Homework 1: Phys 7230 (Spring 2022)

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***Problem* 1:** Consider two (otherwise) closed systems A and B at respective temperatures T_A and T_B in thermal contact with each other, so that heat Q can flow between them.

Using the 2nd law of thermodynamics – total entropy S of a closed system increases under equilibration – show that heat Q flows from the hotter to the colder system as A and B come to thermal equilibrium.

Hint: $TdS \geq Q$.

Solution.

First, assume $T_A > T_B$. Because these two systems are closed, the total energy $U = U_A + U_B$ is constant. Thus $dU_B = -dU_A$. We need to prove that $dU_A = Q < 0$ (the hotter system loses heat Q to the colder one as both systems come to equilibrium).

Now, the total entropy is $S = S_A + S_B$. Since the volume V and number of particles N of each system are constant,

$$dS = \left(\frac{\partial S}{\partial U_A}\right)_{N_A,V_A} dU_A + \left(\frac{\partial S}{\partial U_B}\right) dU_B = \left(\frac{1}{T_A} - \frac{1}{T_B}\right) dU_A \geq 0. \tag{1.1}$$

The last inequality is the 2nd law of thermodynamics. Now, by assumption, $1/T_A - 1/T_B < 0$, so it must be the case that $dU_A < 0$ in order to make $dS \geq 0$. We are done. $\square$

***Problem* 2** (Spin-1/2 paramagnet)**:** Consider a magnet of N noninteracting spin-1/2 magnetic moments in an external magnetic field $\mathbf{B}$, with Hamiltonian given by Zeeman energy,

$$\mathcal{H} = -\sum_{i=1}^{N} \boldsymbol{\mu}_i \cdot \mathbf{B} = -\sum_{i=1}^{N} \mu_B B \sigma_i \equiv -\sum_{i=1}^{N} h\sigma_i \tag{2.1}$$

where μ_B is Bohr magneton (carrying units of magnetic moment) and $\sigma_i = \pm 1$ labels the two Zeeman spin states of nth spin.

(a) For fixed dimensionless magnetization $M = N_\uparrow - N_\downarrow$, (i) what is the multiplicity $\Omega(M, N)$? (ii) What is the corresponding probability $P(M, N)$? Check that $\sum_{M=-N}^{N} P(M, N) = 1$.

(b) Compute the multiplicity $\Omega(E)$ for this system at a total energy E and sketch/plot it as a function of full range of accessible energies.

Hint: Note that the magnetization M is proportional to the energy E.

(c) Derive the relation between temperature $T(E)$ and energy E and plot $T(E)$.

(d) Calculate the (i) magnetization $m(T, B) = \mu_B \sum_{i=1}^{N} \sigma_i$, (ii) obtain its asymptotic forms in the classical $\mu_B B/k_B T \ll 1$ and quantum $\mu_B B/k_B T \gg 1$ limits and (iii) plot it as a function of T at a couple of fixed values of B and as a function of B at a couple of fixed values of T.

Hint: (i) Notice that magnetization is proportional to the energy E, (ii) Eliminate E in favor of T, (iii) Use lowest order Stirling approximation throughout to simplify the factorials in your expression.

(e) Compute the linear magnetic susceptibility $\chi(T, B) = \partial m/\partial B\big|_{B\to 0}$, show that it exhibits Curie form $\chi_{\text{Curie}} = a/T$, extracting the coefficient a.

(f) Compute the heat capacity (specific heat), $C_v(T) = T(\partial S/\partial T)_{V,N}$, extract its low and high temperatures asymptotics, and sketch it, noting its limiting forms and the crossover temperature.

Solution.

(a) Given $M = N_\uparrow - N_\downarrow$ and $N = N_\uparrow + N_\downarrow$, we can write

$$N_\uparrow = \frac{N+M}{2} \qquad \text{and} \qquad N_\downarrow = \frac{N-M}{2}. \tag{2.2}$$

(i) The multiplicity of $\Omega(M, N)$ is just the combination of $N_\uparrow$ in N total paramagnets

$$\Omega(M, N) = \Omega(N_\uparrow, N_\downarrow) = \binom{N}{N_\uparrow} = \frac{N!}{N_\uparrow! N_\downarrow!} = \frac{N!}{\left(\frac{N+M}{2}\right)!\left(\frac{N-M}{2}\right)!}. \tag{2.3}$$

