Solutions Trial Exam “Quantum matter” 2012

1 ^{3}He and ^{4}He Mixtures

1. (a) We have to calculate

$$\left\langle (\Delta N)^2 \right\rangle = \left\langle N^2 - 2N \langle N \rangle + \langle N \rangle^2 \right\rangle = \left\langle N^2 \right\rangle - \langle N \rangle^2 .$$

Now we calculate $\langle N^2 \rangle$ for a fermionic single oribital system with energy ϵ

$$\begin{aligned} \left\langle N^2 \right\rangle &\equiv \frac{1}{Z} \sum_{n=0}^{1} n^2 \exp(-\beta(\epsilon - \mu) n) = \\ &= \frac{1}{1 + \exp(-\beta(\epsilon - \mu))} (0 + \exp(-\beta(\epsilon - \mu))) = f_{FD}(\epsilon - \mu) = \langle N \rangle . \end{aligned} \tag{1}$$

Combining the above results gives the desired result,

$$\left\langle (\Delta N)^2 \right\rangle = \left\langle N^2 \right\rangle - \langle N \rangle^2 = \langle N \rangle (1 - \langle N \rangle).$$

The fluctuations go to 0 for $\langle N \rangle \to 0$ and $\langle N \rangle \to 1$, whereas they are maximal for $\langle N \rangle = \frac{1}{2}$. This can be understood as follows: In the limit $\langle N \rangle \to 1$ (i.e., with energies $\epsilon \ll \mu$), the positive fluctuations are small, since the occupancy may not exceed 1. For a negative fluctuation, the occupancy of the neighbouring states (in terms of energy) has to increase. Since these also have an occupancy close to 1, these fluctuations also have to be suppressed. Hence, since neither positive nor negative fluctuations can be large, the total fluctuation $\langle \Delta N \rangle$ is small. A similar reasoning holds *mutatis mutandis* for the states for which $\langle N \rangle \to 0$ ($\epsilon \gg \mu$), due to the symmetry of the distribution function. For $\langle N \rangle = \frac{1}{2}$ (or: $\epsilon = \mu$), there is a lot of “room” for changing the occupancy—remark that also at the neighbouring energies large fluctuations are possible. Hence, for energies around μ the fluctuations are the largest, with the maximum value $\langle (\Delta N)^2 \rangle = 1/4$ at $\epsilon = \mu$.

2. (a) We recall that we may compute $\langle N \rangle$ as

$$\langle N \rangle = \frac{1}{Z_{\rm gr}} \sum_i N_i \mathrm{e}^{-(\epsilon_i - \mu N_i)/\tau} = \frac{1}{Z_{\rm gr}} \sum_i \tau \frac{\partial}{\partial \mu} \mathrm{e}^{-(\epsilon_i - \mu N_i)/\tau} = \frac{\tau}{Z_{\rm gr}} \frac{\partial Z_{\rm gr}}{\partial \mu},$$

where $Z_{\rm gr} = \sum_i \mathrm{e}^{-(\epsilon_i - \mu N_i)/\tau}$ is the grand-canonical partition sum, where i labels the states. Similarly, we have

$$\langle N^2 \rangle = \frac{1}{Z_{\rm gr}} \sum_i N_i^2 \mathrm{e}^{-(\epsilon_i - \mu N_i)/\tau} = \frac{1}{Z_{\rm gr}} \sum_i \tau^2 \frac{\partial^2}{\partial \mu^2} \mathrm{e}^{-(\epsilon_i - \mu N_i)/\tau} = \frac{\tau^2}{Z_{\rm gr}} \frac{\partial^2 Z_{\rm gr}}{\partial \mu^2}.$$

For the mean-square deviation, we use $\langle(\delta N)^2\rangle = \langle N^2\rangle - \langle N\rangle^2$ to compute

$$\langle(\delta N)^2\rangle = \frac{\tau^2}{Z_{\rm gr}}\frac{\partial^2 Z_{\rm gr}}{\partial\mu^2} - \frac{\tau^2}{Z_{\rm gr}^2}\left(\frac{\partial Z_{\rm gr}}{\partial\mu}\right)^2.$$

