Notes for Lecture 14

Quantum ideal gas (cont.)

Here we continue our exploration of the quantum ideal gas. We will study the quantum regime, where fermions and bosons show their truly peculiar and fascinating behaviors.

14.1 Fermi gas

Although this model sounds very naive, it is actually one of the most important models for the theory of electrons in metals and certain quantum liquids such as ^{3}He. Especially, the importance of this model is that the so-called Landau Fermi liquid is defined as a quantum liquid whose elementary particles can be mapped to free fermions in a Fermi gas.

14.1.1 Sommerfeld expansion

Let us start by stating this important expansion

$$\begin{aligned}\int_{-\infty}^{\infty} H(\varepsilon) f(\varepsilon) d\varepsilon \;&=\; \int_{-\infty}^{\mu} H(\varepsilon) d\varepsilon + \frac{\pi^2}{6} H'(\mu)(k_B T)^2 \\ &+\; \frac{7\pi^2}{360} H'''(\mu)(k_B T)^4 + O\left(\frac{T}{T_F}\right)^6 \end{aligned} \tag{14.1}$$

where $f(\varepsilon)$ is the Fermi-Dirac function[1] and $H(\varepsilon)$ is a function such that its integral ($K(\varepsilon) \equiv \int_{-\infty}^{\varepsilon} dy H(y)$) satisfies the properties that $K(-\infty) = 0$ and $K(\varepsilon)e^{-\beta\varepsilon} \to 0$ as $\varepsilon \to \infty$.

The assumption of this expansion is that

$$\frac{T}{T_F} \ll 1 \tag{14.2}$$

where T_F is the so-called *Fermi temperature*, which we will identify shortly. At this point, it suffices to know that this expansion is valid in the quantum degenerate regime, low T or high n.

The reason that the Sommerfeld expansion works is because $-f'(\varepsilon)$ is a sharply peaked function[2] at $\varepsilon = \mu$ with a unit area (if $T \ll T_F$) and it converges to a Dirac delta function, $\delta(\varepsilon - \mu(T = 0))$, in the limit of T/T_F going to zero. Note that $\mu(T = 0) \equiv \varepsilon_F \equiv k_B T_F$, where ε_F is the so-called *Fermi energy*.

The reason that the perturbation parameter is T/T_F will become clearer as we go along. However, even now, one can note the following. In the order of magnitude, $H'(\mu) \sim H(\mu)/\mu$ and so the order of the magnitude for the second term is $H\mu(k_B T/\mu)^2$. Similarly the fourth order term is of order $H\mu(k_B T/\mu)^4$. So, it is clear that the perturbation parameter is $k_B T/\mu \approx T/T_F$, if $\mu \approx \varepsilon_F = k_B T_F$. We will see shortly that indeed the chemical potential μ is equal to its zero temperature value $k_B T_F$ with a small 2nd order correction.

Once we identify the nature of $-f'(\varepsilon)$, the Sommerfeld expansion follows rather easily.

$$\int_{-\infty}^{\infty} H(\varepsilon) f(\varepsilon) d\varepsilon = K(\varepsilon) f(\varepsilon)|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} K(\varepsilon) f'(\varepsilon) d\varepsilon \tag{14.3}$$

$$= -\int_{-\infty}^{\infty} K(\varepsilon) f'(\varepsilon) d\varepsilon \tag{14.4}$$

due to the assumptions made on $K(\varepsilon)$. Since $-f'(\varepsilon)$ is peaked around $x \equiv \varepsilon - \mu = 0$, we can expand $K(\varepsilon)$ as a power series of x. Noting that $-f'(\varepsilon)$ is an even function

[1] Note that here, we expand the range of ε to $-\infty$, even if the physical spectrum is bounded from below, like $\varepsilon \geq 0$. The reason is the mathematical convenience. Since $f'(\varepsilon)$ is exponentially small at the minimum value of the physical energy spectrum if $T \ll T_F$, it introduces practically no error if we extend $f(\varepsilon)$ to $\varepsilon \to -\infty$.