(ii) For N total paramagnets, each with 2 possible states, the sample size is 2^N. So the probability $P(M, N)$ is

$$P(M, N) = \frac{\Omega(M, N)}{2^N} = 2^{-N} \frac{N!}{\left(\frac{N+M}{2}\right)!\left(\frac{N-M}{2}\right)!}. \tag{2.4}$$

Now, we check for the normalization condition of the probability P. Using the binomial theorem:

$$(1+1)^N = 2^N = \sum_{N_\uparrow=0}^{N} \binom{N}{N_\uparrow} 1^{N_\uparrow} 1^{N-N_\uparrow} = \sum_{N_\uparrow=0}^{N} \Omega(N_\uparrow, N_\downarrow). \tag{2.5}$$

Converting the summation back to M, we get $-N \le M \le N$ for $0 \le N_\uparrow \le N$. Thus,

$$1 = 2^{-N} \sum_{M=-N}^{N} \binom{N}{N_\uparrow} = \sum_{M=-N}^{N} P(M,N). \tag{2.6}$$

(b) By definition, $E = -hM$ with $h = \mu_B B$. So from (2.3),

$$\Omega(E) = \frac{N!}{\left(\frac{N-E/\mu_B B}{2}\right)!\left(\frac{N+E/\mu_B B}{2}\right)!} \tag{2.7}$$

for $-\mu_B BN \le E \le \mu_B BN$. Figure 1(a) shows a plot of (2.7).

(c) By definition, the entropy is

$$\begin{aligned} S/k_B &= \ln\Omega \\ &\approx N\ln N - N - \left(\frac{N-E/\mu_B B}{2}\right)\ln\left(\frac{N-E/\mu_B B}{2}\right) + \frac{N-E/\mu_B B}{2} \\ &\quad - \left(\frac{N+E/\mu_B B}{2}\right)\ln\left(\frac{N+E/\mu_B B}{2}\right) + \frac{N+E/\mu_B B}{2} \\ &= N\ln N - \left(\frac{N-E/\mu_B B}{2}\right)\ln\left(\frac{N-E/\mu_B B}{2}\right) - \left(\frac{N+E/\mu_B B}{2}\right)\ln\left(\frac{N+E/\mu_B B}{2}\right) \end{aligned} \tag{2.8}$$

by Stirling approximation. Using Mathematica to differentiate this wrt E, we get

$$\frac{1}{k_B T} = \frac{\partial(S/k_B)}{\partial E} = \frac{1}{2\mu_B B}\ln\left(\frac{N-E/\mu_B B}{N+E/\mu_B B}\right). \tag{2.9}$$

Thus, the temperature is

$$T = \frac{2\mu_B B}{k_B \ln\left(\frac{N-E/\mu_B B}{N+E/\mu_B B}\right)}. \tag{2.10}$$

Figure 1(b) shows the normalized temperature $k_B T/\mu_B B$.

(d) First, inverting (2.10), we get

$$E = -N\mu_B B\frac{e^{2\mu_B B}k_B T - 1}{e^{2\mu_B B/k_B T}+1} = -N\mu_B B\tanh\left(\frac{\mu_B B}{k_B T}\right). \tag{2.11}$$

But the energy E can also be written in terms of m as $E = -mB$ since $m = \mu_B M$. (i) So, the magnetization is

