[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 give the significance or importance as well, and provide equations if immediately relevant.

a)   fundamental assumption of thermal physics

The fundamental assumption of thermal physics is: "A <u>closed</u> system is <u>equally likely</u> to be in any of the microstates <u>accessible</u> to it". Its importance: by this assumption, and with the number g of accessible states we can calculate the probability of finding the system in a particular microstate: i.e., $1/g$. It's also important because it says basically that thermal physics comes down to the counting of states.

b)   accessible state of a system

An accessible state of a system is: "A system microstate compatible with the state specification of energy, number of particles, etc. – a microstate compatible with the system macrostate." This concept is important for its relation to the fundamental assumption of thermal physics; knowing which states are accessible tells us how to count states and find the statistics.

c)   binary model system

A binary model system is an example system comprised of particles which have only two potential states. An example is the system of up/down spins. This is significant because it's one of the simplest physical models that show the main characteristics of thermal physics: accessible states, total energy, multiplicity function, etc.

 [I did not require definitions/explanations this thorough, for full marks. If you did not pay attention to significance/importance, 2 marks were lost immediately]

[20]   2.   Multiple Choice

i)
A   0
B   0
C   0
D   0
E   0
F   5

ii)
A   2   (first two are OK, last is nonsense but looks like a wavefunction)
B   3   (wrong sign for trapped central potential)
C   0
D   5
E   0
F   0

iii)

A   5

B   1   (if you know two, you find three, always, from the ground-state energy)

C   2   (true, first level comes from the longest dimension)

D   0

E   1   (has a bit of the right sense, without being quite true)

F   0

iv)

A   0   (always the orbital angular moment)

B   2   (true but not best answer)

C   2   (true but not best answer)

D   2   (true but not best answer)

E   3   (almost, but not best answer)

F   5

3 a) Each state of each spin can be represented ↑ or ↓

The system of spins has microstates, each can be represented as

eg. ↑↑↓↑···↓↑   where $N =$ # of spins in system

all such microstates can be generated by a choice for <u>each</u> spin, which choice we write $(\uparrow + \downarrow)_i$ for ith spin

and then for the system:

$$(\uparrow + \downarrow)_1 \, (\uparrow + \downarrow)_2 \, (\uparrow + \downarrow)_3 \cdots (\uparrow + \downarrow)_N$$ ie a choice between 2

states for each of N spins, or 2^N microstates possible.

This choice for one of two possibilities in each factor is the same choice made in the binomial $(x + y)^N$,

for which $(x+y)^N = \sum\limits_{t=0}^{N} \dfrac{N!}{(N-t)! \, t!} \, x^{N-t} y^{t}$

<u>ways to get "t" y's</u>

we write using $t \to \frac{N}{2} - s$

$$(x+y)^N = \sum\limits_{s=-N/2}^{N/2} \dfrac{N!}{(\frac{N}{2}+s)!(\frac{N}{2}-s)!} \, x^{\frac{N}{2}+s} y^{\frac{N}{2}-s}$$

and now we identify $x \Leftrightarrow \uparrow$ & $y \Leftrightarrow \downarrow$

$$(\uparrow + \downarrow)^N = \sum\limits_{s} \dfrac{N!}{(\frac{N}{2}+s)!(\frac{N}{2}-s)!} \, \uparrow^{\frac{N}{2}+s} \downarrow^{\frac{N}{2}-s}$$

from which we see the multiplicity function

$$g(N, s) = \dfrac{N!}{(\frac{N}{2}+s)!(\frac{N}{2}-s)!} = \dfrac{N!}{N_\uparrow! \, N_\downarrow!}$$

$N_\uparrow = \frac{N}{2} - s$
$N_\downarrow = \frac{N}{2} + s$

and the uncancelled spins are the spin excess $N_\uparrow - N_\downarrow = 2s$

b) for N very large we use Stirling's approximation

$$N! \simeq (2\pi N)^{1/2} N^N \exp\left\{ -N + \frac{1}{12N} + \cdots \right\}$$ and keep only 1st term

with this, $\log N! \simeq \frac{1}{2} \log 2\pi + (N+\frac{1}{2}) \log N - N$ ①②

Likewise $\log N_\uparrow! \simeq \frac{1}{2} \log 2\pi + (N_\uparrow + \frac{1}{2}) \log N_\uparrow - N_\uparrow$ ②

