2}} = 2\cosh\left(\beta\frac{\varepsilon}{2}\right)$$

$$Z = (Z_1)^N = 2^N \cosh^N\left(\beta\frac{\varepsilon}{2}\right)$$

From this we get

$$\langle n\rangle = \frac{1}{\beta}\frac{\partial \ln(Z)}{\partial\frac{\varepsilon}{2}} = N\tanh\left(\beta\frac{\varepsilon}{2}\right)$$

We notice that in the limit $\varepsilon \to 0$ we have $\langle n\rangle \to 0$ and in the limit $\varepsilon \to \infty$ we have $\langle n\rangle \to N$, as expected.

$$\text{Var}(n) = \frac{1}{\beta^2}\frac{\partial^2 \ln(Z)}{\partial\frac{\varepsilon}{2}^2} = \frac{N}{\cosh^2\left(\beta\frac{\varepsilon}{2}\right)}$$

If we approximate for small ε we get

$$\langle n\rangle \approx \frac{N}{T}\frac{\varepsilon}{2}$$

$$\text{Var}(n) \approx N\left(1 - \left(\frac{1}{T}\frac{\varepsilon}{2}\right)^2\right)$$

3. The stochastic rate equation

$$\frac{dn}{dt} = -\gamma n + A(t)$$

after averaging we get in steady state

$$\langle n\rangle = \frac{A_0}{\gamma}$$

we require

$$\frac{A_0}{\gamma} = \frac{N}{T}\frac{\varepsilon}{2}$$

$$\to A_0 = \gamma\frac{N}{T}\frac{\varepsilon}{2}$$

4. By taking the Fourier transform of the averaging stochastic rate equation

$$n_\omega = \frac{A_{0\omega}}{(\gamma - i\omega)}$$

$$n_\omega = \frac{\gamma N\beta}{(\gamma - i\omega)} \frac{\varepsilon_\omega}{2}$$

$$\rightarrow \chi(\omega) = \frac{\gamma N\beta}{(\gamma - i\omega)}$$

5.

$$\chi(\omega) = \frac{\gamma N\beta}{(\gamma - i\omega)} = \frac{\gamma^2 N\beta}{(\gamma^2 + \omega^2)} + i\frac{\gamma N\beta\omega}{(\gamma^2 + \omega^2)}$$

From FDT we get

$$\text{Im}\chi(\omega) = \tanh\left(\frac{\omega}{2T}\right) C_{nn}(\omega)$$

in the classical limit $\omega \rightarrow 0$

$$\frac{\text{Im}\chi(\omega)}{\omega} = \frac{1}{2T} C_{nn}(\omega) = \frac{\gamma N\beta}{\gamma^2 + \omega^2}$$

$$C_{nn}(\omega) = N\frac{2\gamma}{\gamma^2 + \omega^2}$$

6.

$$\left\langle |n_\omega|^2 \right\rangle = \frac{\left\langle |A_\omega|^2 \right\rangle}{\gamma^2 + \omega^2}$$

$$C_{nn}(\omega) = \frac{\phi(\omega)}{\gamma^2 + \omega^2}$$

$$\phi(\omega) = N2\gamma$$

Exercise 8034 - Brownian particle on a ring

The motion of a classical Brownian particle on a 1D ring is described by the Langevin equation $m\ddot{\theta} + \eta\dot{\theta} = f(t)$, where $f(t)$ is due to a noisy electromotive force that has a correlation function $\langle f(t')f(t'')\rangle = C_f(t' - t'')$. The power spectrum $\tilde{C}_f(\omega)$ is defined as the Fourier transform of the correlation function. We consider two cases:

1. High temperature white noise $\tilde{C}_f(\omega) = \nu$.
2. Zero temperature noise $\tilde{C}_f(\omega) = c|\omega|$.

