

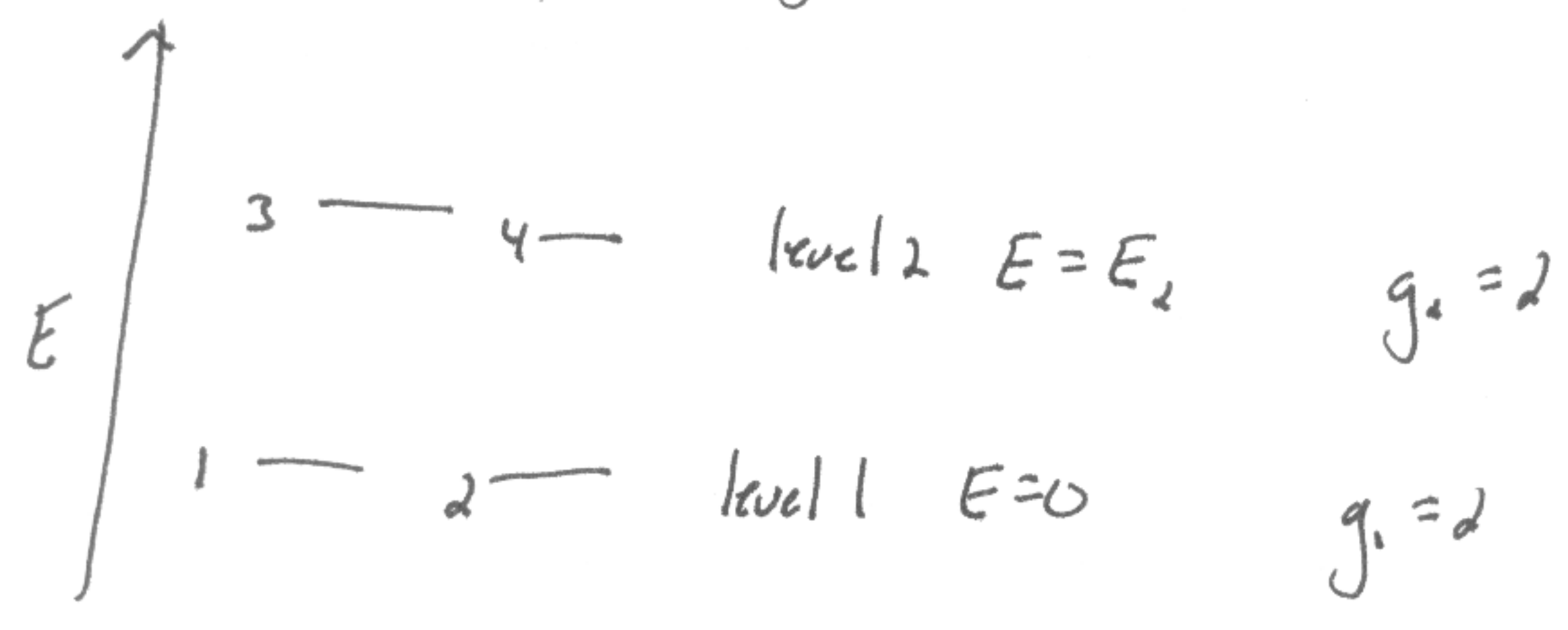
HW11 key

1. a) microscopic property - a property of an individual atom or molecule, or a very small number of molecules. Microscopic properties are known from quantum mechanics.
- b) macroscopic property - a property of a large collection of atoms or molecules that cannot be predicted directly from quantum mechanics but needs additional analytical inputs.
- c) partition function - a mathematical function which describes how energy is distributed (or "partitioned") throughout a system composed of a large # of atoms or molecules.
- d) energy of monoatomic species - a single atom has a non zero energy due to contributions from electronic packing (E_{elec}) and translation through space (E_{trans}).
- e) energy of polyatomic species - a molecule has a non zero energy due to contributions from E_{elec} and E_{trans} , as well as from rotating through space and vibrational oscillations.

f) degeneracy - energy levels that are distinct but have the same energy.

