Physics 313 Quantum Mechanics facts

h is the Planck's constant, $h = 6.626 \times 10^{-34} \; J \cdot s \;=\; 4.136 \times 10^{-15} \; eV \cdot s$

1. Quantum Harmonic Oscillator

For an oscillator with a classical oscillation frequency f, the energy spectrum is $(hf)n$ for $n \geq 0$ an integer (we are ignoring a zero-point energy). The spacing between the energy levels in then hf.

Thermal excitation of the vibration, in accordance with the equipartition theorem occurs only when $kT \gg hf$. When $kT < hf$, the vibration is said to be frozen out and does not contribute to the number of degrees of freedom. Typically, at room temperature, vibrations in small molecules ($H_2 0$, N_2, NH_3, etc...) **are** frozen out. For example, for nitrogen, the period of oscillation is 12fs, and $hf = 0.34eV$, which is larger than $kT = (1/40)eV$ for $T = 300K$ – the vibrations are definitely frozen out.

2. Uncertainty relation

$$\Delta x \Delta p_x \geq \frac{h}{4\pi}$$

In the $x - p$ plane, we should think of every particle as occupying a small tile of area $h/4\pi \approx h$. (h^{-1} is a large number, so we can drop the factor of 4π.)

3. Two state paramagnet

Each site contains a spin which has only two states - $\uparrow$ and $\downarrow$. The energy for these two states is $\pm B\mu$. The total energy for a state with $N_\uparrow$ $\uparrow$s and $N_\downarrow$ $\downarrow$s is $U = (N_\downarrow - N_\uparrow)B\mu$ and the magnetization is $M = (N_\uparrow - N_\downarrow)\mu$ so that $U = -\mu M$. The multiplicity is

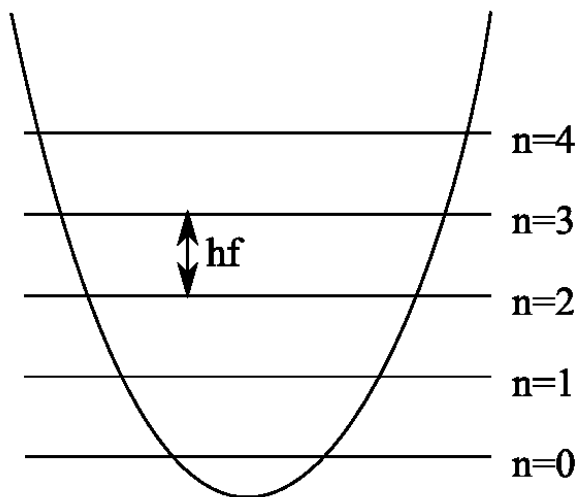$$\Omega = \binom{N_\downarrow + N_\uparrow}{N_\uparrow} = \binom{N}{q}$$

where N is the total number of sites and q is the number of energy quanta in the system (i.e. the number of spins flipped to the state of higher energy).
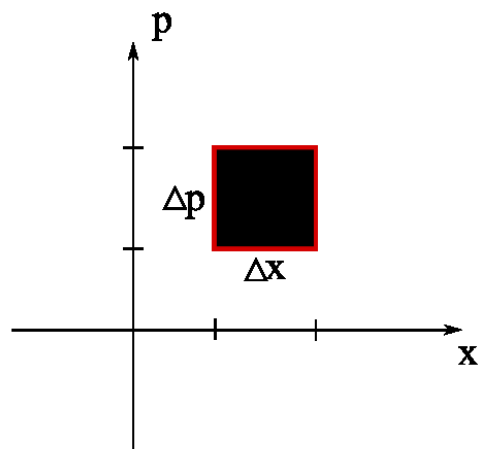
4. Einstein Solid

This is a collection of N QHO (see above). Every QHO has some non-negative number of energy quanta n. If we denote by q the total number of energy quanta in the system, the total internal energy is $U = q(hf)$ and the multiplicity is
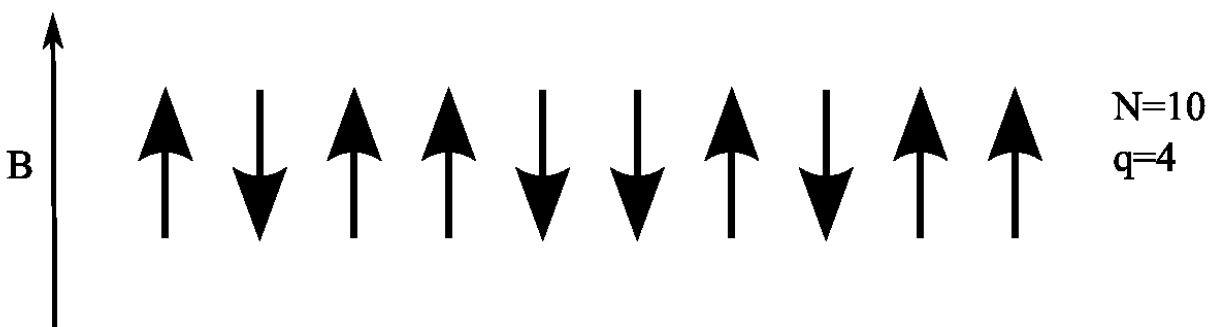
$$\Omega = \binom{N + q - 1}{q}$$

1.

n=4
n=3
hf
n=2
n=1
n=0

2.

p

Δp

Δx

x

3.

B

N=10
q=4

4.

N=10
q=18