[2] Its FWHM is about $4k_B T$.

of x, we see that odd power terms vanish when integrated with $-f'(\varepsilon)$. So, we get

$$\begin{aligned}\int_{-\infty}^{\infty} H(\varepsilon)f(\varepsilon)d\varepsilon &\approx -\int_{-\infty}^{\infty} d\varepsilon K(\mu)f'(\varepsilon) - \int_{-\infty}^{\infty} d\varepsilon \frac{K''(\mu)}{2}(\varepsilon-\mu)^2 f'(\varepsilon) \\ &= K(\mu) + 2H'(\mu)(k_BT)^2 \int_0^{\infty} dy \frac{y}{e^y+1} \end{aligned} \tag{14.5}$$

where in the last step, three things are done concurrently: the variable substitution $y \equiv \beta(\varepsilon-\mu)$, noting the symmetry of the integral and halving the integral range with the introduction of an overall factor of 2, and the integration by parts. The integral is $\pi^2/12$ and thus the Sommerfeld expansion, Eq. 14.1, is proven to the $(T/T_F)^2$ order. This expansion can be carried out more systematically and coefficients for all orders can, in fact, be written down in a closed form, but in practice we hardly need more than what we just derived. The fourth order term is written above in Eq. 14.1, really just for information.

14.1.2 Chemical potential

We use Eq. 13.32 to figure out the chemical potential. We have, after extending the density of states to $\varepsilon = (-\infty, \infty)$ by defining $D(\varepsilon) = 0$ for $\varepsilon < 0$ or the minimum of the physical energy spectrum,

$$N = \int_{-\infty}^{\infty} d\varepsilon D(\varepsilon) f(\varepsilon) \tag{14.6}$$

$$\approx \int_{-\infty}^{\mu} d\varepsilon D(\varepsilon) + \frac{\pi^2}{6} D'(\mu)(k_BT)^2 \qquad \text{Eq. 14.1} \tag{14.7}$$

$$= N + \int_{\varepsilon_F}^{\mu} d\varepsilon D(\varepsilon) + \frac{\pi^2}{6} D'(\mu)(k_BT)^2 \qquad \text{using } \int_{-\infty}^{\varepsilon_F} d\varepsilon D(\varepsilon) = N \tag{14.8}$$

$$\approx N + (\mu - \varepsilon_F) D(\varepsilon_F) + \frac{\pi^2}{6} D'(\varepsilon_F)(k_BT)^2 \qquad \text{assuming } \mu \approx \varepsilon_F \tag{14.9}$$

Thus, we get

$$\mu \approx \varepsilon_F - \frac{\pi^2}{6} \frac{D'(\varepsilon_F)}{D(\varepsilon_F)} (k_BT)^2 \tag{14.10}$$

which justifies the assumption that $\mu \approx \varepsilon_F$ if $T \ll T_F$.

14.1.3 Fermi energy

The Fermi energy is an important energy scale of the Fermi gas problem. If one divides it by k_B, then one gets the temperature scale T_F. This temperature is the

crossover temperature above which the system will behave as a classical system. If $T \ll T_F$, then the system acts as a quantum system. In the quantum system, the energy per particle is about ε_F. It is one of the most striking consequences of the Pauli exclusion principle that even at $T = 0$ the Fermi gas system imparts such a high energy to each particle. For this reason, many properties of the Fermi gas system is essentially a $T = 0$ property: e.g., the pressure, the energy, and the compressibility. Since the free electrons in a metal bind the material together ("metallic bonding"), really the existence of a metallic substance and the reason why it hurts when you kick a metal pole are all due to the $T = 0$ quantum effect of the electron gas in the metallic substance. In this sense, any metallic substance that you see around yourself should be viewed as a quantum matter.

It is plain to see why T_F for a common metal is easily as high as $10,000$ K or $100,000$ K. First of all, note that k_F, the *Fermi momentum* – the maximum value of the magnitude of the momentum for occupied states at $T = 0$ – is determined by the equation:

$$2\frac{\frac{4\pi}{3}k_F^3}{\frac{8\pi^3}{V}} \;=\; N \tag{14.11}$$

where 2 is from the spin degeneracy of the electron. So

$$k_F \;=\; \sqrt[3]{3\pi^2 n} \tag{14.12}$$

Since $n \sim 10^{-1}\text{Å}^{-3}$ for a typical metal, we get $k_F \sim 1$ to 2 Å^{-1}. For a non-relativistic electron, we then get

$$\varepsilon_F \;=\; \frac{\hbar^2}{2m}k_F^2 = 4 \sim 16 \text{ eV} \tag{14.13}$$

which definitely justifies the assumption of the non-relativistic electron. Using $k_B = 0.02585$ meV/300 K we get

$$T_F \;=\; 10,000 \text{ K} \sim 100,000 \text{ K} \tag{14.14}$$

This is the temperature scale corresponding to the typical kinetic energy of the electron in a Fermi gas at $T = 0$.

The Fermi gas problem is important not only for the electron gas in a metal, but for electrons and nucleons in a star or liquid of ^{3}He. The Fermi temperature can range from 10^6 K to a few mK, depending on systems.

14.1.4 Energy and heat capacity

Let us calculate the energy using

$$E = \int_{-\infty}^{\infty} d\varepsilon\, \varepsilon D(\varepsilon) f(\varepsilon) \tag{14.15}$$

$$\approx \int_{-\infty}^{\mu} d\varepsilon\, \varepsilon D(\varepsilon) + \frac{\pi^2}{6} \left(D(\mu) + \mu D'(\mu)\right) (k_B T)^2 \qquad \text{Eq. 14.1} \tag{14.16}$$

$$= E_0 + \int_{\varepsilon_F}^{\mu} d\varepsilon\, \varepsilon D(\varepsilon) + \frac{\pi^2}{6} \left(D(\mu) + \mu D'(\mu)\right) (k_B T)^2 \quad E_0 \equiv \int_{-\infty}^{\varepsilon} d\varepsilon\, \varepsilon_F D(\varepsilon) \tag{14.17}$$

Using the result, Eq. 14.10, we see that $\int_{\varepsilon_F}^{\mu} d\varepsilon\, \varepsilon D(\varepsilon) \approx -\frac{\pi^2}{6} \mu D'(\mu) (k_B T)^2$ cancels one of the terms above, and we have finally (with $\mu \approx \varepsilon_F$)

$$E \approx E_0 + \frac{\pi^2}{6} D(\varepsilon_F) (k_B T)^2 \tag{14.18}$$

The heat capacity is

$$C_V \approx \frac{\pi^2}{3} D(\varepsilon_F) (k_B T) k_B \tag{14.19}$$

These expressions have a very precise qualitative interpretation. With respect to the ground state ("vacuum") at $T = 0$, a finite temperature state is characterized by the electrons excited above μ and the holes[3] excited below μ. Mathematically the presence of these excitations is indicated by the fact that $f(\varepsilon, T)$ deviates from $f(\varepsilon, T = 0)$. Since this deviation occurs in a small sliver of energy of width about $4k_B T$, we can estimate that the number of electrons and holes excited around the chemical potential are given by $\sim D(\varepsilon_F)(k_B T)$. These are particles whose energy relative to the $T = 0$ "vacuum" is less than the temperature – i.e., they act as classical particles with equipartition energy $\sim k_B T$ per particle. This is the reason why $E \sim D(\varepsilon_F)(k_B T)(k_B T)$ up to a numerical factor, and why $C_V \sim D(\varepsilon_F)(k_B T) k_B$ up to a numerical factor.

14.1.5 Order of magnitude and dispersion

As we have been doing the 2nd order perturbation on T/T_F, we expect that $E_0 \gg E - E_0$ and likewise $P_0 \gg P - P_0$ (cf. Eq. 13.34). That this is really true can be

[3] These holes are somewhat different from holes in semiconductors, and should not be confused with them.

analyzed as follows. $D(\varepsilon_F) \sim N/\varepsilon_F$. $E_0 \sim N\varepsilon_F$. And so, from Eq. 14.18, we get $E - E_0 \sim E_0(T/T_F)^2 \ll E_0$.

Purposefully, we did not specify the nature of the Fermion so much in this note so far (with the exception of Section 14.1.3). This leaves all expressions so far applicable regardless of relativistic or non-relativistic particles and the dimensionality of the space.

Here, we take up the non-relativistic case in three dimensions as we did in Section 14.1.3. Note that in this case the density of states is proportional to $\varepsilon^{1/2}$ (Eq. 13.49). Thus, by setting $D(\varepsilon) = A\varepsilon^{1/2}$ and using $\int_0^{\varepsilon_F} d\varepsilon D(\varepsilon) = N$ (the zero temperature particle conservation equation), we get

$$D(\varepsilon) \;=\; \frac{3}{2}\frac{N}{\varepsilon_F}\left(\frac{\varepsilon}{\varepsilon_F}\right)^{1/2} \tag{14.20}$$

Comparing this expression with Eq. 13.49 gives another way to evaluate ε_F in terms of the system parameters. From this expression, it is readily found that

$$E_0 \equiv E(T=0) \;=\; \int_0^{\varepsilon_F} d\varepsilon\, \varepsilon D(\varepsilon) \;=\; \frac{3}{5}N\varepsilon_F \tag{14.21}$$

which means

$$P(T=0)V \;=\; \frac{2}{5}N\varepsilon_F \tag{14.22}$$

Also, we get

$$D(\varepsilon_F) \;=\; \frac{3}{2}\frac{N}{\varepsilon_F} \tag{14.23}$$

$$\frac{D'(\varepsilon_F)}{D(\varepsilon_F)} \;=\; \frac{1}{2}\frac{1}{\varepsilon_F} \tag{14.24}$$

and therefore

$$\mu \;=\; \varepsilon_F\left(1 - \frac{\pi^2}{12}\left(\frac{T}{T_F}\right)^2 + O\left(\frac{T}{T_F}\right)^4\right) \tag{14.25}$$

$$E \;=\; \frac{3}{5}N\varepsilon_F\left(1 + \frac{5\pi^2}{12}\left(\frac{T}{T_F}\right)^2 + O\left(\frac{T}{T_F}\right)^4\right) \tag{14.26}$$

$$C_V \;=\; \frac{\pi^2}{2}Nk_B\frac{T}{T_F} + O\left(\frac{T}{T_F}\right)^3 \tag{14.27}$$

14.1.6 Heavy fermion

The heat capacity for a free fermion system is typically written as

$$C_V = \gamma T \tag{14.28}$$

where according to Eq. 14.19

$$\gamma = \frac{\pi^2}{3} D(\varepsilon_F) k_B^2 \tag{14.29}$$

Here, γ has the dimension of mJ / mole / K^2. For a typical metal, it has the value of $\gamma \sim 1$ mJ / mole / K^2. However, for certain materials called "heavy fermions" (e.g. UPt_3, UBe_{13}, $CeCu_2Si_2$, ...), γ can be as large as 1000! It is as though an electron is as heavy as a neutron! To explain this one notes that $\gamma \propto m$, since $D(\varepsilon_F) \sim N/\varepsilon_F$ and $\varepsilon_F \propto 1/m$. It turns out that what we call "free fermions" are sometimes collective particles that emerge out of very strong interactions. Those particles are called "renormalized particles" or "quasi-particles." In the heavy fermion case, these quasi-particles act just like free electrons except that each heavy fermion, i.e. each quasi-particle, has a very large mass. In this case, the heavy mass originates from the Kondo interaction – the spin-flip scattering of a conduction electron off of a spin impurity. This problem cannot be solved perturbatively and has been vexing physicists for years, before it was masterfully solved by K. G. Wilson.

14.2 Bose gas

14.2.1 General setup

Let us recall, from Eqs. 13.32,13.33, (with $\eta = -1$)

$$N = \int d\varepsilon\, D(\varepsilon) \frac{1}{z^{-1} e^{\beta\varepsilon} - 1} \qquad \text{see below} \tag{14.30}$$

$$E = \int d\varepsilon\, D(\varepsilon) \frac{\varepsilon}{z^{-1} e^{\beta\varepsilon} - 1} \tag{14.31}$$

where $z \equiv \exp(\beta\mu)$. Also, note that we will be considering a spin 0 particle (e.g., ^{4}He). So we shall put the non-orbital degeneracy $g = 1$. For the results below, however, it is easy to put back the non-orbital degeneracy later on: simply multiply g to the function $g_m(z)$, which will be defined shortly below. Also, we shall confine ourselves to the non-relativistic particles. I.e., the dispersion relation of the form

$\varepsilon(\vec{k}) = \frac{\hbar^2 k^2}{2m}$ will be assumed. Finally, we will also assume that the spatial dimension is 3. Then,

$$PV \;=\; \frac{2}{3}\,E \tag{14.32}$$

However, generalizing calculations below to other dispersions and to other spatial dimensions should not be viewed as posing any fundamental difficulty.