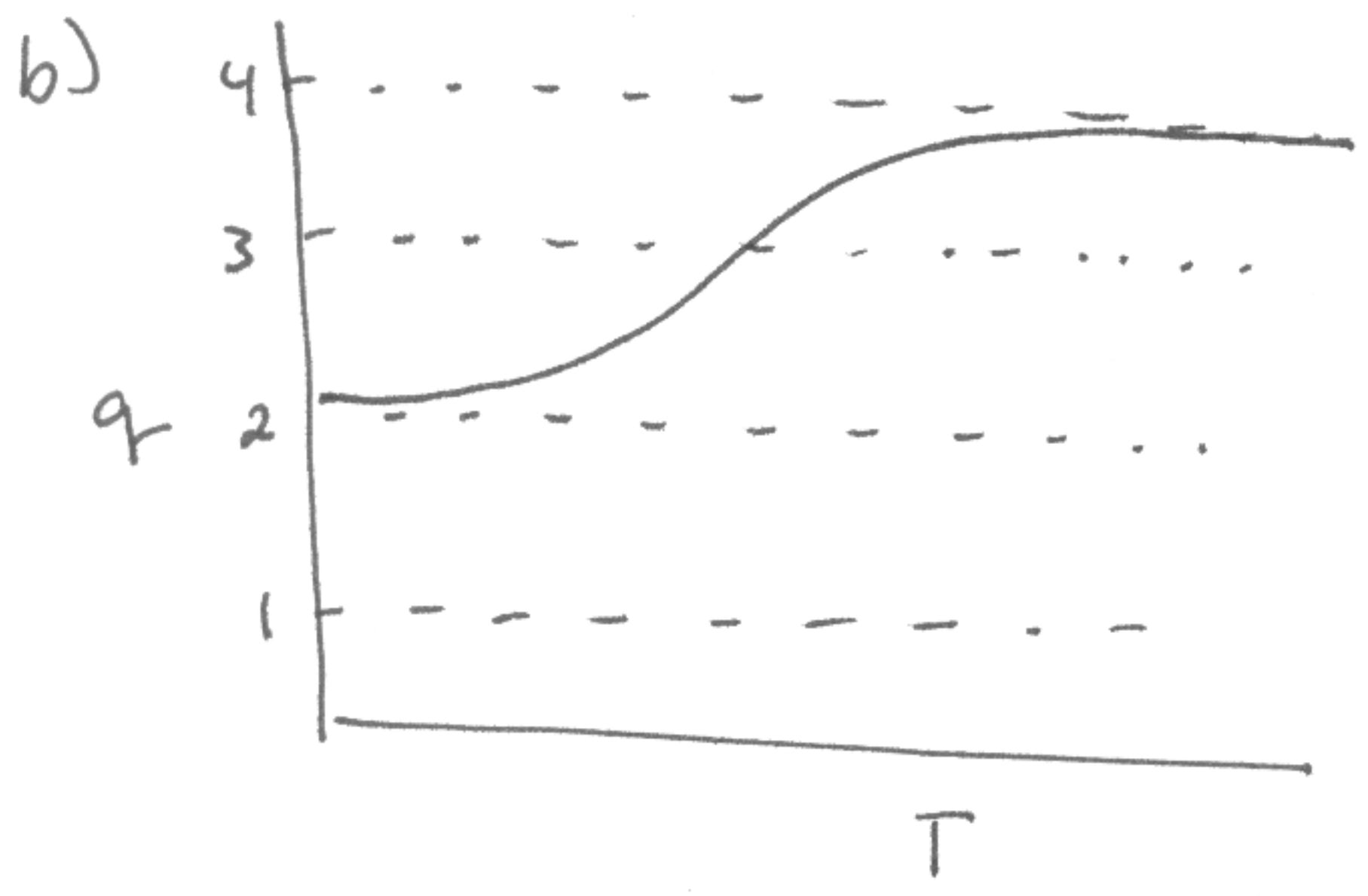
2. NO - each energy level is doubly degenerate

a)



