Solutions to Problem Set 9

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9.1 One Dimensional Paramagnet

(a) We have $\tau_1 = \sigma_1$, $\tau_2 = \sigma_1/\sigma_2$, $\tau_3 = \sigma_3/\tau_1\tau_2 = \sigma_3/\sigma_2$.

Induction: Assume $\tau_i = \sigma_i/\sigma_{i-1}$, for all $i > 1$. if this is true for all $i \leq n$, then we must have

$$\tau_{n+1} = \frac{\sigma_{n+1}}{\prod_{i=1}^{n} \tau_i} = \frac{\sigma_{n+1}}{\sigma_1 \prod_{i=2}^{n} \frac{\sigma_i}{\sigma_{i-1}}} = \frac{\sigma n + 1}{\sigma_n} \ .$$

QED.

(Since $\sigma_i = \pm 1$ we can also write: $\tau_i = \sigma_{i-1}\sigma_i$.

(b)

$$\begin{aligned}
Z &= \sum_{\tau_1 \ldots \tau_N} \exp\left[\frac{J}{2kT}(\sum_{i=1}^{N-1}(\tau_1\tau_2 \ldots \tau_i)(\tau_1 \ldots \tau_i + 1))\right] \\
&= \sum_{\tau_1 \ldots \tau_N} \exp\left[\frac{J}{2kT}(\sum_{i=1}^{N-1}(\tau_1\tau_2 \ldots \tau_i)^2 \tau_{i+1}\right] \\
&= \sum_{\tau_1 \ldots \tau_N} \exp\left[\frac{J}{2kT}\sum_{i=2}^{N}\tau_i\right] \\
&= 2\sum_{\tau_2 \ldots \tau_N} \exp\left[\frac{J}{2kT}\sum_{i=2}^{N}\tau_i\right]
\end{aligned}$$

This is twice that of a partition functino of $N - 1$ particles with $B' = J/2\mu_B$ and $J' = 0$.

$$\Rightarrow \boxed{Z = 2(e^{J/2kT} + e^{-J/2kT})^{N-1} = 2^N \cosh^{N-1}(J/2kT)}$$

(c) We have $\overline{\sigma_1\sigma_{i+p}} = \overline{\tau_{i+1} \ldots \tau_{i+p}}$ since $(\tau_i \ldots \tau_i)^2 = 1$.

This gives us

$$\begin{aligned}
\overline{\sigma_1\sigma_{i+p}} &= \frac{\sum_{\tau_1\ldots\tau_N}\tau_{i+1}\ldots\tau_{i+p}e^{\frac{J}{2kT}\sum_{j=2}^{N}\tau_j}}{\sum_{\tau_1\ldots\tau_N}e^{\frac{J}{2kT}\sum_{j=2}^{N}\tau_j}} \\
&= \frac{\sum_{\tau_{i+1}\ldots\tau_{i+p}}\prod_{j=i+1}^{i+p}\tau_j e^{J\tau_j/2kT}}{\sum_{\tau_{i+1}\ldots\tau_{i+p}}\prod_{j=i+1}^{i+p}e^{J\tau_j/2kT}} \\
&= \frac{(e^{J/2kT}-e^{-J/2kT})^p}{(e^{J/2kT}+e^{-J/2kT})^p} = \tanh^p(J/2kT)
\end{aligned}$$

This implies that

$$\ln\overline{\sigma_i\sigma_{i+p}} = p\ln(\tanh(J/2kT))$$

which gives an exponential dependence of the spin-spin correlation function on the distance p, where the correlation length is given by

$$\zeta = -(\ln[\tanh(J/2kT)])^{-1} = \frac{1}{\ln[\coth(J/2kT)]}$$

□

9.2 Bosons in a Harmonic Trap

Solutions posted next week This problem is very similar to the Bose gas in a container, with hamiltonian

$$\mathcal{H} = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 r^2 \tag{1}$$

(a) The energy of one particle in a single energy level n_x, n_y, n_z is given by

$$\epsilon_n = \frac{3}{2}\hbar\omega + (n_x + n_y + n_z)\hbar\omega = \frac{3}{2}\hbar\omega + n\hbar\omega$$

where $n = n_x + n_y + n_z$.