We define the angular velocity of the particle as $v = \dot{\theta}$, and its Cartesian coordinate as $x = \sin(\theta)$. In the absence of noise the dynamics is characterized by the damping time $t_c = m/\eta$.
In items (3)-(5) you should assume a spreading scenario: the particle is initially ($t = 0$) located at $\theta \sim 0$. The spreading during the transient period $0 < t < t_c$ is assumed to be negligible. In item (6) assume that the particle had been launched in the far past ($t = -\infty$): accordingly there is no preferred location on the ring.

1. Find the exact correlation function $\langle v(t)v(0)\rangle$ in case (a).
2. Find the correlation function $\langle v(t)v(0)\rangle$ for $t \gg t_c$ in case (b).
3. Find the spreading $S(t) \equiv \langle \theta(t)^2 \rangle$ for $t \gg t_c$ in case (a).
4. Find the spreading $S(t) \equiv \langle \theta(t)^2 \rangle$ for $t \gg t_c$ in case (b).
5. Express $\langle x(t)^2 \rangle$ for a spreading scenario given $S(t)$.
6. Express the correlation function $\langle x(t)x(0)\rangle$ given $S(t)$.
7. Write the explicit long time expression for $\langle x(t)x(0)\rangle$ in case (b), and deduce what is the critical value η_c above which a "phase transition" is expected in the response characteristics of the system.

Tips: For a Gaussian variable that has zero average $\langle \exp i\varphi \rangle = \exp[-(1/2)\langle \varphi^2 \rangle]$. The Fourier transform of $|\omega|$ has zero area, with negative tails $-1/(\pi t^2)$.
If you fail to solve (6), assume that the answer is the same as in (5), and proceed to (7).

Answer

1. We will start with writing the Langevin equation for the velocity $m\dot{v} + \eta v = f(t)$, we can solve it with Fourier transform:

$$(-i\omega m + \eta)v_\omega = f(\omega)$$

$$v_\omega = \frac{1}{m}\frac{f(\omega)}{\gamma - i\omega}, \gamma = \frac{\eta}{m}$$

Now we can take square absolute value from both sides and average :

$$\langle |v_\omega|^2 \rangle = \frac{1}{m^2}\frac{\langle |f(\omega)|^2 \rangle}{\gamma^2 + \omega^2}$$

From the Wiener-Khinchin theorem we get that $\langle |f(\omega)|^2 \rangle = \tilde{C}_f(\omega) \times t$, so we get:

$$\tilde{C}_v(\omega) = \frac{1}{m^2}\frac{\tilde{C}_f(\omega)}{\gamma^2 + \omega^2}$$

For case (a) $\tilde{C}_f(\omega) = \nu$ we get:

$$\tilde{C}_v(\omega) = \frac{1}{m^2}\frac{\nu}{\gamma^2 + \omega^2}$$

After inverse Fourier transform:

$$C_v(t) = \int \frac{d\omega'}{2\pi}\frac{1}{m^2}\frac{\nu}{\gamma^2 + \omega'^2}e^{-i\omega' t} = \frac{\nu}{2m^2\gamma}\int d\omega \frac{1}{\pi}\frac{\gamma}{\gamma^2 + \omega'^2}e^{-i\omega' t}$$

This is a Lorentzian, so we get:

$$C_v(t) = \langle v(t)v(0)\rangle = \frac{\nu}{2m^2\gamma}e^{-\gamma|t|} = \frac{\nu}{2m^2\gamma}e^{-\frac{|t|}{t_c}}$$

2. Now we use the same equation but in case (b) $\tilde{C}_f(\omega) = c|\omega|$:

$$\tilde{C}_v(\omega) = \frac{1}{m^2}\frac{\tilde{C}_f(\omega)}{\gamma^2+\omega^2} = \frac{1}{m^2}\frac{c|\omega|}{\gamma^2+\omega^2}$$

we need to do inverse Fourier transform:

$$C_v(t) = \frac{c}{m^2}\int \frac{d\omega'}{2\pi}\frac{|\omega'|}{\gamma^2+\omega'^2}e^{-i\omega' t}$$