$$q_f = 2 \cdot 1 + 2e^{-\beta E_2}$$

\uparrow \nwarrow
 2 states in 2 states in
 level 1 level 2

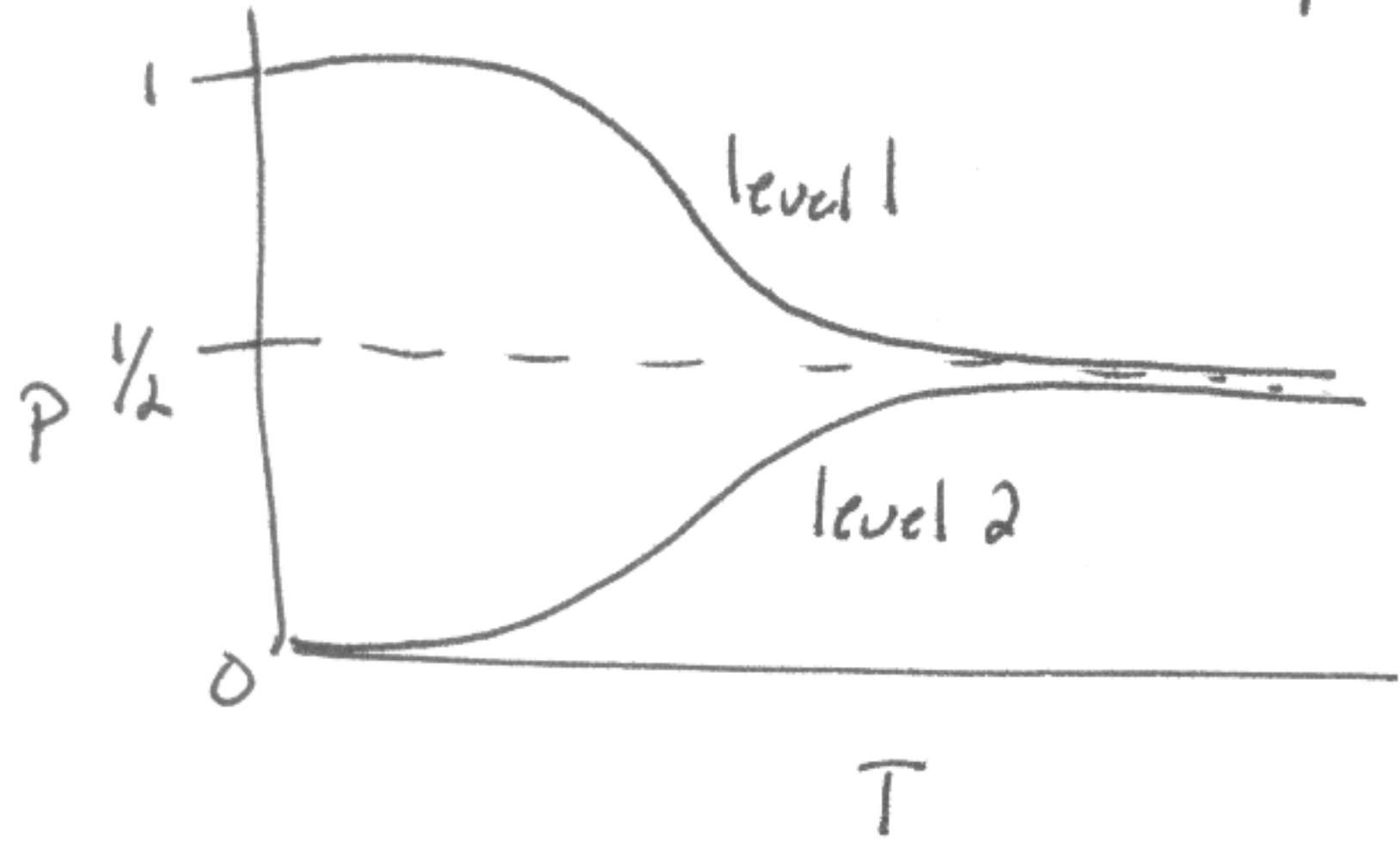


at low T , $e^{-E_2 \beta} \rightarrow 0$
 $q \rightarrow 2$

at high T , $e^{-E_2 \beta} \rightarrow 1$
 $q = 4$

c) $P_{\text{level 1}} = \frac{2}{g}$ $P_{\text{level 2}} = \frac{2e^{-\beta E_2}}{g}$