Let n_r = the # of bosons in the rth energy level. The grand canonical partition function is then

$$\begin{aligned}
\Xi &= \sum_{n_1,n_2,\ldots} e^{-\beta(n_1E_1+n_2E_2+\ldots)}e^{\beta\mu(n_1+n_2+\ldots)} \\
&= \left(\sum_{n_0=0}^{\infty} e^{-\beta(E_0-\mu)n_0}\right)\left(\sum_{n_1=0}^{\infty} e^{-\beta(E_1-\mu)n_1}\right)\left(\sum_{n_2=0}^{\infty} e^{-\beta(E_2-\mu)n_2}\right)\cdots \\
&= \boxed{\prod_{n_x,n_y,n_z=0}^{\infty}\left(\frac{1}{1-e^{-\beta(\epsilon_n-\mu)}}\right)} \qquad \text{by the geometric series}
\end{aligned}$$

(b) We know

$$\bar{N} = \frac{1}{\beta}\left(\frac{\partial}{\partial\mu}\ln\Xi\right)_\beta$$

From part (a) we have

$$\ln\Xi = -\sum_{\substack{n_x,n_y,\\ n_z=0}}^{\infty}\left(1-e^{-\beta(\epsilon_n-\mu)}\right)$$

Therefore

$$\bar{N} = \frac{1}{\beta}\sum_{\substack{n_x,n_y,\\ n_z=0}}^{\infty}\frac{\beta e^{-\beta(\epsilon_n-\mu)}}{1-e^{-\beta(\epsilon_n-\mu)}} = \boxed{\sum_{\substack{n_x,n_y,\\ n_z=0}}^{\infty}\frac{1}{e^{\beta(\epsilon_n-\mu)}-1}}$$

(c) The chemical potential $\mu(N,T)$ must be less than the ground state energy ϵ_0 for all T, otherwise the lowest state would have negative occupation number! At very low T, the chemical potential goes to ϵ_0. Thus the largest number any excited state can have is $1/(e^{(\epsilon_n-\epsilon_0)/kT}-1)$. As $T \to 0$ the number of particles in the excited states will fall below N, and there the remaining particles must occupy the ground state. The highest temperature at which the condensate exists is referred to as the Bose-Einstein tranisition temperature and we shall denote it by T_c.

(d) In order to find the critical temperature T_c we examine the number of particles in the excited state. To find an upper bound on the total number of bosons outside of the groundstate we want to consider

$$\bar{N}_{ex} = \bar{N} - \bar{N}_0 = \sum_{\substack{n_x,n_y,\\ n_z=0}}^{\infty} \frac{1}{e^{\beta(\epsilon_n - \mu)} - 1} - \frac{1}{e^{\beta(\epsilon_0-\mu)} - 1}.$$

it will be useful to rewrite this as

$$\bar{N}_{ex} = \sum_{n=1}^{\infty} \frac{g(n)}{e^{\beta(\epsilon_n-\mu)} - 1}$$

where the degeneracy in choosing $n = n_x + n_y + n_z$ is given by

$$g(n) = \binom{m+2}{2} = \frac{(m+2)(m+1)}{2}$$

since the number of ways of divvying up m parcels of energy into 3 dimensions is equivalent to choosing 2 "dividers" out of a list of $m+2$ possible energy units and dividers.

