[15] 1. *Definitions and terms* — Define each of the following terms or concepts, as used in this course, in one or two sentences written in your test booklet. Then explain the significance or importance, in thermal physics, as well, in one or two sentences. Provide equations if directly relevant.

a) ensemble average over accessible states of a thermal system

An ensemble average is a weighted average of some state property X(s), with weight equal to the probability P(s) of finding the system in that state. The weighted average is taken over all states of the system (all members of the ensemble).

$$\langle X \rangle = \sum_s X(s)P(s)$$

For a closed system this simplifies: only accessible states (i.e., compatible with all specifications for a given system, including energy, external fields, number of particles, etc.) have non-zero P(s), and for those, P(s) is the same:

$$\langle X \rangle = \sum_{\substack{\text{only accessible} \\ \text{states } s}} X(s)\frac{1}{g}$$

where g is the multiplicity.

The significance is that this represents the value of X one would find from repeated measurements.

b) partition function of a thermal system

The partition function is the sum of all Boltzmann factors $\exp(-\varepsilon_s/\tau)$ *of all states s of the system, i.e.:*

$$Z(\tau) = \sum_s \exp(-\varepsilon_s/\tau)$$ *[note that a given energy* ε_s *may appear in multiple terms, if degenerate]*

Its immediate significance is that it normalizes the Boltzmann factor of any state to give the probability P(s) of that state occurring, in thermal equilibrium with a reservoir at temperature τ. *(Beyond that, because it contains the energy of every single state of the system, it can be used to derive many results like the thermal average energy U of the system.)*

c) entropy of a thermal system

In thermal physics we define the entropy σ *to be the natural logarithm of the multiplicity g, where the multiplicity gives the number of accessible microstates of a system.*

It's significant in thermal physics for several reasons (only one good one needed): maximizing this function corresponds to finding the equilibrium state of two systems in contact (most probable configuration); it also gives us our microscopic definition of temperature, $\frac{1}{\tau} = \left(\frac{\partial \sigma}{\partial U}\right)_N$ *; it also gives microscopic physical meaning to the thermodynamic entropy* $S = k_B\sigma$, *which originally was a deduced abstract function in thermodynamics, from which temperature and other thermodynamic variables could be constructed.*

[20] 2. *Multiple Choice* — In each part below, select the *best* single choice, and mark your answer on the special sheet provided for multiple choice answers. No explanations are required; part-marks may be awarded for partially correct answers. All parts (i)–(iv) below have equal marking weight.

i) A particle is confined in a 3D infinite-potential quantum well. All sides have length L, the box is a cube. All together, how many states are degenerate in energy with the state $\psi_{1,1,6}$? (Count $\psi_{1,1,6}$ in your answer.) (from study problems)

need consider only $(n_x^2+n_y^2+n_z^2)$

0 A. 1

2 B. 3 6: $1^2+1^2+6^2=38$ (and 3 ways to place the 6-digit)

3 C. 6 5: $5^2+3^2+2^2=38$ (and $3\times2=6$ ways)

5 D. 9 4: no solution $\Rightarrow 3+6=9$ degenerate states

0 ~~E. 11~~

0 F. it is not possible to find the multiplicity from the information provided

ii) For a collection of hydrogen atoms in equilibrium at the temperature of the sun's photosphere (~5770 K), what fraction of atoms are in a 2s orbital?

0 A. 0.5 $P(s) = \frac{\exp\{-\varepsilon_s/\tau\}}{Z(\tau)}$ $E_n = -\frac{13.6\text{eV}}{n^2}$ $E_1 = -13.6\text{eV}$

1 B. 4×10^{-5} $E_2 = -3.4\text{eV}$

2 C. 4×10^{-7} $P(1) \gg P(2) \gg P(3) \Rightarrow Z(\tau) \simeq \exp(-E_1/\tau)$ $E_3 = -1.5\text{eV}$

4 D. 2×10^{-10} $P(2s) \simeq \frac{\exp(-(-3.4\text{eV})/\tau)}{\exp(-(-13.6\text{eV})/\tau)} = \exp(-10.2\text{eV}/\tau)$

2 E. 2×10^{-14}

5 F. none of the above is correct within a factor of 2 $5770\text{K} \Leftrightarrow 0.497$

$P(2s) \simeq 1.2\times10^{-9}$

For the next two questions, consider a particular system $\mathscr{S}$ made up of 8 particles, each with magnetic moment m, in a uniform magnetic field $\vec{B}$. Each particle can have its magnetic moment aligned with the magnetic field, pointing either the same direction as the magnetic field (↑) or in the direction opposite to the magnetic field (↓). Particles do not interact with each other, but can interact with the magnetic field. A given state of the system can be represented as in lecture, e.g., ↓↓↑↓↑↓↓↓

iii) How many energy macrostates are there of the system $\mathscr{S}$?