$$m = \mu_B N\tanh\left(\frac{\mu_B B}{k_B T}\right). \tag{2.12}$$

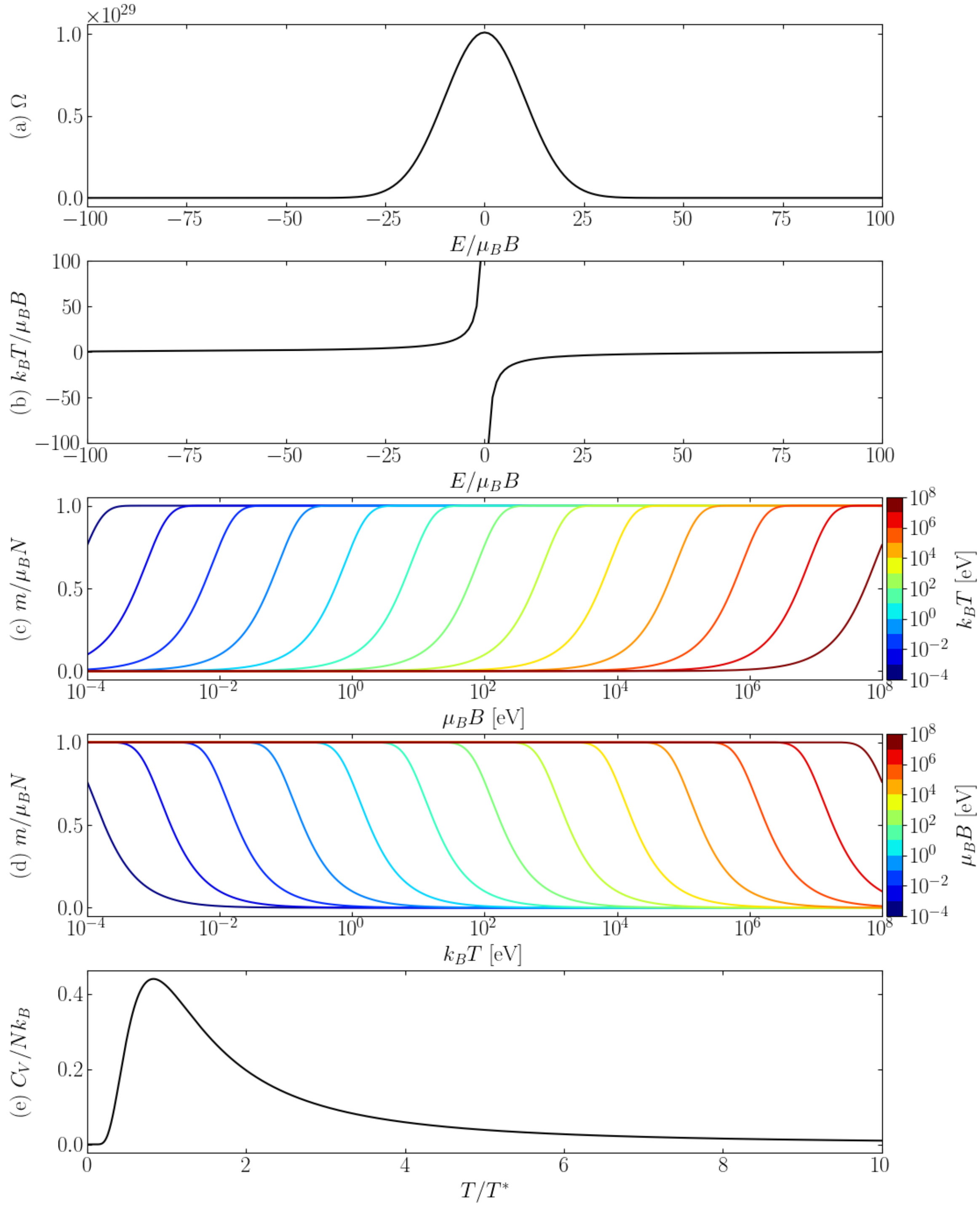

Figure 1: Sketches of quantities in problem 2.

(ii) For $\mu_B B/k_B T \ll 1$, $\tanh(x) \approx x$. Thus,

$$m\left(\frac{\mu_B B}{k_B T} \ll 1\right) = \frac{\mu_B^2 N B}{k_B T}. \tag{2.13}$$

For $\mu_B B/k_B T \gg 1$, $\tanh(x) \to 1$, so the magnetization is a constant

$$m\left(\frac{\mu_B B}{k_B T} \gg 1\right) = \mu_B N. \tag{2.14}$$

(iii) Figure 1(c-d) shows $m(T,B)/\mu_B N$ in various values.

(e) From (2.12), we can calculate

$$\chi = \lim_{B\to 0} \frac{\partial m}{\partial B} = \frac{\mu_B^2 N}{k_B T} \lim_{B\to 0} \operatorname{sech}^2\left(\frac{\mu_B B}{k_B T}\right) = \frac{\mu_B^2 N}{k_B T}. \tag{2.15}$$

So χ follows Curie's law with the constant $a = \mu_B^2 N/k_B$.

