States of a Model System

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- Consider a system of N quantum particles in a stationary quantum state (U, V, N... are independent of time)
- Multiplicity of degeneracy of an energy level ε_n is the number of quantum states, g_n , corresponding to ε_n
- Hydrogen Atom:
 - One proton, one electron

$$-\varepsilon_n = -\frac{13.6[\text{eV}]}{n^2}$$

$$-\psi_{n,l,m,s} = R_{n,l}(r)\Theta_{l,m}(\theta)\Phi_m(\phi)(s)$$

- * n, l, m, s are quantum numbers
- * n is called the principle quantum number
- $\ast \ l$ is the angular momentum quantum number

$$0 \le l \le n-1$$

* m is the magnetic quantum number

$$-l \le m \le l$$

 $*\ s$ is the spin-magnetic quantum number

$$\cdot \ s = \pm \frac{1}{2}$$

$$* g_n = 2n^2$$

• Quantum Particle in a Box $(L \times L \times L)$

- We find
$$\varepsilon_{n_x,n_y,n_z} = \frac{\hbar^2 \pi^2}{2mL^2} (n_x^2 + n_y^2 + n_z^2)$$

$$- \psi_{n_x,n_y,n_z}(x,y,z) = \dots$$

$$-1 \le n_x, n_y, n_z \le \infty$$

| n_x | $\mid n_y \mid$ | n_z | $\varepsilon_{n_x,n_y,n_z}/A$ |
|-------|-----------------|-------|-------------------------------|
| 1 | 1 | 1 | 3 |
| 2 | 1 | 1 | 6 |
| 1 | 2 | 1 | 6 |
| 1 | 1 | 2 | 6 |
| 2 | 2 | 1 | 9 |
| 2 | 1 | 2 | 9 |
| _1_ | 2 | 2 | 9 |

- We can see that the "6" energy level is degenerate, with a multiplicity of 3, just like "9"

• Binary Model System

- Energy of the system, $\varepsilon = -MB$
 - * M is total magnetic moment: $M = (\text{spins up spins down})m \rightarrow M = (N_{\uparrow} N_{\downarrow}) m$
 - * $(N_{\uparrow} N_{\bot}) = 2s$ spin excess
 - * Thus, $\varepsilon = -2mBs$, meaning it is dependent on spin excess
 - * N = 3 example:

$$\cdot \uparrow \uparrow \uparrow -2s = N_{\uparrow} - N_{\downarrow} = 3 \Rightarrow g = 1$$

$$\cdot \uparrow \uparrow \downarrow, \uparrow \downarrow \uparrow, \downarrow \uparrow \uparrow - 2s = N_{\uparrow} - N_{\downarrow} = 1 \Rightarrow g = 3$$

$$\cdot \uparrow \downarrow \downarrow, \downarrow \downarrow \uparrow, \downarrow \uparrow \downarrow - 2s = N_{\uparrow} - N_{\downarrow} = -1 \Rightarrow g = 3$$

$$\cdot \ \downarrow \downarrow \downarrow -2s = N_{\uparrow} - N_{\downarrow} = -3 \Rightarrow g = 1$$

- * In general, there are N+1 values of 2s (or M or ε) and 2^N states of the system in total \Rightarrow same energy levels have very high multiplicity
- Calculation of g(N, s)

$$\begin{cases} N_{\uparrow} - N_{\downarrow} = 2s \\ N_{\uparrow} + N_{\downarrow} = N \end{cases} \qquad \begin{cases} N_{\uparrow} = \frac{N}{2} + s \\ N_{\downarrow} = \frac{N}{2} - s \end{cases}$$

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

- Drawing from combinatorics below, an approximation of g(N, s) for N >> 1 and s << N, we can use the Stirling formula:

$$N! \approx \sqrt{2\pi N} \left(\frac{N}{e}\right)^N$$

$$-\ln(N!) \approx N \ln(N) - N + \frac{1}{2} \ln(N) + \frac{1}{2} \ln(2\pi) + 0 \left(\frac{1}{N}\right)$$

$$-\ln(1+x) \approx x - \frac{1}{2}x^2 + 0x^3, \quad -1 \le x \le 1$$

- Thus,
$$g(N,s) \approx 2^N \sqrt{\frac{2}{\pi N}} e^{-\frac{2s^2}{N}}$$

• Important Combinatorics

–
$$(x+y^n)=\sum_{k=0}^n\binom{n}{k}\,x^ky^{n-k}$$
 — Binomial Expansion
 – $\binom{n}{k}=\frac{n!}{k!(n-k!)}$ — Binomial Coefficient

• Gaussian Probability Density Function (PDF)

$$G(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{x^2}{2\sigma^2}}$$

- σ represents the standard deviation of G
- Macroscopic properties of a large system are well defined (i.e. fluctuations about the mean values are small $\approx O(\sqrt{N})$)