1 A. 8 N+1 macrostates for a binary system

5 B. 9

2 C. 17

1 D. 256 $= (2)^8$ # microstates total

0 E. 257

0 F. none of the above is correct

iv) Consider the system $\mathscr{S}$ to be *closed*, and that it has energy $U = +2mB$. Of the examples illustrated below, which are *accessible states* of this closed system?

2 A. ↓↑↑↓↑↓↓↓ ✓ $U \equiv -(2s)mB \Rightarrow 2s = -2 \Rightarrow 5\downarrow, 3\uparrow$

2 B. ↓↑↓↑↓↓↑↓ ✓

1 C. ↑↑↓↑↑↑↓↓ $2s = +2$

1 D. ↓↑↓↑↑↑↓↓ $2s = +2$

0 E. ↑↓↑↑↓↑↑↑ $2s = +4$

5 F. exactly two examples above are accessible states

[20] 3. *Equilibrium* — Consider two closed systems $\mathscr{S}_1$ and $\mathscr{S}_2$, which have particle numbers N_1 and N_2 respectively. These two are brought into thermal contact with other, so they can exchange energy with each other but nothing else. The combined system $\mathscr{S}$ is still closed.

[6] a) If the original multiplicity function for $\mathscr{S}_1$ when it has energy U_1 is $g_1(N_1, U_1)$ and similarly for $\mathscr{S}_2$, with $g_2(N_2, U_2)$, what is $g(N, U)$ of the combined system before thermal contact? What is it after thermal contact?

before: $g(N,U) = g_1(N_1,U_1)\,g_2(N_2,U_2)$ $U_1+U_2=U$ (non contact)

after: $g(N,U) = \sum_{U_1} g_1(N_1,U_1)\,g_2(N_2,U-U_1)$ (with contact)

includes every new macrostate of S_1 & S_2 once they can rearrange energies.

[10] b) Derive the condition shown in class for the most probable configuration, and show how this leads to conditions for the entropy and the temperature of each of $\mathscr{S}_1$ and $\mathscr{S}_2$ at equilibrium.

see lecture notes or text pp. 39-40

[4] c) Prove that the entropy σ of the combined system, made up of $\mathscr{S}_1$ and $\mathscr{S}_2$ in thermal contact, must be at least as large as $\sigma_1+\sigma_2$ of $\mathscr{S}_1$ and $\mathscr{S}_2$ before thermal contact.

$$\sigma_{final} \equiv \log\left(\sum_{U_1} g_1 g_2\right) \geq \log(g_1 g_2)_0 \equiv \sigma_{initial}$$

new options, more microstates, become possible
one energy may be shared, but original sharing
is one option still

[20] 4. *System with three states of spin* — Consider a system $\mathscr{S}$ made up of N particles with magnetic moment of magnitude m, in the case that each magnetic moment must now be in one of *three* states: up ($\uparrow$), down ($\downarrow$), and neither ($\rightarrow$).

[5] a) How many *microstates* are there of this system with N particles? The system is now put in a magnetic field $\vec{B}$ which points in the same direction as $\uparrow$. How does the energy of each particle depend on its state? How many *macrostates* of different energy are there for this system?

o $(\uparrow + \downarrow + \rightarrow)^N$ generating function $\Rightarrow 3^N$ total microstates
o each particle $U_{particle} = -\vec{m}\cdot\vec{B}$ mB for spin $\downarrow$, $-mB$ for $\uparrow$
o System energy $U_{system} = -(\text{spin excess})\, mB$
Since we have $\rightarrow$ we can have every integer value of spin-excess from $-N$ to $+N$ including 0, thus $\boxed{2N+1}$

[5] b) Consider a closed system with $N = 4$, and $U = -mB$. What is the multiplicity of this macrostate? Write out all accessible microstates.