We know that the change of $|\omega|$ is slow except near the $\omega = 0$, so the shape of $\omega \approx 0$ is determined by the higher t and the shape of $\omega \gg 0$ is determined by the lower t. We take the limit $t \gg t_c$ so we can neglect $\omega > \frac{1}{t_c}$ and get:

$$C_v(t) = \langle v(t)v(0)\rangle = \frac{c}{m^2}\int \frac{d\omega'}{2\pi}\frac{|\omega'|}{\gamma^2+\omega'^2}e^{-i\omega' t} = \frac{c}{\eta^2}\int \frac{d\omega'}{2\pi}\frac{|\omega'|}{1+t_c^2\omega'^2}e^{-i\omega' t} \approx \frac{c}{\eta^2}\int \frac{d\omega'}{2\pi}|\omega'|e^{-i\omega' t}$$

We know that the Fourier transform of $|\omega|$ has zero area, with negative tails $-\frac{1}{\pi t^2}$, so we get:

$$\begin{aligned}
\int \frac{d\omega'}{2\pi}|\omega'|e^{-i\omega' t} &= -\int_{-\infty}^{0}\frac{d\omega'}{2\pi}\omega' e^{-i\omega' t} + \int_{0}^{\infty}\frac{d\omega'}{2\pi}\omega' e^{-i\omega' t} \\
&= i\partial_t \lim_{\eta\to 0}\int_{-\infty}^{0}\frac{d\omega'}{2\pi}e^{-i\omega' t+\eta\omega'} + i\partial_t \lim_{\eta\to 0}\int_{0}^{\infty}\frac{d\omega'}{2\pi}e^{-i\omega' t-\eta\omega'} \\
&= -i\partial_t \lim_{\eta\to 0}\frac{1}{2\pi}\frac{1}{-it+\eta} - i\partial_t \lim_{\eta\to 0}\frac{1}{2\pi}\frac{1}{-it-\eta} = \frac{1}{\pi}\partial_t\frac{1}{t} = -\frac{1}{\pi t^2}
\end{aligned}$$

$$C_v(t) = \langle v(t)v(0)\rangle \approx \frac{c}{\eta^2}\int \frac{d\omega'}{2\pi}|\omega'|e^{-i\omega' t} = -\frac{c}{\eta^2\pi t^2}$$

3. In the beginning we define $\dot{\theta} = v$, so we get:

$$\theta(t) = \int_0^t dt' v(t')$$

$$\theta^2(t) = \int_0^t\int_0^t dt' dt'' v(t')v(t'')$$

$$\langle\theta^2(t)\rangle = \int_0^t\int_0^t dt' dt'' \langle v(t')v(t'')\rangle = \int_0^t\int_0^t dt' dt'' C_v(t'-t'')$$

We can see that t', t'' are independent variables, so we can choose that $t' > t''$ and double the result. We can do a change of variables to two dependent variables $T = t' \to 0 < T < t, \tau = t' - t'' \to 0 < \tau < T$.

$$\langle\theta^2(t)\rangle = 2\int_0^t dT\int_0^T d\tau C_v(\tau) = 2\int_0^t dT\int_0^T d\tau \frac{\nu}{2m\eta}e^{-\frac{|\tau|}{\left(\frac{m}{\eta}\right)}}$$

The correlation decay very fast so in the limit $t \gg t_c$ we can take the integral to infinite:

$$\langle\theta^2(t)\rangle = 2\int_0^t dT\int_0^\infty d\tau \frac{\nu}{2m\eta}e^{-\frac{|\tau|}{\left(\frac{m}{\eta}\right)}} = 2t\frac{\nu}{2m\eta}\left(\frac{m}{\eta}\right) = \frac{\nu}{\eta^2}t$$