On the other hand, we have

$$\frac{\partial\langle N\rangle}{\partial\mu} = \frac{\partial}{\partial\mu}\left(\frac{\tau}{Z_{\rm gr}}\frac{\partial Z_{\rm gr}}{\partial\mu}\right) = -\frac{\tau}{Z_{\rm gr}^2}\frac{\partial Z_{\rm gr}}{\partial\mu} + \frac{\tau}{Z_{\rm gr}}\frac{\partial^2 Z_{\rm gr}}{\partial\mu^2}.$$

Combining the two last equations, we find the result

$$\langle(\delta N)^2\rangle = \tau\frac{\partial\langle N\rangle}{\partial\mu}.$$

Now we take the single-orbital expression

$$\begin{aligned}\langle N\rangle &= \frac{\tau}{Z_{\rm gr}}\frac{\partial Z_{\rm gr}}{\partial\mu} = \frac{\tau}{Z_{\rm gr}}\frac{\partial}{\partial\mu}\frac{1}{1-{\rm e}^{-(\epsilon-\mu)/\tau}}\\ &= \frac{1}{Z_{\rm gr}}\frac{{\rm e}^{-(\epsilon-\mu)/\tau}}{\left(1-{\rm e}^{-(\epsilon-\mu)/\tau}\right)^2} = \frac{1}{{\rm e}^{(\epsilon-\mu)/\tau}-1},\end{aligned}$$

where the partition sum is

$$Z_{\rm gr} = \sum_{n=0}^{\infty}{\rm e}^{-n(\epsilon-\mu)/\tau} = \frac{1}{1-{\rm e}^{-(\epsilon-\mu)/\tau}}.$$

Substituting the expression for $\langle N\rangle$, we find

$$\langle(\delta N)^2\rangle = \tau\frac{\partial\langle N\rangle}{\partial\mu} = \tau\frac{\partial}{\partial\mu}\frac{1}{{\rm e}^{(\epsilon-\mu)/\tau}-1} = \frac{{\rm e}^{(\epsilon-\mu)/\tau}-1}{\left({\rm e}^{(\epsilon-\mu)/\tau}-1\right)^2}.$$

Writing the numerator as ${\rm e}^{(\epsilon-\mu)/\tau-1}-1+1$, we observe that this is equal to

$$\langle(\delta N)^2\rangle = \frac{1}{{\rm e}^{(\epsilon-\mu)/\tau}-1} + \frac{1}{\left({\rm e}^{(\epsilon-\mu)/\tau}-1\right)^2} = \langle N\rangle + \langle N\rangle^2,$$

which is the desired expression.

Alternative way:

Since the only quantity in $\langle N\rangle$ that depends on μ is the distribution function $f(\epsilon,\mu,\tau)$, we can take the derivative into the integral, as

$$\langle(\delta N)^2\rangle = \tau\frac{\partial}{\partial\mu}\int {\rm d}\epsilon\, D(\epsilon)f(\epsilon,\mu,\tau) = \tau\int {\rm d}\epsilon\, D(\epsilon)\frac{\partial f(\epsilon,\mu,\tau)}{\partial\mu}. \qquad (2)$$

The derivative of the boson distribution function $f(\epsilon,\mu,\tau) = \left(e^{(\epsilon-\mu)/\tau} - 1\right)^{-1}$ is computed as

$$\frac{\partial f(\epsilon,\mu,\tau)}{\partial\mu} = \frac{\partial}{\partial\mu}\frac{1}{e^{(\epsilon-\mu)/\tau} - 1} = \frac{1}{\tau}\frac{e^{(\epsilon-\mu)/\tau}}{\left(e^{(\epsilon-\mu)/\tau} - 1\right)^2}.$$

Writing the numerator in the last expression as $e^{(\epsilon-\mu)/\tau} - 1 + 1$, we find that

$$\frac{\partial f(\epsilon,\mu,\tau)}{\partial\mu} = \frac{1}{\tau}\left[f(\epsilon,\mu,\tau) + \left(f(\epsilon,\mu,\tau)\right)^2\right].$$

Plugging this result into (2), we obtain

$$\langle(\delta N)^2\rangle = \int d\epsilon\, D(\epsilon)\left[f(\epsilon,\mu,\tau) + \left(f(\epsilon,\mu,\tau)\right)^2\right].$$

