PHYS 427 - Thermal and Statistical Physics - Discussion 08

March 25, 2025

- 1. **Phonons in one dimension**: In lecture, you saw that the Debye model accurately predicts the heat capacity of solids for the high and low temperature limits. You showed that, in 3D, $C_V \propto T^3$ at low temperature. In this problem, you will find the dependence of the heat capacity on the temperature for a one-dimensional system.
 - (a) What is the density of states in one dimension? How does it differ from $D(\omega)$ in 3D? How many phonon modes are there?
 - (b) Calculate the internal energy of this system for the low temperature and the high temperature limits. Find the Debye temperature in the process.
 - (c) Finally, calculate the heat capacity at constant volume, C_V , for each limit.

Consider a system consisting of two particles of the same type, i.e. they have the same mass, charge, etc. *In classical mechanics*, the two particles, despite being "the same", are distinguishable. I'll let Griffiths take it from here:

"You can always tell the particles apart, in principle—just paint one of them red and the other one blue, or stamp identification numbers on them, or hire private detectives to follow them around. But in quantum mechanics the situation is fundamentally different: You can't paint an electron red, or pin a label on it, and a detective's observations will inevitably and unpredictably alter its state, raising doubts as to whether the two had perhaps switched places. The fact is, all electrons are utterly identical, in a way that no two classical objects can ever be. It's not just that we don't happen to know which electron is which; God doesn't know which is which, because there is no such thing as "this" electron, or "that" electron; all we can legitimately speak about is "an" electron." - David J. Griffiths, Introduction to Quantum Mechanics

In other words, in quantum mechanics particles which are "the same" are fundamentally *indistinguishable*. This has profound consequences. The basic result¹ is that particles can be divided into two categories: **bosons** and **fermions**.² Bosons are particles whose wavefunction is <u>symmetric</u> under the exchange of any two particle labels, whereas fermions are particles whose wavefunction is antisymmetric under this exchange. For example, for

¹Derivations can be found in any quantum mechanics textbook.

²Note: more exotic types of particles which are neither bosons nor fermions do exist as excitations in condensed matter systems (e.g. anyons), but we won't discuss them in this course.

a system of two identical particles, this means

$$\psi(x_1, x_2) = \psi(x_2, x_1)$$
 if the particles are identical bosons or
$$\psi(x_1, x_2) = -\psi(x_2, x_1)$$
 if the particles are identical fermions, (2)

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where ψ is the wavefunction of the two-particle system.

For fermions, the antisymmetry of the wavefunction implies the Pauli exclusion principle: no two identical fermions can occupy the same state. For example, if we put a bunch of identical non-interacting fermions into a one-dimensional harmonic potential, where the eigenstates have energy $\varepsilon_n = \hbar\omega(n+1/2)$, then no two fermions can have the same value of the quantum number n.

Bosons aren't subject to an exclusion principle, so any number of identical bosons can simultaneously occupy a single quantum state. If we put a bunch of identical non-interacting bosons into a one-dimensional harmonic potential, it's perfectly fine for two (or three or more) bosons to have the same value of n.

It turns out there is a deep relationship between the intrinsic spin of a particle and whether that particle is a boson or a fermion. Particles with integer spin (like photons) are bosons, whereas particles with half-integer spin (like electrons) are fermions. This is the content of the spin-statistics theorem³ one encounters in a course on quantum field theory.

2. Non-interacting bosons: Consider a system of identical non-interacting bosons. The bosons can be in many different single-particle quantum states which are labelled by an index $m = 0, 1, 2, \dots$ The energy of a single boson in the singleparticle state m will be denoted ε_m .

In order to specify a microstate state of the whole system, we just have to specify N_m , the number of particles in the $m^{\rm th}$ single-particle state. Then, for example, the energy of the microstate is $\sum_{m} \varepsilon_{m} N_{m}$. Note that this scheme for specifying microstates automatically takes into account the fact that the bosons are indistinguishable.

Let ε_0 denote the lowest energy level (it may be degenerate).