Or, in the short way

$$\langle\theta^2(t)\rangle = \int_0^t\int_0^t dt'dt''\langle v(t')v(t'')\rangle = \int_0^t\int_0^t dt'dt''C_v(t'-t'') = \tilde{C}_v(\omega=0)\cdot t = \frac{\nu}{\eta^2}t$$

4. In the same way:

$$\langle\theta^2(t)\rangle = 2\int_0^t dT\int_0^T d\tau C_v(\tau)$$

We can neglect the spreading during the transient period $0 < t < t_c$, so we take the limit:

$$\langle\theta^2(t)\rangle = 2\int_{t_c}^t dT\int_0^T d\tau C_v(\tau)$$

The solution we found to $C_v(t)$ in case (b) is good just for $t \gg t_c$, so we need to divide the integral to two parts (we assume that the limit $T = t_c$ is the lower limit to our solution):

$$\langle\theta^2(t)\rangle = 2\int_{t_c}^t dT\left(\int_0^\infty d\tau C_v(\tau) - \int_T^\infty d\tau C_v(\tau)\right)$$

The part $\int_0^\infty d\tau C_v(\tau) = \tilde{C}_v(\omega=0) = 0$, so we get:

$$\langle\theta^2(t)\rangle = -2\int_{t_c}^t dT\int_T^\infty d\tau C_v(\tau) = 2\int_{t_c}^t dT\int_T^\infty d\tau\frac{c}{\eta^2\pi\tau^2} = 2\int_{t_c}^t dT\frac{c}{\eta^2\pi T} = \frac{2c}{\pi\eta^2}\ln\frac{|t|}{t_c}$$

5. We defined $x = \sin\theta$:

$$\langle x^2(t)\rangle = \langle\sin^2\theta(t)\rangle = \langle\frac{\left(e^{i\theta}-e^{-i\theta}\right)^2}{-4}\rangle = \frac{1}{4}\langle\left(2-e^{i2\theta}-e^{-i2\theta}\right)\rangle = \frac{1}{2}-\frac{1}{4}\langle e^{i2\theta}\rangle-\frac{1}{4}\langle e^{-i2\theta}\rangle$$

We get a tip that for a Gaussian variable that has zero average $\langle e^{i\varphi}\rangle = e^{-(1/2)\langle\varphi^2\rangle}$. Because θ is a Gaussian variable and it has zero average we get:

$$\langle x^2(t)\rangle = \frac{1}{2}-\frac{1}{4}\langle e^{i2\theta}\rangle-\frac{1}{4}\langle e^{-i2\theta}\rangle = \frac{1}{2}-\frac{1}{4}e^{-2\langle\theta^2\rangle}-\frac{1}{4}e^{-2\langle\theta^2\rangle} = \frac{1}{2}\left(1-e^{-2\langle\theta^2\rangle}\right) = \frac{1}{2}\left(1-e^{-2S(t)}\right)$$

Note that $\langle(2\theta)^2\rangle = \langle(-2\theta)^2\rangle = 4\langle\theta^2\rangle$

6. In the previous sections we assumed that $\theta(0) \approx 0$ and we talked about short times, so we could treat θ like a coordinate and calculate $\langle\theta(t)^2\rangle$. Now there isn't a preferred location on the ring so we can't calculate $S(t) = \langle\theta(t)^2\rangle$, because θ is not well defined. So we can't calculate $\langle x^2(t)\rangle$ like before, just the correlation between two different times $\langle x(t)x(0)\rangle$.
By definition:

$$\langle x(t)x(0)\rangle = \int_0^{2\pi}\int_0^{2\pi}\sin(\theta_t)\sin(\theta_0)\rho(\theta_t,\theta_0)d\theta_t d\theta_0$$

The formula for conditional probability is:

$$\rho(A|B) = \frac{\rho(A,B)}{\rho(B)} \to \rho(A,B) = \rho(A|B)\rho(B)$$

$$\langle x(t)x(0)\rangle = \int_0^{2\pi}\int_0^{2\pi} \sin(\theta_t)\sin(\theta_0)\rho(\theta_t|\theta_0)\rho(\theta_0)d\theta_t d\theta_0$$