Here, we note that in a single-orbital system, there is only one energy level ϵ_0, so that the density of states satisfies $D(\epsilon) = \delta(\epsilon - \epsilon_0)$. Then

$$\langle(\delta N)^2\rangle = f(\epsilon_0,\mu,\tau) + \left(f(\epsilon_0,\mu,\tau)\right)^2,$$

while on the other hand, $\langle N\rangle = f(\epsilon_0,\mu,\tau)$. Hence we find $\langle(\delta N)^2\rangle = \langle N\rangle + \langle N\rangle^2$, our conclusion. Note that with this density of states, this reasoning is essentially equivalent to the former solution.

2. (b) When the average number of particles in an orbital is high, we get enormous fluctuations in the number. This is stark contrast to the fermionic case of ^{3}He.

3. (a) One can describe a second order phase transition within the Landau free energy formalism:

$$f = \alpha x^2 + \beta x^4 + \gamma x^6,$$

where $\gamma > 0$ for both first and second order transitions. In the case of the second order phase transition, $\beta > 0$, while α changes the sign when the transition occurs.

The order parameter here is the superfluid density (it is zero in the normal phase and finite in the superfluid phase).

The fact that the transition is second order also means that the second derivative of the Gibbs free energy is discontinuous.

3. (b) For a first order phase transition, the first derivative of the Gibbs free energy is discontinuous. In the Landau free energy f, $\alpha > 0$ and $\beta < 0$ and a new minimum develops at x_0. However, at the phase transition point $f(x_0) = f(0)$. The point where the three phases coexist is called the tricritical point.

2 Infinite Range Ising Model

(a) **(0.5)** The solution is found by straightforward algebra

$$\begin{aligned}\sum_{\{\sigma_i\}} e^{\beta(J\mu+H)\sum_i \sigma_i} &= \sum_{\{\sigma_i\}} \prod_{i=1}^{N} e^{\beta(J\mu+H)\sigma_i} \\ &= \prod_{i=1}^{N} \sum_{\sigma_i=\pm 1} e^{\beta(J\mu+H)\sigma_i} \\ &= \prod_{i=1}^{N} \left(e^{\beta(J\mu+H)} + e^{-\beta(J\mu+H)}\right) \\ &= \prod_{i=1}^{N} \{2\cosh\left[\beta(J\mu+H)\right]\}.\end{aligned}$$

(b) **(0.5)** The double sum can be written as

$$\sum_{i,j} \sigma_i \sigma_j = \sum_i \sum_j \sigma_i \sigma_j = \sum_i \sigma_i \sum_j \sigma_j = \left(\sum_i \sigma_i\right)^2.$$

We can bring the partition function $Z(\beta, H, N)$ into the form

$$\begin{aligned}Z(\beta, H, N) &= \sum_{\{\sigma_i\}} \exp\left\{\frac{\beta J}{2N} \sum_{i,j} \sigma_i \sigma_j + \beta H \sum_i \sigma_i\right\} \\ &= \sum_{\{\sigma_i\}} \exp\left\{\frac{\beta J}{2N} \left(\sum_i \sigma_i\right)^2 + \beta H \sum_i \sigma_i\right\}.\end{aligned}$$

Now we insert the Gaussian identity,

$$e^{\frac{\beta J}{2N}\left(\sum_i \sigma_i\right)^2} = \int_{-\infty}^{\infty} \frac{d\mu}{\sqrt{\frac{2\pi}{N\beta J}}} \exp\left\{-\frac{N\beta J}{2}\mu^2 + \beta J \mu \sum_{i=1}^{N} \sigma_i\right\},$$

and obtain

$$
\begin{aligned}
Z(\beta, H, N) = \sum_{\{\sigma_i\}} \Bigg[\exp\left\{\beta H \sum_i \sigma_i\right\} \\
\times \int_{-\infty}^{\infty} \frac{d\mu}{\sqrt{\frac{2\pi}{N\beta J}}} \exp\left\{-\frac{N\beta J}{2}\mu^2 + \beta J\mu \sum_{i=1}^{N} \sigma_i\right\}\Bigg] \\
= \sum_{\{\sigma_i\}} \int_{-\infty}^{\infty} \frac{d\mu}{\sqrt{\frac{2\pi}{N\beta J}}} \exp\left\{-\frac{N\beta J}{2}\mu^2 + \beta(J\mu + H) \sum_{i=1}^{N} \sigma_i\right\}.
\end{aligned}
$$