With the dispersion and the dimensionality thus assumed, we recall the handy *operator identity*, Eq. 13.53,

$$\frac{1}{V}\int_0^\infty d\varepsilon D(\varepsilon)\,[\;\cdot\;] \;=\; \frac{1}{\lambda^3\left(\frac{1}{2}\right)!}\int_0^\infty dx x^{1/2}\,[\;\cdot\;] \qquad\qquad x \equiv \beta\varepsilon \tag{14.33}$$

where $[\;\cdot\;]$ means an arbitrary integrand that this operator acts on. Using this identity, the above expressions for N and E can be written as

$$n \;=\; \frac{N}{V} \;=\; \frac{1}{\lambda^3\left(\frac{1}{2}\right)!}\int_0^\infty dx \frac{x^{1/2}}{z^{-1}\,e^x - 1} \qquad \text{see below} \tag{14.34}$$

$$\frac{E}{V} \;=\; \frac{k_B T}{\lambda^3\left(\frac{1}{2}\right)!}\int_0^\infty dx \frac{x^{3/2}}{z^{-1}\,e^x - 1} \tag{14.35}$$

Now, we define the following function[4] $g_m(z)$

$$g_m(z) \;=\; \frac{1}{(m-1)!}\int_0^\infty dx \frac{x^{m-1}}{z^{-1}e^x - 1} \tag{14.36}$$

Note that $1/(z^{-1}e^x - 1) = ze^{-x}/(1 - ze^{-x}) = \sum_{n=1}^\infty z^n e^{-nx}$. And so, $g_m(z) = \sum_{n=1}^\infty \frac{z^n}{(m-1)!}\int_0^\infty dx x^{m-1}e^{-nx}$. By changing the variable to $y = nx$, it is seen that the integral is $(m-1)!\,n^{-m}$. Therefore, we get the following simple result

$$g_m(z) \;=\; \sum_{n=1}^\infty \frac{z^n}{n^m} \tag{14.37}$$

$$g_m(z=1) \;=\; \zeta(m) \qquad \text{Riemann zeta function} \tag{14.38}$$

$$\frac{dg_m(z)}{dz} \;=\; \frac{g_{m-1}}{z} \tag{14.39}$$

$$g_m(z=0) \;=\; 0 \quad \text{and} \quad \frac{dg_m(z>0)}{dz} > 0 \qquad \text{mononotic for } z \geq 0 \tag{14.40}$$

It can be noted that the Riemann zeta function diverges if $m \leq 1$. From the recursion relation, Eq. 14.39, then, one sees that the function $g_m(z)$ is *not* a nice function around $z = 1$. A derivative will diverge (eventually), and thus g_m is not analytic

[4] This is what is defined as $f_m^+(z)$ in the textbook.

around $z = 1$. Now, in terms of g_m's we get from the above two equations for $n, E/V$ and from Eq. 14.32,

$$n = \frac{1}{\lambda^3} g_{3/2}(z) \qquad \text{see below} \tag{14.41}$$

$$\frac{E}{V} = \frac{3k_BT}{2\lambda^3} g_{5/2}(z) \tag{14.42}$$

$$P = \frac{k_BT}{\lambda^3} g_{5/2}(z) \tag{14.43}$$

14.2.2 Chemical potential

Here, we will use the equation for N (Eq. 14.41) to try solving for the chemical potential, as usual.

First of all, though, let us note the following simple fact about the chemical potential (and thus the fugacity) in the case of the boson gas. Since the Bose-Einstein occupation number $n(\varepsilon) = 1/(e^{\beta(\varepsilon-\mu)} - 1)$ must be non-negative for any ε, and since $\varepsilon \geq 0$ for the current case, it follows that at any temperature

$$\mu \leq 0 \qquad \text{Bose gas} \tag{14.44}$$

This is *much* different from the fermion case, where μ at $T = 0$ is a very large positive number. Of course, as the temperature is raised, or the volume is expanded, the chemical potential for boson or fermion must tend to its classical value – a large negative value (Section 13.4). We will see shortly that in the case of the Bose gas

$$\mu \to 0^- \qquad \text{as } T \to 0^+ \tag{14.45}$$

In any case, the non-positive chemical potential means that the fugacity is limited to

$$0 \leq z \leq 1 \tag{14.46}$$

As we saw above (Eq. 14.40), the function $g_m(z)$ is zero at $z = 0$ and monotonically increases as z increases from zero. If $m \leq 2$, then g_m has a divergent derivative at $z = 1$, while its value at $z = 1$ is finite if $m > 1$. Such is the case for $g_{3/2}(z)$. From Eq. 14.41, we can see, then, that

$$n = \frac{g_{3/2}(z)}{\lambda^3} \leq \frac{g_{3/2}(1)}{\lambda^3} = \frac{\zeta(3/2)}{\lambda^3} \approx \frac{2.612}{\lambda^3} \qquad \text{see below} \tag{14.47}$$

This is a curious inequality! And it turns out to be *incorrect*! This is the reason for the "see below" tags in the equations for N or n. That this must be incorrect is seen by noting that $\lambda = h/\sqrt{2\pi m k_B T}$. So, as $T \to 0$, the right hand side vanishes as $T^{3/2}$.

