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HW 10	Introduction to Statistical and Thermal Physics	November 27, 2023

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### Schroeder 7.55

Suppose that the concentration of infrared-absorbing gases in earth's atmosphere were to double, effectively creating a second "blanket" to warm the surface. Estimate the equilibrium surface temperature of the earth that would result from this catastrophe. (Hint: First show that the lower atmospheric blanket is warmer than the upper one by a factor of  $2^{1/4}$ . The surface is warmer than the lower blanket by a smaller factor.)

While the Debye results were obtained assuming a linear dispersion  $\omega = v|\mathbf{k}|$ , a more accurate description of a phonon in a cubic crystal is the frequency relation

$$\omega(\mathbf{k}) = \frac{v}{a} \sqrt{6 - 2\cos(k_x a) - 2\cos(k_y a) - 2\cos(k_z a)}$$

where *a* is the lattice spacing of the crystal.

- a) Sketch  $\omega(k_x, 0, 0)$  across the Broullin zone, and use a Taylor expansion to show the phonon velocity is v.
- b) Within the Debye approximation developed in lecture / Schroeder, what is the debye temperature  $T_D$  and the expected heat capacity as  $T \to 0$  and  $T \to \infty$ ?
- c) The heat capacity of the phonons takes the general form  $C_V = 3\sum_{\mathbf{k}} f(\mathbf{k})$ . What is f in terms of  $\hbar\omega(\mathbf{k})$  and  $k_BT$ ?
- d) When the system is placed on a cube of linear dimension L = aN, there are  $N^3$  terms in  $\sum_k$ . Using the result of the previous question, write a Python script to compute  $C_V(T, N)$  as such as sum, working in units where  $a = v = \hbar = k_B = 1$ .
- e) Use the script to plot  $C_V(T, N)/N^3$  for N = 40, 0 < T < 5. Annotate the graph with your prediction of  $T_D$  and the high low limits of  $C_V$ . Do they agree?
- f) Strictly speaking, Debye's  $T^3$  law only holds when  $L \to \infty$ . For finite L, for what  $T < T_L$  do you expect to see deviations? Can you see this effect in your result for the previous part?

Consider a gas of non=interacting spin 1 bosons, each subject to a Hamiltonian

$$\mathcal{H}_1(\mathbf{p}, s_z) = \frac{p^2}{2m} - \mu_0 s_z B$$

where  $\mu_0 = e\hbar/mc$  and  $s_z$  takes three possible values of (-1, 0, 1). (The orbital effect,  $\mathbf{p} \to \mathbf{p} - \epsilon \mathbf{A}$  has been ignored.) Denote n = N/V to be the total gas density.

- a) In a grand canonical ensemble of chemical potential  $\mu$ , what are the average occupation numbers  $\{\overline{n}_+(\mathbf{k}), \overline{n}_0(\mathbf{k}), \overline{n}_-(\mathbf{k})\}$  of one-particle states of wavenumber  $\mathbf{k}/\hbar$ ?
- b) Calculate the average total numbers  $\{N^+, N^0, N^-\}$  of bosons with the three possible values of  $s_z$ .
- c) Wrie down the expression for the magnetization  $M(T, \mu) = \mu_0(N_+ N_-)$ , and by expanding the result for small B find the zero field suscptibility  $\chi(T, \mu) = \partial M/\partial B|_{B=0}$
- d) For B = 0, find the high temperature expansion for  $z(\beta, n) = e^{\beta u}$ , correct to second order in n. Hence obtain the first correction from quantm statistics to  $\chi(T, n)$  at high temperatures.
- e) Find the temperature  $T_c(n, B = 0)$  of Bose-Einstein condensation. What happens to  $\chi(T, n)$  on approaching  $T_c(n)$  from the high=temperature side?
- f) What is the chemical potential  $\mu$  for  $T < T_c(n)$ , at a small but finite value of B? Which one-particle state has a macroscopic occupation number?
- g) Find the spontaneous magnetization

$$M(T,n) = \lim_{B\to 0} M(T,n,B)$$

Electromagnetic radiation at temperature  $T_i$  fills a cavity of volulme V. If the volume of the thermally insulated cavity is expanded quasistatically to a volume 8V, what is the final temperature  $T_f$ ? Neglect the heat capacity of the cavity walls.

- a) Write the integral for the number of bosons in the excited energy states  $N_e$  in a one-dimensional gas of non-interacting bosons with the usual dispersion  $\epsilon = \frac{p^2}{2m}$ .
- b) Argue that your result implies the absence of a BEC in 1D. Hint: Show that in this case the number equation can always be satisfied with "fugacity"  $e^{\beta\mu} < 1$ , and explain how this implies the absence of a BEC.

Consider bosons moving in a 3D harmonic potential, with single particle energies  $E = \frac{p^2}{2m} + \frac{kr^2}{2} = \hbar\omega(n_x + n_y + n_z + 3/2)$  with  $n_{x/y/z} = 0, 1, 2, ...$  The integers  $n_i$  then replace the momenta  $\mathbf{k}$  when summing over single-particle states. For simplicity, for the rest of this problem we will subtract off  $\frac{3}{2}\hbar\omega$  from E, so that the ground state has energy  $E_0 = 0$ . As we'll see, the nice thing about this version of the BEC problem is that it is straightforward to compute the thermodynamics via a summation, so we can skip the approximation inherent in replacing sums by integrals  $\sum_{E_n} \approx \int dE g(E)$ .

- a) Defining  $n = n_x + n_y + n_z$ , give a pictoral (or rigorous) argument that the degeneracy of level  $E_n = \hbar \omega n$  is g(n) = (n+2)(n+1)/2. It will be sufficient to show it is true just for e first couple n.
- b) Write a Python or Mathematica function to evaluate  $N(T,\mu) = \sum_{n=0}^{\infty} \frac{g(n)}{e^{\beta(E_n-\mu)}-1}$ . To keep things simple, henceforth we'll choose units in which  $\hbar\omega = k_B = 1$ .
  - Hint: To evaluate the sum, in practice you'll cutoff the series at some large enough  $n_*$ ,  $\sum_{n=0}^{\infty} \approx \sum_{n=0}^{n_*}$ . Include some logic to determine a "good enough" value of  $n_*(T, \mu)$ .
- c) Now write a Python or etc. function whihe evaluates  $\mu(T, N = 2000)$ . Plot the result for  $1 \le T \le 20$ . As a check of your result, compare with the classical expectation for  $T \to \infty$  (Midterm Problem 2) and the low-T expectation  $\mu \approx -k_BT/N$ .
  - Hint: I would do it like this.  $\mu$  is implicitly defined by the condition  $N(T,\mu)-2000=0$ . To find the  $\mu$  which satisfies this condition, you can apply sp.optimize.root\_scalar to the function  $f(\mu)=N(T,\mu)-2000$ . This function requires a "bracket", which means an interval  $\mu \in [a,b]$  in which the zero exists. a=-40 will be sufficient for this problem and for b use your knowledge of the low-T limit.
- d) Now that we know  $\mu(T, N = 2000)$ , use the Bose distribution to plot the occupation of the n = 0, 1, 2, 3 states (not including g(n)) for  $1 \le T \le 20$ . Do you find evidence for a BEC transition? At approximately what T?