(f) By definition,

$$C_v = T\frac{\partial S}{\partial T} = \frac{\partial E}{\partial T} = N k_B \left(\frac{\mu_B B}{k_B T}\right)^2 \operatorname{sech}^2\left(\frac{\mu_B B}{k_B T}\right). \tag{2.16}$$

For $x = \mu_B B/k_B T \ll 1$ (high temperature), $\operatorname{sech}(x) \to 1$ and the heat capacity is

$$C_v\left(\frac{\mu_B B}{k_B T} \ll 1\right) \approx N k_B \left(\frac{\mu_B B}{k_B T}\right)^2. \tag{2.17}$$

For $x \gg 1$ (low temperature), $\operatorname{sech}^2(x)$ dominates and so $C_v \to 0$. Letting the crossover temperature be $T^* = \mu_B B/k_B$, we can rewrite the heat capacity in normalized form

$$\frac{C_v}{N k_B} = \left(\frac{T^*}{T}\right)^2 \operatorname{sech}^2\left(\frac{T^*}{T}\right). \tag{2.18}$$

Figure 1(e) shows a plot of (2.18). □

***Problem* 3** (Quamtum harmonic oscillators: Einstein solid)**:** Consider N decoupled 3D quantum harmonic oscillators as a model of atomic vibrations in a crystalline solid (Einstein phonons), described by the familiar quantum Hamiltonian

$$\hat{\mathcal{H}} = \sum_i^N \left[\frac{\hat{p}_i^2}{2m} + \frac{1}{2} m\omega_0^2 \hat{r}_i^2 - \frac{3}{2}\hbar\omega_0 \right] \tag{3.1}$$

where for convenience I defined $\hat{\mathcal{H}}$ with zero point energy subtracted off.

(a) Let's warm up on a single harmonic oscillator, computing its degeneracy $g(n) = \Omega(E = \hbar\omega_0 n)$ a fixed total energy $E \equiv \hbar\omega_0 n = \hbar\omega_0 \sum_{\alpha=1}^{d} n_\alpha$ (where $n_\alpha \in \mathbb{Z}$ are integer quantum numbers for $\alpha = x, y, \ldots$) for the cases of (i) 2D and (ii) 3D.

(b) Recalling the eigenvalues $E[\{n_\alpha\}] = \hbar\omega_0 \sum_{\alpha=1}^{3N} n_\alpha$ ($\alpha = x_1, y_1, z_1, x_2, y_2, z_2, \ldots$ ranging from 1 to $3N$) for the harmonic oscillator Hamiltonian, compute the multiplicity

$$\Omega(E) = \sum_{\{n_\alpha\}} \delta_{E,E[\{n_\alpha\}]} \tag{3.2}$$

taking $E = \hbar\omega_0 n$ ($n \in \mathbb{Z}$).

Hint: Think about how to distribute n total quanta of excitations among $3N$ 1D oscillators, and use the lowest Stirling formula approximation for $N \gg 1$ and $n \gg 1$.

(c) Compute the entropy $S(E)$ and the corresponding $T(E)$, thereby extracting energy $E(T)$ as a function of temperature T, exploring its classical $\hbar\omega_0/k_BT \ll 1$ and quantum $\hbar\omega_0/k_BT \gg 1$ limiting functional forms. Plot $E(T)$, noting limiting forms.

(d) Compute heat capacity $C_v = T(\partial S/\partial T)_{V,N} = \partial E/\partial T$ and explore its classical (high T) and quantum (low T) limits, showing the expected equipartition $C_v = N_{\text{dof}}k_B$ in the former and its breakdown in the latter limits. Plot $C_v(T)$, noting the crossover temperature.

(e) Consider a classical limit of the problem with small $\hbar\omega_0/k_BT$ such that $E[\{n_\alpha\}] = \sum_{\alpha=1}^{3N} \epsilon_\alpha$ and oscillator eigenvalues ϵ_α vary nearly continuously. Using this simplification compute

$$\Omega(E) = \Delta \prod_{\alpha=1}^{3N} \int \frac{d\epsilon_\alpha}{\hbar\omega_0} \delta(E - E[\{\epsilon_\alpha\}]) \tag{3.3}$$

as a multidimensional integral over ϵ_α.

Hint: It is helpful to use a result for a hypervolume of an N-dimensional space spanned by positive values of x_i coordinates, limited by a hyperplane $x_1 + x_2 + \ldots + x_N = R$,

$$V(R) = \int_{[\sum_{i=1}^N x_i] \le R} dx_1 dx_2 \ldots dx_N = \int_0^R dr S(r) = R^N/N!, \tag{3.4}$$

where $S(R) = R^{N-1}/(N-1)!$ is the corresponding hyper-area at radius R needed for computation of the multiplicity $\Omega(E)$ and above integral is a constrained one indicated by a prime.

