5.11: Appendix III- Example Bose Condensation Problem

A three-dimensional gas of noninteracting bosonic particles obeys the dispersion relation $\varepsilon(\mathbf{k}) = A\,|\mathbf{k}|^{1/2}$.

- Obtain an expression for the density $n(T,z)$ where $z=\exp(\mu/k_BT)$ is the fugacity. Simplify your expression as best you can, adimensionalizing any integral or infinite sum which may appear. You may find it convenient to define

$$Li_\nu(z) \equiv \frac{1}{\Gamma(\nu)}\int_0^\infty dt\,\frac{t^{\nu-1}}{z^{-1}\,e^t-1} = \sum_{k=1}^\infty \frac{z^k}{k^\nu}\ . \tag{5.11.1}$$

  Note $Li_\nu(1)=\zeta(\nu)$, the Riemann zeta function.
- Find the critical temperature for Bose condensation, $T_c(n)$. Your expression should only include the density n, the constant A, physical constants, and numerical factors (which may be expressed in terms of integrals or infinite sums).
- What is the condensate density n_0 when $T=\frac{1}{2}\,T_c$?
- Do you expect the second virial coefficient to be positive or negative? Explain your reasoning. (You don't have to do any calculation.)

We work in the grand canonical ensemble, using Bose-Einstein statistics.

- The density for Bose-Einstein particles are given by

$$\begin{aligned} n(T,z) &= \int\!\frac{d^3\!k}{(2\pi)^3}\,\frac{1}{z^{-1}\,\exp(Ak^{1/2}/k_BT)-1} \\ &= \frac{1}{\pi^2}\bigg(\frac{k_BT}{A}\bigg)^6\int_0^\infty ds\,\frac{s^5}{z^{-1}\,e^s-1} \\ &= \frac{120}{\pi^2}\bigg(\frac{k_BT}{A}\bigg)^6 Li_6(z)\ , \end{aligned}$$

  where we have changed integration variables from k to $s=Ak^{1/2}/k_BT$, and we have defined the functions $Li_\nu(z)$ as above, in Equation [zetadef]. Note $Li_\nu(1)=\zeta(\nu)$, the Riemann zeta function.
- Bose condensation sets in for $z=1$, $\mu=0$. Thus, the critical temperature T_c and the density n are related by

$$n = \frac{120\,\zeta(6)}{\pi^2}\bigg(\frac{k_BT_c}{A}\bigg)^6, \tag{5.11.2}$$

  or

$$T_c(n) = \frac{A}{k_B}\bigg(\frac{\pi^2\,n}{120\,\zeta(6)}\bigg)^{1/6}\ . \tag{5.11.3}$$

- For $T<T_c$, we have

$$\begin{aligned} n &= n_0 + \frac{120\,\zeta(6)}{\pi^2}\bigg(\frac{k_BT}{A}\bigg)^6 \\ &= n_0 + \bigg(\frac{T}{T_c}\bigg)^6 n\ , \end{aligned}$$

  where n_0 is the condensate density. Thus, at $T=\frac{1}{2}\,T_c$,

$$n_0\big(T=\tfrac{1}{2}T_c\big) = \frac{63}{64}\,n. \tag{5.11.4}$$

- The virial expansion of the equation of state is

$$p = nk_BT\Big(1+B_2(T)\,n+B_3(T)\,n^2+\ldots\Big)\ . \tag{5.11.5}$$

We expect $B_2(T) < 0$ for noninteracting bosons, reflecting the tendency of the bosons to condense. (Correspondingly, for noninteracting fermions we expect $B_2(T) > 0$.)

For the curious, we compute $B_2(T)$ by eliminating the fugacity z from the equations for $n(T,z)$ and $p(T,z)$. First, we find $p(T,z)$:

$$\begin{aligned} p(T,z) &= -k_B T \int \frac{d^3k}{(2\pi)^3} \ln\Big(1 - z\,\exp(-Ak^{1/2}/k_B T)\Big) \\ &= -\frac{k_B T}{\pi^2}\left(\frac{k_B T}{A}\right)^6 \int\limits_0^\infty ds\, s^5 \,\ln\left(1 - z\, e^{-s}\right) \\ &= \frac{120\, k_B T}{\pi^2}\left(\frac{k_B T}{A}\right)^6 Li_7(z). \end{aligned}$$

Expanding in powers of the fugacity, we have

$$\begin{aligned} n &= \frac{120}{\pi^2}\left(\frac{k_B T}{A}\right)^6 \left\{ z + \frac{z^2}{2^6} + \frac{z^3}{3^6} + \dots \right\} \\ \frac{p}{k_B T} &= \frac{120}{\pi^2}\left(\frac{k_B T}{A}\right)^6 \left\{ z + \frac{z^2}{2^7} + \frac{z^3}{3^7} + \dots \right\}. \end{aligned}$$