This means that $n \to 0$ as $T \to 0$! This is clearly absurd as the (massive) particles cannot just disappear, simply because the temperature is lowered. Where did things go wrong? This is a subtle and importance question. The answer is easy to find, if one considers the case when $T = 0^+$. Physically, what would happen? At zero temperature, the system will seek out the minimum energy state, and that is simply all particles occupying the lowest possible energy state, i.e. the zero energy state. Let us see that the fugacity must be in this case.

$$N = \sum_i \frac{1}{z^{-1}e^{\beta\varepsilon_i} - 1} \qquad \text{at any } T \tag{14.48}$$

$$\to \frac{1}{z^{-1} - 1} \qquad \text{as } T \to 0^+ \tag{14.49}$$

Therefore

$$z \to \frac{1}{1 + N^{-1}} \approx 1 - \frac{1}{N} \qquad \text{as } T \to 0^+ \tag{14.50}$$

$$\mu \to -\frac{k_B T}{N} \qquad \text{as } T \to 0^+ \tag{14.51}$$

This is the proof of Eq. 14.45. The point here is that the zero energy occupancy $n(\varepsilon = 0) = 1/(z^{-1}-1)$ becomes macroscopically large at low temperatures.[5] However, this singular value at $\varepsilon = 0$ is completely ignored, when the formula for N as a sum, Eq. 14.48, is converted to the formula for N as an integral, Eq. 14.30!

14.2.3 Fixing the N, n formulae

Fortunately, to fix this problem is easy. All we need to do is to separately include $n(\varepsilon = 0)$, for N, or $n(\varepsilon = 0)/V$, for $n = N/V$, in all equations tagged "see below." In other words, all equations tagged "see below" must be interpreted as representing only one-particle excited states, $\varepsilon > 0$, excluding the one-particle ground state, $\varepsilon = 0$. In particular, let us fix Eq. 14.41

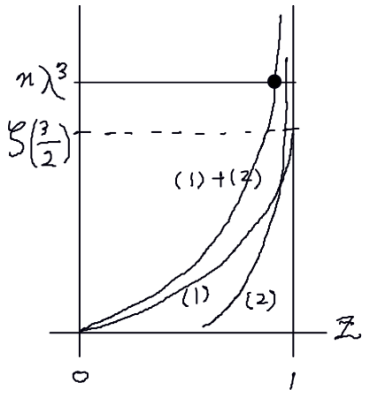
$$n = \frac{g_{3/2}(z)}{\lambda^3} + \frac{1}{V}\frac{z}{1-z} \tag{14.52}$$

A better form of this equation is

$$n\lambda^3 = g_{3/2}(z) + \frac{n\lambda^3}{N}\frac{z}{1-z} \tag{14.53}$$

[5] You might worry whether only the zero energy matters here. Only it matters. You can show that for any non-zero energy value the occupancy cannot be macroscopic, i.e. $n(\varepsilon > 0)/N \to 0$ as $N \to \infty$.

One reason that this new form is better is that it can be seen to consist of three parameters, $N, n\lambda^3, z$. Since N is a constant, this equation is an implicit equation to solve for z (and thus the chemical potential) given a value of $n\lambda^3$. This is what we set out to do in the previous section! Due to the non-analyticity of $g_{3/2}(z)$, this equation must be solved numerically in general. However, we can already learn generic behaviors by graphing the above equation.



As this figure shows, the solution (filled circle) for z can be obtained by the intersection of the horizontal line $n\lambda^3$ and the sum of two curves (1) $g_{3/2}(z)$ and (2) $\frac{n\lambda^3}{N}\frac{z}{1-z}$. Consider scaling up $n\lambda^3 \to An\lambda^3$ with $A > 1$. Then, the horizontal line scales up by A, and so does part (2). But, part (1) remains constant. Since both (1) and (2) are positive, it follows that (1) + (2) $\to$ (1) + A(2) $< A$((1) + (2)).