Subsequently we use the result of (2) to obtain

$$
\begin{aligned}
Z(\beta, H, N) &= \sum_{\{\sigma_i\}} \int_{-\infty}^{\infty} \frac{d\mu}{\sqrt{\frac{2\pi}{N\beta J}}} \exp\left\{-\frac{N\beta J}{2}\mu^2 + \beta(J\mu + H) \sum_{i=1}^{N} \sigma_i\right\} \\
&= \int_{-\infty}^{\infty} \frac{d\mu}{\sqrt{\frac{2\pi}{N\beta J}}} \exp\left\{-\frac{N\beta J}{2}\mu^2 + N\log\left[2\cosh\left(\beta(J\mu + H)\right)\right]\right\}.
\end{aligned}
$$

(c) **(0.5)** The average magnetization $\langle m\rangle$ can be found be differentiating the partition function with respect to the magnetic field H, explicitly we have

$$
\begin{aligned}
\langle m\rangle &= \frac{1}{N\beta}\frac{\partial \log Z}{\partial H} = \frac{1}{N\beta}\frac{1}{Z}\frac{\partial Z(\beta, H, N)}{\partial H} \\
&= \frac{1}{N\beta}\frac{1}{Z}\frac{\partial}{\partial H}\left[\int_{-\infty}^{\infty} \frac{d\mu}{\sqrt{\frac{2\pi}{N\beta J}}} \exp\left\{-\frac{N\beta J}{2}\mu^2 + N\log\left[2\cosh\left(\beta(J\mu + H)\right)\right]\right\}\right].
\end{aligned}
$$

The derivative can be pulled through the integral. We need to calculate

$$
\frac{\partial}{\partial H} e^{N\log[2\cosh(\beta(J\mu+H))]} = N\frac{2\beta\sinh(\beta(J\mu + H))}{2\cosh(\beta(J\mu + H))}e^{\cdots} = N\beta\tanh(\beta(J\mu + H))e^{\cdots}.
$$

Now we put the above result into our expression for m and obtain the desired result

$$
\langle m\rangle = \langle \tanh(\beta(J\mu + H))\rangle,
$$

where

$$
\langle\ldots\rangle = \frac{1}{Z}\int_{-\infty}^{\infty} \frac{d\mu}{\sqrt{\frac{2\pi}{N\beta J}}} \ldots \exp\left\{-\frac{N\beta J}{2}\mu^2 + N\log\left[2\cosh\left(\beta(J\mu + H)\right)\right]\right\}.
$$

(d) **(0.5)** The magnetic susceptibility χ is given by

$$\begin{aligned}\chi &= \frac{1}{N}\frac{\partial\langle m\rangle}{\partial H}\\ &= \frac{1}{\beta N^2}\frac{\partial^2 \log Z}{\partial H^2}\\ &= \frac{1}{\beta N^2}\left[\frac{1}{Z}\frac{\partial^2 Z}{\partial H^2} - \left(\frac{1}{Z}\frac{\partial Z}{\partial H}\right)^2\right].\end{aligned}$$

In the following we write $x = \beta(J\mu + H)$. The second derivative of the partition function w.r.t. H yields

$$\begin{aligned}\frac{\partial^2 Z}{\partial H^2} &= \int_{-\infty}^{\infty} \frac{d\mu}{\sqrt{\frac{2\pi}{N\beta J}}} e^{-\frac{N\beta J}{2}\mu^2} \frac{\partial^2}{\partial H^2} e^{N\log[2\cosh x]}\\ &= \int_{-\infty}^{\infty} \frac{d\mu}{\sqrt{\frac{2\pi}{N\beta J}}} e^{-\frac{N\beta J}{2}\mu^2} N\beta \frac{\partial}{\partial H}\tanh(x) e^{N\log[2\cosh x]}\\ &= \int_{-\infty}^{\infty} \frac{d\mu e^{-\frac{N\beta J}{2}\mu^2}}{\sqrt{\frac{2\pi}{N\beta J}}} N\beta\Big(N\beta\tanh^2(x) + \beta - \beta\tanh^2(x)\Big) e^{N\log[2\cosh x]}.\end{aligned}$$