Now, we approximate the sum by an integral,

$$\begin{aligned}
\bar{N}_{ex} &= \frac{1}{2}\sum_{n=1}^{\infty} \frac{(n+2)(n+1)}{e^{\beta(\hbar\omega n + \frac{3}{2}\hbar\omega - \mu)} - 1} \approx \frac{1}{2}\int_{n=1}^{\infty} dn \frac{(n+2)(n+1)}{e^{\beta(\hbar\omega n + \frac{3}{2}\hbar\omega-\mu)} - 1} \\
&= \frac{1}{2}\frac{1}{\beta\hbar\omega}\int_{\beta\hbar\omega}^{\infty} dx \frac{1}{e^{x+y}-1}\left[\left(\frac{x}{\beta\hbar\omega}\right)^2 + 3\left(\frac{x}{\beta\hbar\omega}\right) + 2\right] \\
&= \frac{1}{2}\frac{1}{\beta\hbar\omega}\int_{\beta\hbar\omega}^{\infty} dx \frac{1}{e^{x+y}-1}\left[\left(\frac{x}{\beta\hbar\omega}\right)^2 + (3-2y)\left(\frac{x}{\beta\hbar\omega}\right) + (y-1)(y-2)\right]
\end{aligned}$$

where $x = \beta\hbar\omega m$, $y = \frac{3}{2}\hbar\omega - \mu$.

The integrals evaluate to

$$\begin{aligned}
\int_{\alpha}^{\infty} dx \frac{1}{e^x - 1} &= -\ln(1-e^{-\alpha}) = \ln(1/\alpha) + O(\alpha) \\
\int_{\alpha}^{\infty} dx \frac{x}{e^x - 1} &= \frac{\pi^2}{6} - O(\alpha) \\
\int_{\alpha}^{\infty} dx \frac{x}{e^x - 1} &= 2\zeta(3) - O(\alpha) \approx 2.4 - O(\alpha)
\end{aligned}$$

And so, if $\beta\hbar\omega \ll 1, y \ll 1$ (more on these assumptions later)

$$\bar{N}_{ex} = \frac{1}{(\beta\hbar\omega)^3}\left[\zeta(3) + O(\beta\hbar\omega + y)\right].$$

Bose Einstein condensation occurs when there is a macroscopic number of atoms in the ground state, that is, when

$$\bar{N}_{ex} < \bar{N}$$

or

$$kT_c = \frac{\hbar\omega}{(\zeta(3))^{1/3}} \bar{N}^{1/3}.$$

Are the parameters we assumed to be small actually small? We took $\beta\hbar\omega \ll 1$; we just found that at the critical temperature $\beta_c\hbar\omega \sim 1/\bar{N}^3$. That's very small. We also know that the number of particles in the ground state is given by $\bar{N}_0 = \frac{1}{e^y - 1}$ or $y = \ln(1 + \frac{1}{\bar{N}_0}) \approx \frac{1}{\bar{N}_0}$. This is a small number even if the condensate has 10 particles, but at this point it has a number on the order of $\bar{N}$, so it's even smaller.

(e) What happens in lower dimensions? The calculation is similar, except that $g(n)$ changes. In two dimensions this simply leads to $kT_c^{2D} = \frac{\hbar\omega}{\sqrt{3}\pi} \bar{N}^{1/2}$.

Things are more complicated in one dimension. Here, $g(n) = 1$ and the integral is

$$\bar{N}_{ex}^{1D} = \frac{1}{2} \frac{1}{\beta\hbar\omega} \int_{\beta\hbar\omega}^{\infty} dx \frac{1}{e^{x+y} - 1} \approx \frac{1}{2} \frac{\ln(1/\beta\hbar\omega)}{\beta\hbar\omega}$$

from which we find

$$kT_c^{1D} \approx 2\hbar\omega \frac{\bar{N}}{\ln \bar{N}}.$$

This is a condensation temperature, and we can calculate it for any finite system. But what happens as we increase the number of particles in the system? If we simply take $\bar{N} \to \infty$, the term $\bar{N}/\ln \bar{N}$ still increases. However, we should increase not just the particle number but all extrinsic sizes, like the volume. In particular, if we write the Hamiltonian as