Solution.

(a) For the 2D case, there are two groups (n_x, n_y). The problem can be understood in terms of a sequence of 0's (quanta) and 1's (partitions separting groups). For example, if

$n = 5$, 000100 is a possible sequence. Thus, there are $n+1$ objects in total to shuffle and the (i) degeneracy is

$$g_{2D}(n) = \binom{n+1}{n} = n+1. \tag{3.5}$$

(ii) For the 3D case, there needs to be 2 partitions to separate the 0's into three groups (n_x, n_y, n_z). So the degeneracy is

$$g_{3D}(n) = \binom{n+2}{n} = \frac{(n+1)(n+2)}{2}. \tag{3.6}$$

(b) Generalizing the previous results into the $3N$-dimensional case, there needs to be $3N-1$ partitions to separate the 0's into $3N$ groups. The multiplicity is thus

$$\Omega = \binom{n+3N-1}{n} = \frac{(n+3N-1)!}{n!(3N-1)!} \approx \frac{(n+3N)!}{n!(3N)!} \tag{3.7}$$

where we have assumed $n, N \gg 1$. Using the lowest order Stirling approximation ($N! \approx N^N$), we can simplify this result into

$$\Omega(E) \approx \left(1 + \frac{3N\hbar\omega_0}{E}\right)^{E/\hbar\omega_0} \left(1 + \frac{E}{3N\hbar\omega_0}\right)^{3N} \tag{3.8}$$

where we have also written $n = E/\hbar\omega_0$.

(c) By definition, the entropy is

$$\begin{aligned} S/k_B &= \ln\Omega \\ &= \frac{E}{\hbar\omega_0}\ln\left(1 + \frac{3N\hbar\omega_0}{E}\right) + 3N\ln\left(1 + \frac{E}{3N\hbar\omega_0}\right) \\ &= 3N\left[\epsilon\ln\left(1 + \frac{1}{\epsilon}\right) + \ln(1+\epsilon)\right] \end{aligned} \tag{3.9}$$

where $\epsilon = E/3N\hbar\omega_0$. Differentiate wrt E,

$$\frac{3N\hbar\omega_0}{k_B T} = \frac{\partial(S/k_B)}{\partial\epsilon} = 3N\ln\left(1 + \frac{1}{\epsilon}\right) \tag{3.10}$$

Thus, the temperature is

$$T(E) = \frac{\hbar\omega_0}{k_B\ln\left(1 + 3N\hbar\omega_0/E\right)} \tag{3.11}$$

Inverting this result, we get

$$E(T) = \frac{3N\hbar\omega_0}{e^{\hbar\omega_0/k_B T} - 1} \tag{3.12}$$

For the classical limit ($x = \hbar\omega_0/k_B T \ll 1$), $e^x - 1 \approx x$ and $E(T) = 3Nk_B T$. For the quantum limit ($x \gg 1$), $e^x \to \infty$ and $E \sim e^{-x} \to 0$. The crossover temperature is

$T^* = \hbar\omega_0/k_B$. Figure 2 shows that E grows linearly at high temperature and decreases to 0 in the quantum limit, as expected.

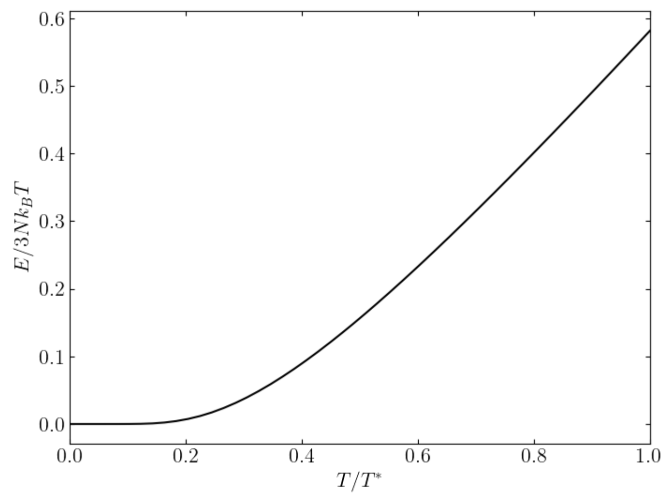

Figure 2: $E(T)$ of N decoupled 3D quantum harmonic oscillators.

(d) By definition,

$$C_v = \frac{\partial E}{\partial T} = 3Nk_B\left(\frac{T^*}{T}\right)^2 \frac{e^{T^*/T}}{(e^{T^*/T}-1)^2} \tag{3.13}$$

For the quantum limit, C_v grows as $(T^*/T)^2 e^{-T^*/T} \sim 0$ because of the exponential term. At large T (classical limit), we can set $x = T^*/T$ and write C_v as

$$C_v = 3Nk_B x^2 \frac{e^x}{(e^x-1)^2} \approx 3Nk_B x^2 \frac{1+x}{x^2} = 3Nk_B \tag{3.14}$$

as $x \to 0$. This is the expected equipartition where $N_{\text{dof}} = 3N$. Figure 3 shows that the formal break occurs at $T = T^*$ as expected. Also, C_v is asymptotically constant as $T \to \infty$ as predicted in (3.14) and decreases to 0 as $T \to 0$.

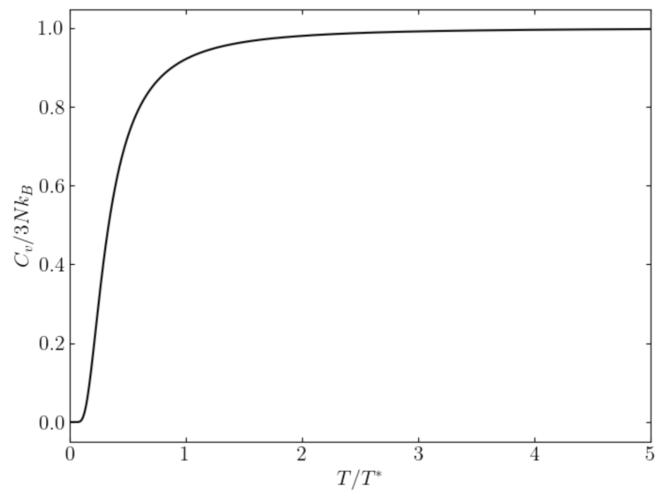

Figure 3: $C_v(T)$ of N decoupled 3D quantum harmonic oscillators.

(e) First, we can isolate the integration

$$\Omega(E) = \frac{\Delta}{(\hbar\omega_0)^{3N}} \prod_{\alpha=1}^{3N} \int d\epsilon_\alpha \delta\big(E - E[\{\epsilon_\alpha\}]\big) = \frac{\Delta}{(\hbar\omega_0)^{3N}} I_{3N} \tag{3.15}$$

I_{3N} is just the $(3N-1)$-dimensiona hyper-area restricted by the constraint $E = \sum_{\beta=1}^{3N} \epsilon_\beta$ when integrating over a $3N$-dimensional space $\mathbb{R}_+^{3N}$ where $R_+ = [0, \infty)$. Thus,

$$\Omega(E) = \frac{\Delta}{(\hbar\omega_0)^{3N}} S_{3N}(E) = \frac{1}{(3N-1)!} \frac{\Delta}{E} \left(\frac{E}{\hbar\omega_0}\right)^{3N}. \tag{3.16}$$

But $(3N-1)! \approx (3N)! \approx (3N)^{3N}$ for $N \gg 1$. So

$$\Omega(E) \approx \frac{\Delta}{E} \left(\frac{E}{3N\hbar\omega_0}\right)^{3N}. \tag{3.17}$$

□

***Problem* 4** (Boltzmann gas)**:** Consider N identical noninteracting particles in a 3D box of linear size L, described by a Hamiltonian

$$\mathcal{H}(\{\mathbf{p}_i\}) = \sum_i^N \frac{p_i^2}{2m} \tag{4.1}$$

(a) By integrating over $6N$ dimensional phase space, compute the multiplicity (number of microstates) in a shell of width Δ around energy E,

$$\Omega(E) = \frac{\Delta}{N!}\prod_i^N \left[\int \frac{d\mathbf{r}_i d\mathbf{p}_i}{(2\pi\hbar)^3}\right]\delta(E - \mathcal{H}(\{\mathbf{p}_i\})] \tag{4.2}$$

where $1/N!$ is the Gibbs "fudge" factor to crudely (we will see later why this fix fails at low temperatures; also see below) account for the identity of these classical particles, and we used the fact that 1 state corresponds to phase space area $dxdp = 2\pi\hbar$ to normalize the integration measure.