It follows that *as $n\lambda^3$ increases, z increases monotonically.*
z goes monotonically from 0 ($\mu = -\infty$) to 1 ($\mu = 0$) as $n\lambda^3$ goes from 0 (classical limit) to ∞ (quantum limit: low T or high n).

An important thing to note in the above figure is that the graph (2) is highly exaggerated, unless $n(\varepsilon = 0)/N = z/(N(1-z)) \to$ finite.

14.2.4 The BEC condition

The Bose-Einstein condensate (BEC) refers to the macroscopic occupation of the zero energy level. That is, when a BEC forms

$$\frac{n(\varepsilon = 0)}{N} = \text{finite} \tag{14.54}$$

When does this transition into the BEC start? Roughly speaking, it is when the excited states cannot hold all the particles any more. This condition is

$$n\lambda^3 \;=\; g_{3/2}(1) \;=\; \zeta(3/2) \;\approx\; 2.612 \tag{14.55}$$

This condition can be interpreted as the condition that the maximum number of particles stored in excited states is equal to N. However, this condition needs some more explanation, since strictly speaking the condition that the excited states can hold all particles is $n\lambda^3 \;=\; g_{3/2}(z)$, strictly speaking (Eq. 14.53). How is it that z can be replaced by 1 here?

14.2.5 Perturbation explanation for the BEC condition

Apparently, the nice thing about the form of Eq. 14.53 is that it contains very sensible perturbation parameters. In the classical regime, $n\lambda^3$ is the small perturbation parameter. Although we could discuss the classical regime with this equation, since our discussion so far has been very general, we have already done that in a previous lecture and so we won't repeat it. In the quantum regime, $n\lambda^3$ is large (as we already saw above in Eq. 14.47) but $n\lambda^3/N = \lambda^3/V$ looks to be a promising perturbation parameter.

Now how good a perturbation parameter is this λ^3/V? A short answer is very good, since one can always send $V \to \infty$ in the thermodynamic limit. This is unsatisfactory, though, since what we really want is to compare λ^3 and V for a reasonably estimated T and V values. For instance, if we take $T \sim 1$ K, and take the boson to be the ^{4}He atom, then one can calculate that $\lambda \sim 10$ Å. Even taking the sample size to be very small, a micron along each axis, we get $\lambda^3/V \sim 10^{-9}$, which is very small.

However, even with this small parameter, we *cannot* really do the perturbation theory here: the reason is that near the region of the most interest, $z \approx 1$, $g_{3/2}$ is not an analytic function, and that, inside the BEC condensate regime ($n\lambda^3 > \zeta(3/2)$), the zeroth order equation does not have a solution (see the figure above; ignoring (2) would correspond to the zeroth order). Instead, we need to to analyze Eq. 14.53 in more general terms. We will see that we can indeed justify the BEC condition as stated in Eq. 14.55 and that the *answer* is a perturbative statement, while the process to the answer is not.

The problem is quite subtle. In the vicinity of $z = 1$, λ^3/V is small, but the term $\frac{\lambda^3}{V}\frac{z}{1-z}$ might be very large since $z \approx 1$. Also, in general, this term will not be small at all as $T \to 0$. On the other hand, the physical intuition is that this term must be very small in the vicinity of the BEC transition since there the zero energy level

has a low occupancy. The subtlety is that, near the BEC transition, the value of z is essentially 1.

First, let us consider the case when $n\lambda^3 \leq g_{3/2}(1) = \zeta(3/2) \approx 2.612$. This is the non-BEC phase at high temperature or low density. We can re-write the above equation as

$$g_{3/2}(z) \;=\; n\lambda^3 \left(1 - \frac{1}{N}\frac{1}{z^{-1}-1}\right) \tag{14.56}$$

Since the temperature is finite (as λ has an upper bound), we should expect that z is not exactly 1. Thus, the second term should not be too large. In fact, it is clear that the second term on the right hand side can be safely ignored if $\frac{1}{z^{-1}-1} \ll N$. As we shall see shortly, this is indeed the case. And, so we get

$$g_{3/2}(z) \;=\; n\lambda^3 \left[1 - O(1/N)\right] \qquad\qquad \text{if } n\lambda^3 \leq \zeta(3/2) \tag{14.57}$$