$U = -mB$ means one net spin against B field direction

How? case I : exactly 1 spin down $\Rightarrow$ 3 spins "$\rightarrow$" $\binom{4}{1} = 4$ way

case II : exactly 2 spins down $\Rightarrow$ 1 "$\uparrow$", 1 "$\rightarrow$" $\binom{4}{1}\binom{3}{1} = 12$ way
"$\uparrow$" "$\rightarrow$"

3 or 4 spins down impossible

$\Rightarrow$ 16 accessible states

(4)

case I: $\uparrow\rightarrow\rightarrow\rightarrow$, $\rightarrow\uparrow\rightarrow\rightarrow$, $\rightarrow\rightarrow\uparrow\rightarrow$, $\rightarrow\rightarrow\rightarrow\uparrow$

(4) 4 ways to place "$\rightarrow$"

case II:	$\rightarrow\times\times\times$	$\times\rightarrow\times\times$	$\times\times\rightarrow\times$	$\times\times\times\rightarrow$
$\circ\,\circ\,\uparrow$	$\rightarrow\downarrow\downarrow\uparrow$	$\downarrow\rightarrow\downarrow\uparrow$	$\downarrow\downarrow\rightarrow\uparrow$	$\downarrow\downarrow\uparrow\rightarrow$
$\circ\,\uparrow\,\circ$	$\rightarrow\downarrow\uparrow\downarrow$	$\downarrow\rightarrow\uparrow\downarrow$	$\downarrow\uparrow\rightarrow\downarrow$	$\downarrow\uparrow\downarrow\rightarrow$
$\uparrow\,\circ\,\circ$	$\rightarrow\uparrow\downarrow\downarrow$	$\uparrow\rightarrow\downarrow\downarrow$	$\uparrow\downarrow\rightarrow\downarrow$	$\uparrow\downarrow\downarrow\rightarrow$

then 3 spots left for $\uparrow$

(12)

[5] c) This system $\mathscr{S}$ is now put into thermal contact with a reservoir $\mathscr{R}$ at temperature τ. What is the ratio $P(s_2)/P(s_1)$ of probability of finding the system in the single microstate $s_2 = \uparrow\uparrow\uparrow\rightarrow$ versus the probability of finding the system in the microstate $s_1 = \uparrow\uparrow\uparrow\uparrow$ (no derivation required)?

Individual states – multiplicity does not enter in, here.

$E_2 = -3mB$

$E_1 = -4mB$

$$\frac{P(s_2)}{P(s_1)} = \frac{e^{-E_2/\tau}}{e^{-E_1/\tau}} = e^{(E_1-E_2)/\tau} = e^{-mB/\tau}$$

[5] d) Now consider a magnetic moment and B-field such that mB = 10 meV. For a fundamental temperature τ = 1 meV (11.6 K), what is the ratio $P(U_2)/P(U_1)$ of probability of finding the system in the macrostate of energy $U_2 = -3mB$ versus the probability of finding the system in the macrostate of energy $U_1 = -4mB$? Repeat for a fundamental temperature τ = 100 meV (1160 K).

macrostates – now multiplicity matters

$\uparrow\uparrow\uparrow\uparrow$ $\quad g(U_1) = 1$

$\uparrow\uparrow\uparrow\rightarrow$; $\uparrow\uparrow\rightarrow\uparrow$; $\uparrow\rightarrow\uparrow\uparrow$; $\rightarrow\uparrow\uparrow\uparrow$ $\quad g(U_2) = 4$

$$\frac{P(U_2)}{P(U_1)} = \frac{g(U_2)\,e^{-U_2/\tau}}{g(U_1)\,e^{-U_1/\tau}} = \frac{4\,e^{-(-3mB/\tau)}}{1\,e^{-(-4mB/\tau)}} = 4e^{-mB/\tau}$$

$\underline{\tau = 1\text{meV}}$ $\quad \dfrac{P(U_2)}{P(U_1)} = 4e^{-10\text{meV}/1\text{meV}} = 4e^{-10} = 1.8\times10^{-4}$

$\underline{\tau = 100\text{ meV}}$ $\quad \dfrac{P(U_2)}{P(U_1)} = 4e^{-10\text{meV}/100\text{meV}} = 4e^{-0.1} = 3.62$

Because of multiplicity (degeneracy), at high relative temperature system is more likely to be found in one of the higher-energy states

(END OF TEST)

[75] TOTAL MARKS