Hint: Use the expression for a surface area of a d-dimensional unit hypersphere, $S_d = 2\pi^{d/2}/\Gamma(d/2)$ (with $S_2 = 2\pi, S_3 = 4\pi, \ldots$).

(b) Compute the corresponding (i) entropy $S(E, V, N) = k_B \ln \Omega$, and (ii) find the temperature T_c at which the entropy becomes negative, i.e., unphysical.

(c) Using the expression for $S(E, V, N)$ found above, calculate the pressure $P(V, N) = T(\partial S/\partial V)_{E,N}$ for the Boltzmann gas, and show that it leads to the familiar ideal gas law, $PV = Nk_BT$.

(d) Compute the corresponding chemical potential $\mu = -T(\partial S/\partial N)_{E,V}$, expressing in terms of the thermal deBroglie wavelength $\lambda_{dB}(T) = h/\sqrt{2\pi m k_B T}$, T and density n.

Solution.

(a) First, we can simplify

$$\begin{aligned}
\Omega(E) &= \frac{\Delta}{E}\frac{V^N}{N!}\frac{1}{h^{3N}}\prod_i^N \int d\mathbf{p}_i \delta\left(1 - \sum_j^N \frac{p_j^2}{2mE}\right) \\
&= \frac{\Delta}{E}\frac{V^N}{N!}\left(\frac{2mE}{h^2}\right)^{3N/2}\prod_i^N \int d\overline{\mathbf{p}}_i \delta\left(1 - \sum_j^N \overline{p}_j^2\right) \qquad (\overline{p}_j^2 = p_j^2/2mE)
\end{aligned}$$

The integration is now just the surface area of a $3N$-dimensional unit hypersphere, since it is constrained to the surface $1 = \sum_j^N \overline{p}_j^2$. So we can write

$$\begin{aligned}
\Omega(E) &= \frac{\Delta}{E}\frac{V^N}{N!}\left(\frac{2mE}{h^2}\right)^{3N/2}\frac{2\pi^{3N/2}}{\Gamma(3N/2)} \\
&\approx \frac{\Delta}{E}\frac{V^N}{\sqrt{2\pi N}e^{-N}N^N}\left(\frac{2\pi mE}{h^2}\right)^{3N/2}\frac{2}{\sqrt{3\pi N}e^{-3N/2}(3N/2)^{3N/2}} \\
&= \frac{2\Delta}{\sqrt{6}\pi NE}e^{5N/2}\frac{V^N}{N^N}\left(\frac{4\pi mE}{3Nh^2}\right)^{3N/2}
\end{aligned} \tag{4.3}$$

where we have written $\Gamma(3N/2) = (3N/2-1)! \approx (3N/2)!$ and used Stirling approximation on the factorials.

(b) By definition, the (i) entropy is

$$S/k_B = \ln \Omega = \ln\left(\frac{2\Delta}{\sqrt{6}\pi N E}\right) + N\left\{\frac{5}{2} + \ln\left[\frac{V}{N}\left(\frac{4\pi m E}{3Nh^2}\right)^{3/2}\right]\right\} \tag{4.4}$$

the first term is small compared to N and we retrieve the Sackur-Tetrode equation in the last two terms. Also, the temperature (calculated with Mathematica) is

$$\frac{1}{k_B T} = \frac{\partial(S/k_B)}{\partial E} = \frac{3}{2}\frac{N}{E} \Rightarrow \frac{E}{N} = \frac{3}{2}k_B T \tag{4.5}$$

Now, from (4.4), $S < 0$ only when

$$\frac{V}{N}\left(\frac{4\pi m E}{3Nh^2}\right)^{3/2} = \frac{V}{N}\left(\frac{2\pi m k_B T}{h^2}\right)^{3/2} < e^{-5/2} \tag{4.6}$$

(ii) Solving this inequality, we get

$$T_c < \frac{h^2}{2\pi m k_B}\left(\frac{N}{V}\right)^{2/3} e^{-5/3} \tag{4.7}$$

(c) Differentiating S wrt V (in Mathematica), we get

$$\frac{P}{T} = \frac{\partial S}{\partial V} = \frac{N k_B}{V} \Rightarrow PV = N k_B T \tag{4.8}$$

This is the ideal gas law.