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 = \frac{p^2}{2m} + \frac{1}{2} V \left(\frac{x}{L}\right)^2$$

we can rewrite

$$\begin{aligned} kT_c^{3D} &= \frac{\hbar\sqrt{V/m}}{(\zeta(3)^{1/3}} \left(\frac{\bar{N}}{L}\right)^{1/3}, \\ kT_c^{2D} &= \frac{\hbar\sqrt{V/m}}{\sqrt{3}\pi} \left(\frac{\bar{N}}{L}\right)^{1/2}, \\ kT_c^{1D} &= \frac{2\hbar\sqrt{V/m}}{\ln \bar{N}} \left(\frac{\bar{N}}{L}\right). \end{aligned}$$

In two or more dimensions, the critical temperature remains constant. In one dimension, the critical temperature drops logarithmically as we increase the size of the system, and in the thermodynamic limit, with $\bar{N} \to \infty, \bar{L} \to \infty, \bar{N}/\bar{L} = const.$, it goes to zero. So we say that a harmonic oscillator is only condensed at zero temperature in one dimension.

The calculation is very similar for an unconfined gas, except that the correct quantum numbers to use are the momenta, k, and the energies are given by $\epsilon \propto k^2$. We get

$$\bar{N}_{ex} = \int_{k_{\min}}^{k_{\max}} d^D k \frac{1}{e^{\beta\epsilon_k} - 1} \propto \int_{\epsilon_{\min}}^{\epsilon_{\max}} d\epsilon \frac{\epsilon^{\frac{D}{2}-1}}{e^{\beta\epsilon} - 1}.$$

Compare this to what we had above:

- In three dimensions we have ϵ in the numerator, and we will have regular condensation.
- In two dimensions we have 1 in the numerator, like we had for a one-dimensional trap above. This means we only have a BEC at zero temperature.
- In one dimension, things are even worse - we have $1/\epsilon$ in the numerator. This means there is no condensation in the thermodynamic limit!

□

9.3 Velocity Distribution of a Fermi Gas

(a) Clearly $\bar{v}_x = 0$ since each particle is as likely to be moving forward as backwards.

We do not have a velocity distribution but we have calculated the energy dependent density of states $g(E)$. From class and from Reif, we know for a Fermi gas $g(E) \propto E^{1/2}$. We also know

$$\bar{E} = \frac{1}{2}m(\overline{v_x^2} + \overline{v_y^2} + \overline{v_z^2}) = \frac{3}{2}m\overline{v_x^2}. \tag{2}$$

Thus we have $\overline{v_x^2} = 2\bar{E}/3m$.

Let $g(E) = CE^{1/2}$ where C is a constant to be determined by the normalization condition

$$1 = \int_0^\infty g(e)dE = \int_0^\mu CE^{1/2}dE = \frac{2}{3}C\mu^{3/2} \tag{3}$$

since only the levels up to energy μ are filled at $T = 0$. Hence $C = \frac{3}{2}\mu^{-3/2}$.

Now to calculate $\bar{E}$:

$$\begin{aligned} \bar{E} &= \int_0^{mu} g(E)EdE = \int_0^\mu \frac{3}{2}\mu^{-3/2}E^{3/2}dE \\ &= \frac{3}{2}mu^{-3/2}\left(\frac{2}{5}mu^{5/2}\right) = \frac{3}{5}\mu \ . \end{aligned}$$

Thus we have

$$\overline{v_x^2} = \frac{2\mu}{5m}. \tag{4}$$

(b) If the temperature were not zero, but still much smaller than the Germi temperature, $\overline{v_x^2}$ would increase. This can be understood with the following picture:

For T ¿ 0, electrons move from low energy states to higher energy states. The temperature dependence of this increase in *barE* can be estimated as follows

$$\Delta\bar{E} \approx [g(\mu)(kT)](kT) \propto T^2 \tag{5}$$

where the term in square brackets is approximately the number of energy levels that shift, which are shifted by the amount (kT).

The exact calculation is more difficult (see Reif p.396-397), which gives the result

$$\Delta \bar{E} = \frac{1}{N} \frac{\pi^2}{3} (kT)^2 \frac{Vm}{2\pi^2 \hbar^2} \left(3\pi^2 \frac{N}{V} \right)^{1/3}. \tag{6}$$

With $\Delta \overline{v_x^2} = \frac{2}{3m} \Delta \bar{E}$ the increase in $\overline{v_x^2}$.