(a) Show the grand partition function is

$$\mathcal{Z} = \prod_{m} \frac{1}{1 - e^{-\beta(\varepsilon_m - \mu)}} \tag{3}$$

as long as the chemical potential obeys $\mu < \varepsilon_0$. What goes wrong if $\mu > \varepsilon_0$?

(b) Using the result from part (a), show that the number of particles in the system is

$$N = \sum_{m} f(\varepsilon_m), \tag{4}$$

where

$$f(\varepsilon) = \frac{1}{e^{\beta(\varepsilon - \mu)} - 1} \tag{5}$$

is called the **Bose-Einstein** distribution function.

³In this context, the "statistics" of a particle refers to whether it is a boson or a fermion.

- (c) Sketch the Bose-Einstein distribution function at some positive temperature. Which single-particle state(s) contains the most particles on average?
- (d) Using the result from part (a), show that the energy of the system is

$$U = \sum_{m} \varepsilon_{m} f(\varepsilon_{m}). \tag{6}$$

(e) Suppose you have actually created a gas of N^* non-interacting bosons in the lab which is in equilibrium at a temperature T. Briefly explain how you could use (4) to solve for μ (although in practice you would need to do it numerically or make further approximations).

Note that you could plug this μ into (6), hence determining $U(T, N^*)$.

This gives another perspective on the meaning of μ . If you have the ability to choose (or measure) the number of particles in your system, μ can be thought of as a value which is tuned such that (4) correctly gives the chosen (or measured) number of particles in the system. Then all other thermodynamic quantities could in principle be expressed in terms of the number of particles instead of μ . However, it is generally much more convenient to continue working with μ .

- 3. Non-interacting ultra-relativistic gas: Consider a collection of massive spin-1 particles in two dimensions confined to a square of area $A=L^2$. Suppose the particles are moving very quickly; in this so-called "ultra-relativistic" limit, the relation between a particle's energy and wavevector is $\varepsilon_{\vec{k}} = c\hbar |\vec{k}|$, where c is the speed of light and the wavevector is quantized as $\vec{k} = \pi \vec{n}/L$ with $n_x, n_y = 1, 2, ..., \infty$.
 - (a) Show that when L is sufficiently large we can approximate a sum over single-particle eigenstates by an integral over energy, i.e. show

$$\sum_{m_s=-1}^{1} \sum_{\vec{k}} F(\varepsilon_{\vec{k}}) \to \frac{3}{2\pi} \frac{L^2}{(\hbar c)^2} \int_{0}^{\infty} d\varepsilon \, \varepsilon F(\varepsilon)$$
 (7)

for any function F. It is customary to define the so-called *density of states*

$$\mathcal{D}(\varepsilon) = \frac{3}{2\pi} \left(\frac{L}{\hbar c}\right)^2 \varepsilon,\tag{8}$$

so that the result can be written as

$$\sum_{m_s=-1}^{1} \sum_{\vec{k}} F(\varepsilon_{\vec{k}}) \to \int_{0}^{\infty} d\varepsilon \, \mathcal{D}(\varepsilon) F(\varepsilon). \tag{9}$$

Explain why $\mathcal{D}(\varepsilon)$ is called the density of states.

Note: you have calculated the density of states of ultrarelativistic massive spin-1 particles in 2 dimensions. For other dispersion relations in different number of dimensions, the expression for $\mathcal{D}(\varepsilon)$ will look different from (8).

- (b) Consider the special case where $\mu \to 0$. Using your result from part (a), compute the energy of the system as a function of T in the infinite-area limit.
 - i. First, without evaluating the integral all the way, show that $U(T) \propto T^3$.

ii. Then evaluate the integral to find the exact constant of proportionality, namely

$$U(T) = \frac{3}{2\pi} \frac{L^2}{(\hbar c)^2} (k_B T)^3 \Gamma(3) \zeta(3), \tag{10}$$

where the gamma function is defined as

$$\Gamma(s) = \int_0^\infty dt \ t^{s-1} e^{-t} \tag{11}$$

and the Riemann zeta function is defined as

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}.$$
 (12)

Hint: At some point in the calculation, use $\frac{1}{1-e^{-x}} = \sum_{n=0}^{\infty} e^{-nx}$. Why is this true?