We get that in $t=0$, θ_0 has a Uniform distribution, namely $\rho(\theta_0) = \frac{1}{2\pi}$.
Additionally $\rho(\theta_t|\theta_0)$ is the probability to find θ_t when we know where is θ_0, and this is like the previous section, when we assumed that $\theta_0 = 0$.
The probability $\rho(\theta_t|\theta_0)$ depends only on the difference between θ_t and θ_0, it doesn't depends on one of them, so let's define $\delta\theta = \theta_t - \theta_0$, when $\rho(\theta_t|\theta_0)d\theta_t = \rho(\delta\theta)d\delta\theta$
By using a trigonometric identities we get:

$$\int_0^{2\pi}\int_0^{2\pi} \sin(\theta_t)\sin(\theta_0)\rho(\theta_t|\theta_0)\rho(\theta_0)d\theta_t d\theta_0 = \frac{1}{4\pi}\int_0^{2\pi}\int_0^{2\pi}\left(\cos(\delta\theta) - \cos(2\theta_0+\delta\theta)\right)\rho(\delta\theta)d\delta\theta d\theta_0 =$$

$$= \frac{1}{4\pi}\int_0^{2\pi}\int_0^{2\pi}\cos(\delta\theta)\rho(\delta\theta)d\delta\theta d\theta_0 - \frac{1}{4\pi}\int_0^{2\pi}\int_0^{2\pi}\cos(2\theta_0+\delta\theta)\rho(\delta\theta)d\delta\theta d\theta_0 =$$

The first integral doesn't depend on θ_0, the integral on θ_0 in the second term give 0, and we get:

$$= \frac{1}{4\pi}\int_0^{2\pi}\int_0^{2\pi}\cos(\delta\theta)\rho(\delta\theta)d\delta\theta d\theta_0 = \frac{1}{2}\int_0^{2\pi}\cos(\delta\theta)\rho(\delta\theta)d\delta\theta = \frac{1}{2}\langle\cos(\delta\theta)\rangle$$

When we take $\theta_0 = 0$ we get that $\delta\theta$ is the same θ we define in the previous section and get:

$$\frac{1}{2}\langle\cos(\delta\theta)\rangle = \frac{1}{4}\langle e^{i\delta\theta} + e^{-i\delta\theta}\rangle = \frac{1}{4}\left(\langle e^{i\delta\theta}\rangle + \langle e^{-i\delta\theta}\rangle\right) = \frac{1}{2}e^{-\frac{1}{2}\langle\delta\theta^2\rangle} = \frac{1}{2}e^{-\frac{1}{2}S(t)}$$

7. For case (b):

$$S(t) = \frac{2c}{\pi\eta^2}\ln\frac{t}{t_c}$$

$$\langle x(t)x(0)\rangle = \frac{1}{2}e^{-\frac{1}{2}S(t)} = \frac{1}{2}\left(\frac{t}{t_c}\right)^{-\frac{c}{\pi\eta^2}}$$

From the FDT we get the relationship between the correlation function and the response:

$$\text{Im}\chi \sim \frac{\omega}{2T}\tilde{C}_{xx}(\omega)$$

In the DC limit, we get:

$$\text{Im}\chi = \frac{\omega}{2T}\tilde{C}_{xx}(\omega=0)$$

When:

$$\tilde{C}_{xx}(\omega=0) = \int_{-\infty}^{\infty} C_{xx}(t)dt = \int_{-\infty}^{\infty}\frac{1}{2}\left(\frac{t}{t_c}\right)^{-\frac{c}{\pi\eta^2}} dt$$

We define "phase transition" as When the response diverges. this will happen when $\frac{c}{\pi\eta^2} \le 1$, so we get:

$$\eta_c = \sqrt{\frac{c}{\pi}}$$