□

9.4 Electron Gas

Reif §9.17: Consider an ideal gas of N electrons in a volume V at absolute zero.

(a) Calculate the total mean energy $\bar{E}$ of this gas.

(b) Express $\bar{E}$ in terms of the Fermi energy μ.

(c) Show that $\bar{E}$ is properly an extensive quantity, but that for a fixed volume V, $\bar{E}$ is not proportional to the number N of particles in the container. How do you account for this last result despite the fact that there is no interaction potential between the particles?

(a) We have

$$\bar{E} = \int_0^\mu \epsilon\rho(\epsilon)d\epsilon \qquad \text{where } \rho(\epsilon) = \left(\frac{2m}{\hbar^2}\right)^{3/2} \frac{V}{2\pi}\epsilon^{1/2}$$

where we've included the spin in the density of states. Carrying out hte integral we see

$$\bar{E} = \left(\frac{2m}{\hbar^2}\right)^{3/2} \frac{V}{2\pi^2} \int_0^\mu \epsilon^{3/2} d\epsilon = \left(\frac{2m}{\hbar^2}\right)^{3/2} \frac{V}{2\pi^2}\frac{2}{5}\mu^{5/2}$$

Giving us a chemical potential

$$\mu(T = 0) = \frac{\hbar^2}{2m}(3\pi^2 N/V)^{2/3} \tag{7}$$

and the average energy

$$\boxed{\bar{E} = \frac{\hbar^2}{2m}\frac{V}{5\pi^2}\left(3\pi^2 N/V\right)^{5/3}}$$

(b) Rewriting we see that

$$\bar{E} = \frac{3}{5}\mu N$$

which matches with our result from problem 10.3.

(c) If we start adding electrons to the box without changing the volume we are foricing the electrons to fill up the lowest energy states, without expanding the number of these energy states. Thus we expect that the energy should not scale proportionally with number, if the volume isn't also scaled. Indeed we see that if we scale both volume and number by α we get

$$\bar{E}(\alpha N, \alpha V) = \frac{\hbar^2}{2m}\frac{\alpha V}{5\pi^2}\left(3\pi^2 \alpha N/\alpha V\right)^{5/3} = \alpha\bar{E} \tag{8}$$

$$\bar{E}(\alpha N, V) = \frac{\hbar^2}{2m}\frac{V}{5\pi^2}\left(3\pi^2 \alpha N/V\right)^{5/3} = \bar{E}\alpha^{5/3} \tag{9}$$

which clearly is not linear.

□

9.5 Two Particles

(a) Distinguishable Particles Possible states:

ϵ_1	ϵ_2
0	0
ϵ	ϵ
3ϵ	3ϵ
0	ϵ
ϵ	0
0	3ϵ
3ϵ	0
ϵ	3ϵ
3ϵ	ϵ

$$Z = e^0 + e^{-2\beta\epsilon} + e^{-6\beta\epsilon} + 2e^{-\beta\epsilon} + 2e^{-3\beta\epsilon} + 2e^{-4\beta\epsilon}$$

(b) Fermions are indistinguishable and do not want to be in the same energy level. Possible states:

ϵ_1	ϵ_2
0	ϵ
0	3ϵ
ϵ	3ϵ

$$Z = e^{-\beta\epsilon} + e^{-3\beta\epsilon} + e^{-4\beta\epsilon}$$

(c) Bosons are indistinguishable but can be in the same energy level. Possible states:

ϵ_1	ϵ_2
0	0
0	ϵ
0	3ϵ
ϵ	3ϵ
3ϵ	3ϵ

$$Z = e^0 + e^{-\beta\epsilon} + e^{-2\beta\epsilon} + e^{-3\beta\epsilon} + e^{-4\beta\epsilon} + e^{-6\beta\epsilon}$$