(d) Differentiating S wrt N (in Mathematica), we get

$$\mu = -k_B T \ln\left[\frac{8}{3\sqrt{3}}\frac{V}{N}\left(\frac{\pi m E}{h^2 N}\right)^{3/2}\right] = -k_B T \ln\left[\frac{1}{n}\left(\frac{2\pi m k_B T}{h^2}\right)^{3/2}\right] = k_B T \ln\left(n \lambda_{dB}^3\right) \tag{4.9}$$

$\square$

***Problem* 5** (Classical harmonic oscillators: Einstein solid)**:** Consider N decouped 3D classical harmonic oscillators, described by the familiar Hamiltonian

$$\mathcal{H} = \sum_i^N \left[\frac{p_i^2}{2m} + \frac{1}{2} m\omega_0^2 r_i^2 \right] \tag{5.1}$$

as the classical version of the problem above, with $\mathbf{r}_i, \mathbf{p}_i$ the classical phase space coordinates. Let's repeat the analysis utilizing and generalizing the analysis for the Boltzmann gas, above.

(a) By integrating over $6N$ dimensional phase space, compute the multiplicity (number of microstates) in a shell of width Δ around energy E,

$$\Omega(E, N) = \Delta \prod_i^N \left[\int \frac{d\mathbf{r}_i d\mathbf{p}_i}{(2\pi\hbar)^3} \right] \delta[E - \mathcal{H}(\{\mathbf{p}_i\})], \tag{5.2}$$

where there is no $1/N!$ Gibbs "fudge" factor. Why?

(b) Compare your classical result with the high T classical limit ($\hbar\omega_0/k_B T$ is the relevant dimensionless parameter) of the quantum treatment of the system in problem 3(c,d,e) above.

(c) What is the relation of this classical analysis to the classical limit analysis in problem 3e?

Solution.

(a)

$$\begin{aligned}
\Omega(E, N) &= \Delta \prod_i^N \left[\int \frac{d^3 r_i d^3 p_i}{(2\pi\hbar)^3} \right] \delta(E - \mathcal{H}(\{\mathbf{p}_i\})) \\
&= \frac{\Delta}{E} \frac{1}{h^{3N}} \prod_i \int d^3 r_i d^3 p_i \delta \left[1 - \sum_j^N \left(\frac{p_j^2}{2mE} + \frac{m\omega_0^2 r_j^2}{2E} \right) \right] \\
&= \frac{\Delta}{E} \left(\frac{4E^2}{(2\pi\hbar\omega_0)^2} \right)^{3N/2} \prod_i^N \int d^3 \overline{r}_i d^3 \overline{p}_i \delta \left(1 - \sum_j^N \overline{p}_j^2 + \overline{r}_j^2 \right) \\
&\qquad (\overline{r}_j^2 = m\omega_0^2 r_j^2/2E, \overline{p}_j^2 = p_j^2/2mE) \\
&= \frac{\Delta}{E} \left(\frac{4E^2}{(2\pi\hbar\omega_0)^2} \right)^{3N/2} \frac{2\pi^{3N}}{\Gamma(3N)} \\
&\approx \frac{\Delta}{E} \left(\frac{4E^2}{(2\pi\hbar\omega_0)^2} \right)^{3N/2} \frac{2\pi^{3N}}{(3N)^{3N}} \\
&= \frac{\Delta}{E} \left(\frac{E}{3N\hbar\omega_0} \right)^{3N}
\end{aligned} \tag{5.3}$$

There is no fudge factor because the particles are distinguishable because of the position in the Hamiltonian.

(b) From the previous results, the entropy is

$$S = 3Nk_B \ln \left(\frac{E}{3N\hbar\omega_0} \right) \tag{5.4}$$

Then

$$\frac{1}{T} = \frac{\partial S}{\partial E} = \frac{3Nk_B}{E} \tag{5.5}$$

and the temperature is

$$T = \frac{E}{3Nk_B} \tag{5.6}$$

and the energy in terms of temperature is

$$E = 3Nk_B T \tag{5.7}$$

This agrees with the classical limit of problem 3(c). Similarly,

$$C_v = \frac{\partial E}{\partial T} = 3Nk_B \tag{5.8}$$

which is the asymptotic limit that we've seen in (3.14). The multiplicity in Problem 3(e) is the exact same result that we derived in part (a).

(c) We're integrating over the entire 6D phase space here, while in problem 3(e), we integrate over the energies of each macrostate. □