Putting this into the expression for the susceptibility we obtain

$$\chi = \beta\left(\langle\tanh^2(x) + \frac{1}{N}(1-\tanh^2(x))\rangle - \langle\tanh(x)\rangle^2\right).$$

In the limit that $N \to \infty$ we obtain the result

$$\chi = \beta\left(\langle\tanh^2(\beta(J\mu + H))\rangle - \langle\tanh(\beta(J\mu + H))\rangle^2\right).$$

(e) **(1.0)** The answer is not surprising since the fluctuation-dissipation theorem tells us that the fluctuations in the magnetization indicate the systems response to an external magnetic field. The fluctuations in the magnetic field are given by

$$\delta m^2 = \langle m^2\rangle - \langle m\rangle^2,$$

which is equal to χ/β.

(f) **(0.5)** The stationarity condition

$$\frac{\partial}{\partial\mu}\mathcal{F}(\mu, H) = 0,$$

can be found by differentiating $\mathcal{F}$, we obtain

$$\begin{aligned}\frac{\partial}{\partial\mu}\mathcal{F}(\mu,H) &= \frac{\partial}{\partial\mu}\frac{J}{2}\mu^2 - \frac{1}{\beta}\log\left[2\cosh(\beta(J\mu+H))\right] \\ &= J\mu - \frac{1}{\beta}\frac{2\beta J\sinh(\beta(J\mu+H))}{2\cosh(\beta(J\mu+H))} \\ &= J\mu - J\tanh(\beta(J\mu+H)).\end{aligned}$$

This gives the desired result.

(g) **(0.8)** The minimum of the Landau free energy shifts from zero to a nonzero value in a continuous way upon lowering the temperature. This implies that it is a second order phase transition.

(h) **(0.7)** We have the equation for the magnetization as a function of H given by

$$m(H) = \tanh(\beta(Jm(H)+H)).$$

Now we differentiate this equation w.r.t. H and obtain

$$\frac{\partial m(H)}{\partial H} = \left(1-\tanh^2(\beta(Jm(H)+H))\right)\beta\left(J\frac{\partial m(H)}{\partial H}+1\right).$$

By putting the field to zero, $H=0$, and rearanging terms we have

$$\left.\frac{\partial m(H)}{\partial H}\right|_{H=0} = \beta\frac{1-\tanh^2(\beta Jm)}{1-\beta J(1-\tanh^2(\beta Jm))}.$$

We arrive at the susceptibility at zero field by realizing $m=\tanh(\beta Jm)$, thus we have

$$\chi_0 = \frac{1}{\beta}\left.\frac{\partial m(H)}{\partial H}\right|_{H=0} = \frac{1-m^2}{1-\beta J(1-m^2)}.$$

(i) **(1.0)** One way to find the critical temperature is solve the equation

$$\left.\frac{\partial^2\mathcal{F}}{\partial\mu^2}\right|_{\mu=0} = 0$$

for temperature. One has

$$\beta_c = \cosh^2(\beta_c H)/J$$

which in the limit $H=0$ is just $k_B T_c = J$.

In a second-order phase transition the susceptibility diverges at the critical temperature so we could have expected this divergence. We see that the susceptibility diverges for $T = T_c = J/k_B$.

(j) **(0.5)** We have seen that this is a second order phase transition, in a second order phase transition the order parameter changes continuously from zero to a nonzero value at the critical temperature. In this figure the horizontal axis is T/T_c and the vertical axis is the magnetization per particle which is the order parameter for this system.

(k) **(0.5)** We again start with the equation

$$\mu = \tanh(\beta J \mu),$$

and expand it around $T = T_c$, which yields

$$m = \frac{mT_c}{T} - \frac{1}{3}\left(\frac{mT_c}{T}\right)^3,$$

thus we find $m^2 \propto (T_c - T)$. The critical exponent is found to be $\nu = 1/2$.