Solving for $z(n)$ using the first equation, we obtain, to order n^2,

$$z = \left(\frac{\pi^2 A^6\, n}{120\,(k_B T)^6}\right) - \frac{1}{2^6}\left(\frac{\pi^2 A^6\, n}{120\,(k_B T)^6}\right)^2 + \mathcal{O}(n^3)\,. \tag{5.11.6}$$

Plugging this into the equation for $p(T,z)$, we obtain the first nontrivial term in the virial expansion, with

$$B_2(T) = -\frac{\pi^2}{15360}\left(\frac{A}{k_B T}\right)^6, \tag{5.11.7}$$

which is negative, as expected. Note that the ideal gas law is recovered for $T \to \infty$, for fixed n.

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1. For a review of the formalism of second quantization, see the appendix in §9.↩
2. Several texts, such as Pathria and Reichl, write $g_q(z)$ for $Li_q(z)$. I adopt the latter notation since we are already using the symbol g for the density of states function $g(\varepsilon)$ and for the internal degeneracy g.↩
3. Note the dimensions of $g(\omega)$ are $(frequency)^{-1}$. By contrast, the dimensions of $g(\varepsilon)$ in Equation [BDOS] are $(energy)^{-1} \cdot (volume)^{-1}$. The difference lies in the a factor of $\mathcal{V}_0 \cdot \hbar$, where $\mathcal{V}_0$ is the unit cell volume.↩
4. If $\omega(\mathbf{k}) = Ak^\sigma$, then $\mathcal{C} = 2^{1-d}\,\pi^{-\frac{d}{2}}\,\sigma^{-1}\,A^{-\frac{d}{\sigma}}\,\mathsf{g}\,/\,\Gamma(d/2)$.↩
5. OK, that isn't quite true. For example, if $g(\varepsilon) \sim 1/\ln\varepsilon$, then the integral has a very weak $\ln\ln(1/\eta)$ divergence, where η is the lower cutoff. But for any power law density of states $g(\varepsilon) \propto \varepsilon^r$ with $r > 0$, the integral converges.↩
6. It is easy to see that the chemical potential for noninteracting bosons can never exceed the minimum value ε_0 of the single particle dispersion.↩
7. Note that in the thermodynamics chapter we used v to denote the molar volume, $N_A\, V/N$.↩
8. The $\mathbf{k} \neq 0$ particles are sometimes called the *overcondensate*.↩
9. IBG condensation is in the universality class of the spherical model. The λ-transition is in the universality class of the XY model.↩
10. Recall that two bodies in thermal equilibrium will have identical temperatures *if they are free to exchange energy*.↩
11. The phonon velocity c is slightly temperature dependent.↩
12. Many reliable descriptions may be found on the web. Check Wikipedia, for example.↩
13. Explicitly, one replaces $\zeta(3)$ with $\zeta(2) = \frac{\pi^2}{6}$, $Li_3(y)$ with $Li_2(y)$, and $\left(k_B T/\hbar\bar{\omega}\right)^3$ with $\left(k_B T/\hbar\bar{\omega}\right)^2$.↩
14. Note that writing $v = (2n+1)\,i\pi + \epsilon$ we have $e^{\pm v} = -1 \mp \epsilon - \frac{1}{2}\epsilon^2 + \dots$ We then expand), so\((e^v+1)(e^{-v}+1) = -\epsilon^2 + \dots$ $e^{vD} = e^{(2n+1)i\pi D}(1 + \epsilon D + \dots)$ to find the residue: $Res = -D\,e^{(2n+1)i\pi D}$.↩
15. I thank my colleague Tarun Grover for this observation.↩

16. We've used $-\frac{2}{V} Q'(\mu) = -\frac{1}{V} \frac{\partial^2 \Omega}{\partial \mu^2} = n^2 \kappa_T$.↩
17. Note that we have written $\mu n = \bar{\mu} n + \frac{1}{2} U n^2$, which explains the sign of the coefficient of n^2.↩
18. The Gibbs-Duhem relation guarantees that such an equation of state exists, relating any three intensive thermodynamic quantities.↩
19. A theorem due to Nagaoka establishes that the ground state is ferromagnetic for the case of a single hole in the $U = \infty$ system on bipartite lattices.↩
20. See J. P. F. LeBlanc , *Phys. Rev. X* **5**, 041041 (2015) and B. Zheng , *Science* **358**, 1155 (2017).↩
21. The best case for stripe order has been made at $T = 0$, $U/t = 8$, and hold doping $x = \frac{1}{8}$ ($n = \frac{7}{8}$).↩
22. In the normalization integrals, each $\int d^d x$ implicitly includes a sum $\sum_\zeta$ over any internal indices that may be present.↩