Second, let us consider the case when $n\lambda^3 \geq g_{3/2}(1) = \zeta(3/2) \approx 2.612$. Assuming that the temperature is not exactly zero (but can be very small), we should, again, expect that z is not exactly 1. Thus, $\Delta \equiv n\lambda^3 - g_{3/2}(z) > n\lambda^3 - g_{3/2}(1) \geq 0$. Eq. 14.53 then becomes

$$\Delta \;=\; \frac{n\lambda^3}{N}\frac{1}{z^{-1}-1} \tag{14.58}$$

which means

$$z \;=\; \frac{1}{1+\frac{n\lambda^3}{N\Delta}} \tag{14.59}$$

In the limit of $N \to \infty$, we get

$$z \;\approx\; 1 - \frac{n\lambda^3}{N\Delta} \;\approx\; 1 \tag{14.60}$$

One might worry whether it is possible to have a small enough Δ so that z is substantially smaller than 1. But this is impossible, due to the fact that Δ is also a function of z. Since $\Delta = n\lambda^3 - g_{3/2}(z)$, it follows that, if z is substantially smaller than 1, then Δ would be of order 1 or larger since $g_{3/2}(z)$ will be much different from $g_{3/2}(1)$, and since $n\lambda^3 \geq g_{3/2}(1) = \zeta(3/2)$.[6] So, it follows that

$$\frac{n\lambda^3}{N\Delta} \ll 1 \;\text{ and }\; z \;\approx\; 1 - O(1/N) \qquad\qquad \text{if } n\lambda^3 \geq \zeta(3/2) \tag{14.61}$$

[6] This is more so, since the derivative of $g_{3/2}(z)$ at $z = 1$ is infinite!

From Eq. 14.50, note that we must have

$$n\lambda^3/\Delta \to 1 \qquad \text{as } T \to 0 \text{ or } n \to \infty, \text{ that is, as } n\lambda^3 \to \infty \tag{14.62}$$

which is very sensible. From the fact that z is a monotonically increasing function of $n\lambda^3$, it follows that $n\lambda^3/\Delta$ is a monotonically decreasing function of $n\lambda^3$, while the condition $n\lambda^3/\Delta \ll N$ remaining true in this regime defined by $n\lambda^3 \geq \zeta(3/2)$.

To summarize the two cases examined here, we get this very important result:

If $n\lambda^3 \geq \zeta(3/2)$, then the chemical potential gets stuck at 0. If $n\lambda^3 \leq \zeta(3/2)$, then the chemical potential is determined by $g_{3/2}(z) = n\lambda^3$.

Note that the solution for $g_{3/2}(z) = n\lambda^3$ must be obtained numerically. In any case, it is clear from the above discussion that the point at which $n\lambda^3 = \zeta(3/2)$ becomes true defines the transition point. Thus, we have achieved our goal of explaining this BEC condition, already stated in Eq. 14.55. If n is held constant, then this equation defines T_c, the Bose-Einstein condensate transition temperature, as

$$T_c = \frac{h^2}{2\pi m k_B}\left(\frac{n}{\zeta(3/2)}\right)^{2/3} \tag{14.63}$$

In this case, the BEC sets in at $T \leq T_c$. If the temperature is held constant, and the volume is varied, then the above equation defines the critical volume per particle

$$v_c = \frac{\lambda^3}{\zeta(3/2)} \tag{14.64}$$

such that the BEC sets in at $v \leq v_c$.

In the condensed regime ($n\lambda^3 \geq \zeta(3/2)$), we can calculate the occupancy of the zero energy level from Eq. 14.53:

$$\frac{n(\varepsilon = 0)}{N} = \frac{z}{N(1-z)} \tag{14.65}$$

$$= 1 - \frac{g_{3/2}(z)}{n\lambda^3} \tag{14.66}$$

$$\approx 1 - \frac{g_{3/2}(1)}{n\lambda^3} \qquad \text{Eq. 14.61} \tag{14.67}$$

$$= 1 - \left(\frac{T}{T_c}\right)^{3/2} \qquad \text{Eq. 14.63} \tag{14.68}$$

$$= 1 - \frac{v}{v_c} \qquad \text{Eq. 14.64} \tag{14.69}$$

So as the transition point is approached from below, $n(\varepsilon = 0)/N \to 0$. Above the transition, the occupancy $n(\varepsilon = 0)$ will further decrease (as the fugacity is a monotonic function of $n\lambda^3$), proving the assertion made just before Eq. 14.57.