$\log N_\downarrow! \simeq \frac{1}{2} \log 2\pi + (N_\downarrow + \frac{1}{2}) \log N_\downarrow - N_\downarrow$ ③

$N = N_\uparrow + N_\downarrow$ so we rewrite the 1st

$$\log N! \simeq \frac{1}{2} \log (2\pi/N) + (N_\uparrow + \frac{1}{2} + N_\downarrow + \frac{1}{2}) \log N - (N_\uparrow + N_\downarrow)$$ ④

④ − ② − ③ gives

$$\log g \simeq \frac{1}{2} \log \left(\frac{1}{2\pi N}\right) - (N_\uparrow + \frac{1}{2}) \log (N_\uparrow/N) - (N_\downarrow + \frac{1}{2}) \log \frac{N_\downarrow}{N}$$

then $\log (N_\uparrow/N) = \log \frac{1}{2}(1 + \frac{2s}{N}) = -\log 2 + \log (1 + 2s/N)$

$\simeq -\log 2 + 2s/N - (2s^2/N^2)$

$(\cdots \quad \log (1+x) \simeq x - \frac{1}{2} x^2 + \cdots$

whence $\log(N\downarrow/N) \cong \log 2 - (2S/N) - (2S^2/N^2)$

Thus $\log g \cong \frac{1}{2}\log\left(\frac{2}{\pi N}\right) + N\log 2 - 2S^2/N$

finally $g(N,S) \cong \left(\frac{2}{\pi N}\right)^{1/2} 2^N \exp\left\{-2S^2/N\right\}$

c) we can take the width to be the full width at $1/e$ max

$$\frac{1}{e} = \frac{g(N,S_+)}{g(N,0)} \exp\left\{-\frac{2(S_+)^2}{N}\right\}$$

$$\Rightarrow \quad 1 = \left(\sqrt{\frac{2}{N}}\, S_+\right)^2 \quad \text{or} \quad S_+ = \sqrt{\frac{N}{2}}$$

$1/e$ max
S_+

Thus $\delta = 2S_+ = \sqrt{2N}$
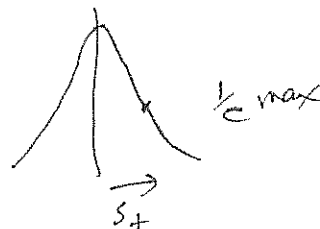
for $N = 10^{20}$ $\quad \delta = \sqrt{2} \times 10^{10}$

Fractional width $\frac{\delta}{N} = \frac{\sqrt{2N}}{N} = \sqrt{\frac{2}{N}} = \sqrt{2}\, 10^{-10}$

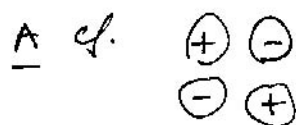a very tiny range centred on $S = 0$, 50-50 spins
up/down.

(4) Crystal of Charges

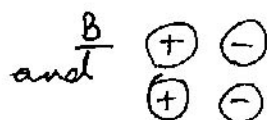NB: ions distinct, locations distinct

a) (4 places for Na^+) (3 places for K^+) (2 places for Cl^-) (1 place for F^-)

$= 4! = 24$ microstates, many degenerate.

(makes no difference, the order of ions being placed)

b) 2 macrostates

$\underline{A}$ cf. ⊕ ⊖ and $\frac{B}{}$ ⊕ ⊖
        ⊖ ⊕   ⊕ ⊖

A: like charges diagonally opposite

B: like charges adjacent

(ie & all rotations reflections)   (ie with all rotations/reflections)

multiplicities

A: (4 ~~states by rotations~~ corners for Na^+) × (1 choice opposite $^{+ve}$) × (2 choices for $-ves$) ~~×(2 mirror images)~~ = 8
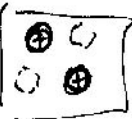
B: (4 corners for Na^+) (2 choices of adjacent $^{+ve}$) (2 choices for $-ves$)

$= 16$

energies

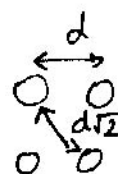add one particle at a time, and keep track of potential energy needed for each addition $V = \frac{kq}{r}$
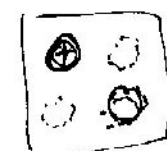
A: Na^+ - 0