probability of being in a level, not a state



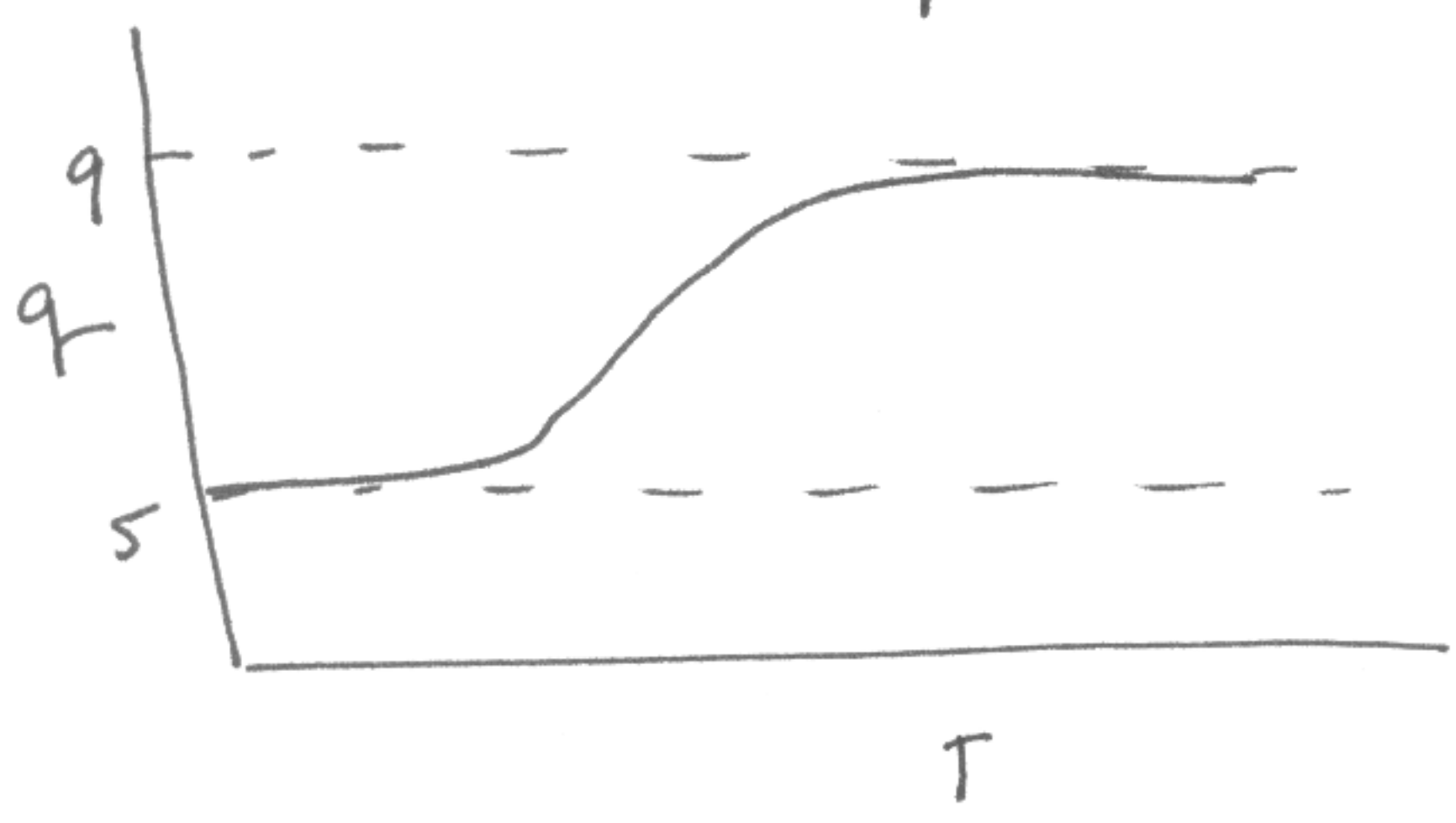
So at high T , all levels are filled equally.

3. $g = \sum_i g_i e^{-\beta E_i}$ $\beta = \frac{1}{k_B T}$

a) 3 levels: $g = 5e^{-\beta 0} + e^{-\beta \Delta} + 3e^{-2\beta \Delta}$

$g = 5 + e^{-\beta \Delta} + 3e^{-2\beta \Delta}$

b) as $T \rightarrow 0$, $e^{-\beta x} \rightarrow 0$, $g \rightarrow 5$
 as $T \rightarrow \infty$, $e^{-\beta x} \rightarrow 1$, $g = 9$



c) probability: level 1: $\frac{5}{5 + e^{-\beta\Delta} + 3e^{-2\beta\Delta}}$

as $T \rightarrow 0$, $e^{-\beta x} \rightarrow 0$, $P_1 = \frac{5}{5} = 1$

as $T \rightarrow \infty$, $e^{-\beta x} \rightarrow 1$, $P_1 = \frac{5}{9}$

level 2: $\frac{e^{-\beta\Delta}}{5 + e^{-\beta\Delta} + 3e^{-2\beta\Delta}}$

as $T \rightarrow 0$, $P_2 \rightarrow 0$

as $T \rightarrow \infty$, $P_2 \rightarrow \frac{1}{2}$

level 3: $\frac{3e^{-2\beta\Delta}}{5 + e^{-\beta\Delta} + 3e^{-2\beta\Delta}}$

as $T \rightarrow 0$, $P_3 \rightarrow 0$

as $T \rightarrow \infty$, $P_3 \rightarrow \frac{3}{9} = \frac{1}{3}$

Put all this together:

