

PHYS 427 - Discussion 02

Feb. 4, 2025

1. **2D ideal gas.** In lecture last week, you derived the entropy of a monatomic ideal gas in a 3D box. Steps from that derivation will show up again later in the the course, so we need to understand them well. In this problem, we repeat those arguments for a gas confined to a two-dimensional box¹ (also known as a rectangle).

Our box is a square rectangle with side length L . The gas particles are non-interacting (“ideal”), so at first we just consider one monatomic² particle in the box. From Schrödinger’s equation, one finds that the quantum states of the particle (eigenstates of the Hamiltonian) are uniquely labelled by two numbers $n_x = 1, 2, \dots, \infty$ and $n_y = 1, 2, \dots, \infty$. That is, if you tell me the values of n_x and n_y , I will know exactly what state the particle is in. The particle’s momentum in this state is $\vec{p} = \hbar \vec{k}$ where $\vec{k} = \frac{\pi n_x}{L} \hat{x} + \frac{\pi n_y}{L} \hat{y}$, so the particle’s energy is

$$\varepsilon_{n_x, n_y} = \frac{p^2}{2m} = \frac{\hbar^2 \pi^2}{2mL^2} (n_x^2 + n_y^2), \quad (1)$$

where m is the particle’s mass. This is all the quantum mechanics we will need.

- (a) Draw a graph with axes labelled k_x and k_y (the components of the vector \vec{k}). Draw the possible quantum states of a single gas particle as dots on this graph. Indicate the values of the horizontal and vertical spacings between the dots. How many states are there per unit \vec{k} -space area?
- (b) How many states are there with energy between ε and $\varepsilon + d\varepsilon$? *Hint: Use your graph from part (a). You might find yourself drawing two quarter-circles in \vec{k} -space with very similar radii. . .*
Optional challenge: justify the approximations you made³.
- (c) If you were to divide your answer to part (b) by $d\varepsilon$, you would get the *density of states per unit energy*, denoted $\mathcal{D}(\varepsilon)$. Briefly explain why it deserves this name. We will use this construction *very* often later in the course. What happens to $\mathcal{D}(\varepsilon)$ as $L \rightarrow \infty$? Does the limit make sense?

Now consider a gas of N particles. The quantum state of the gas is specified by $2N$ positive integers $n_{x1}, n_{y1}, n_{x2}, n_{y2}, \dots, n_{xN}, n_{yN}$. The total energy of the gas in such a state is

$$U_{\{n\}} = \frac{\hbar^2 \pi^2}{2mL^2} (n_{x1}^2 + n_{y1}^2 + n_{x2}^2 + n_{y2}^2 + \dots + n_{xN}^2 + n_{yN}^2). \quad (2)$$

The last factor is the square of the radius of a $2N$ -dimensional sphere. The volume of a D -dimensional sphere with radius R is

$$V_D(R) = \frac{\pi^{D/2}}{\Gamma(\frac{D}{2} + 1)} R^D. \quad (3)$$

For the purposes of this problem, the constants are not important and it is enough to write

$$V_D(R) = \frac{(CR)^D}{N!}, \quad (4)$$

for some constant C .

¹Studying a 2D gas is not only an academic exercise—refinements of this model can describe the mobile electrons trapped on an interface between two different materials. Google “2DEG” after class.

²Our particle isn’t necessarily an atom. It just doesn’t have any internal structure (or such structure must be negligible).

³The answer is valid when $\frac{\hbar}{L} \sqrt{\frac{\varepsilon}{m}} \ll d\varepsilon \ll \varepsilon$. It’s possible to find such a $d\varepsilon$ if the box is big enough, namely if $L \gg \hbar/\sqrt{m\varepsilon}$.

- (d) How many states does the gas have with energies between U and $U + dU$? *Hint: The particles are indistinguishable, so in your final answer you should include an additional factor of $1/N!$ by hand to compensate for overcounting.*
- (e) In part (e), you found that there are $\Omega \approx f(N)V^N U^N dU$ states accessible to a gas of N non-interacting particles in a 2D box when the energy is restricted to a tiny interval $(U, U + dU)$. Here $V = L^2$ is the “volume” (actually area) of the 2D box and $f(N)$ is some complicated function of N that is unimportant for this problem. Compute the temperature $1/T \equiv (\partial S/\partial U)_{V,N}$. If you remember the equipartition theorem from PHYS 213, comment on how it relates to your answer (if you don’t remember, don’t worry, we’ll study it later in the course). Compute the pressure $p \equiv T(\partial S/\partial V)_{U,N}$ of the gas and appreciate how familiar the result is.

2. **Fun with multiplicity functions.** Find the multiplicity Ω for the following closed systems.

- (a) One 3D harmonic oscillator with frequency ω and total energy $U = \hbar\omega\tilde{n}$, where \tilde{n} is a non-negative integer. The microstates of this system are uniquely specified by three integers, n_x , n_y , and n_z , each of which can take any integer value from zero to infinity. The energies of the microstates are given by $\varepsilon_{n_x, n_y, n_z} = \hbar\omega(n_x + n_y + n_z)$.
- (b) N non-interacting 3D harmonic oscillators sitting in a row, sharing a total energy $U = \hbar\omega\tilde{n}$. Each oscillator has the same frequency ω . Note that the oscillators are distinguishable (by their position in the row).
- (c) **(Optional)** One quantum dumbbell⁴ with moment of inertia I and total energy $U = \frac{\hbar^2}{2I}\tilde{\ell}(\tilde{\ell} + 1)$, where $\tilde{\ell}$ is a non-negative integer. A quantum dumbbell is a rod with two equal weights on the end. It can rotate about its center in two independent directions, but it cannot spin about the rod’s axis. From the Schrödinger equation, one finds that the microstates of a quantum dumbbell are uniquely specified by two integers, ℓ and m , where $\ell = 0, 1, 2, \dots, \infty$ and $m = -\ell, -\ell + 1, \dots, \ell - 1, \ell$. The energies of the microstates only depend on ℓ ; they are given by $\varepsilon_{\ell m} = \frac{\hbar^2}{2I}\ell(\ell + 1)$.
- (d) **(Optional)** Two quantum dumbbells sitting in a row, sharing a total energy $U = \frac{\hbar^2}{2I}\tilde{n}$, where \tilde{n} is a non-negative integer. Each dumbbell has the same moment of inertia I . Note that the dumbbells are distinguishable (by their position in the row). First, explicitly work out the multiplicities when $\tilde{n} = 0, 2, 4, 6, 8, 10$, then do it for arbitrary \tilde{n} . *Hint: Give up on this problem when you become convinced that it is very difficult (probably impossible) for arbitrary \tilde{n} ! We have learned: 1) a small adjustment of an easy counting problem can make it impossibly hard, which means 2) the microcanonical ensemble (i.e. the multiplicity-based approach for closed systems), which relies on counting large numbers of arrangements, is difficult to work with for all but the simplest models. That said, a collection of N quantum dumbbells can be studied with relative ease using the so-called canonical ensemble, which will be introduced soon in the lectures.*

3. **Einstein solid.** Consider the system defined in problem 2(b). We say that n quanta are shared among the oscillators. A *quantum* refers to a packet of energy equal to $\hbar\omega$. Assume $N, n \gg 1$, but do not assume any relationship between N and n .

- (a) Compute the entropy using Stirling’s approximation.
- (b) Compute the number of quanta per oscillator as a function of N and the temperature T . Observe the appearance of the *Bose-Einstein distribution function* $f(x) = 1/(e^x - 1)$ in your answer. This function is important and it will appear a lot in this course. What are the limits of your answer when T is big or small? (Compared to what? Always ask yourself this when someone claims a dimensionful quantity is big or small.)
- (c) Compute the heat capacity⁵ at constant volume, $C_V = (\partial U/\partial T)_{V,N}$. Show that $\lim_{T \rightarrow \infty} C_V = 3Nk_B$, which is the celebrated Dulong-Petit law. The Dulong-Petit law agrees well with experi-

⁴More precisely, a quantum mechanical linear rigid rotor. This is a model for the rotational states of a diatomic molecule.

⁵Quick review of heat capacity from PHYS 213. Let dQ be the amount of heat we need to add to the system to change the temperature by dT . The heat capacity is *defined* as the ratio $C \equiv dQ/dT$. If we perform the heating process while keeping the volume (and particle number) constant, then work done by the system on its surroundings is $dW = -pdV = 0$, so the 1st law of thermodynamics tells us the change in internal energy is $dU = dQ + dW = dQ$. That’s why $C_V = (\partial U/\partial T)_{V,N}$.

ments, but the Einstein solid fails to predict the experimentally observed C_V at low temperatures. We'll do better later in the course with the so-called Debye model.