K^+ opposite : $+\frac{kq^2}{d\sqrt{2}}$

Cl^- corner : $+\left(-\frac{kq^2}{d} - \frac{kq^2}{d}\right)$

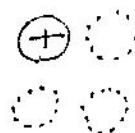F^- corner $+\left(-\frac{kq^2}{d} - \frac{kq^2}{d} + \frac{kq^2}{d\sqrt{2}}\right)$

$\varepsilon_A = \frac{kq^2}{d}\left(\frac{1}{\sqrt{2}} - 1 - 1 - 1 - 1 + \frac{1}{\sqrt{2}}\right) = \frac{kq^2}{d}(\sqrt{2} - 4)$

$= -5.949 \times 10^{-19}$ J

$= -3.718$ eV

④ (cnt'd)   energies (cnt'd)
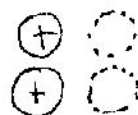
CONTRIBUTION

B: Na^+ :   0   ⊕ ◌
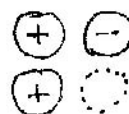◌ ◌

first ion,
no potential

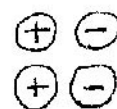$K^+_{adjacent}$: $+\dfrac{kq^2}{d}$ ⊕ ◌
⊕ ◌

potential to add
a +ve charge
adjacent to 1st

Cl^- : $+\left(-\dfrac{kq^2}{d\sqrt{2}} - \dfrac{kq^2}{d}\right)$ ⊕ ⊖
⊕ ◌

pairwise to the 2
+ve charges ...

F^- $+\left(-\dfrac{kq^2}{d} - \dfrac{kq^2}{d\sqrt{2}} + \dfrac{kq^2}{d}\right)$ ⊕ ⊖
⊕ ⊖

$$\varepsilon_B = \frac{kq^2}{d}\left(1 - \frac{1}{\sqrt{2}} - 1 - 1 - \frac{1}{\sqrt{2}} + 1\right) = \frac{kq^2}{d}\left(-\frac{1}{\sqrt{2}}\right) = -3.254 \times 10^{-19} J$$
$$= -2.034\ eV$$

bonus
marks

c) For each state 8 having energy ε_A (8 of these)

$$P(8_{\varepsilon_A}, \tau) = \frac{e^{-\varepsilon_A/\tau}}{Z(\tau)} = \frac{e^{-\varepsilon_A/\tau}}{8e^{-\varepsilon_A/\tau} + 16e^{-\varepsilon_B/\tau}} = \frac{1}{8(1 + 2e^{-\Delta\varepsilon/\tau})}$$

so, probability of an ε_A state

$$P_{\varepsilon_A}^{(\tau)} = 8\,P(8_{\varepsilon_A}, \tau) = \frac{1}{1 + 2e^{-\Delta\varepsilon/\tau}}$$

$\Delta\varepsilon \equiv \varepsilon_B - \varepsilon_A$
$= 1.684\,eV$

$$\boxed{P_{\varepsilon_A}(3K) \doteq 1 \qquad P_{\varepsilon_B}(3K) = 1 - P_{\varepsilon_A}(3K) \doteq 0}$$

$3K = 2.588 \times 10^{-4} eV$

$$\boxed{\begin{array}{l} P_{\varepsilon_A}(1,000K) = \dfrac{1}{1 + 2(1.49 \times 10^{-3})} \approx 1 - 2.98 \times 10^{-3} = \cancel{\text{4.62×10}} \\ \hspace{6cm} = 0.997 \\ P_{\varepsilon_B}(1,000K) = 1 - P_{\varepsilon_A}(1,000K) = 0.003 \end{array}}$$

→ NOT REQUIRED ←

NB: what of 10,000K?

$$\boxed{\begin{array}{l} P_{\varepsilon_A}(10,000K) = \dfrac{1}{1 + 2(0.5217)} = 0.489 \\ P_{\varepsilon_B}(10,000K) = 1 - P_{\varepsilon_A}(10,000K) = 0.511 \end{array}}$$

FYI; most ionic
crystals melt at
high temperatures;
this rearrangement
from $^+_-\,^-_+$ to $^+_-\,^-_-$
is a step towards that.