Lecture 4 Phys 404, Spring 2011

Newton's laws of motion and the Schrodinger equation in quantum mechanics are not well suited to describe the macroscopic properties of common objects (e.g. a block of copper, a glass of water, etc.) at room temperature. It is too cumbersome to use these equations to understand the behavior of a collection of Avagodro's number ($N_A \sim 6.02\ 10^{23}$) of particles. In particular it is hard to understand how macroscopic objects interact with each other. Most importantly, quantum mechanics cannot tell us why heat flows from hot things to cold things spontaneously (without the intervention of an agent). We need another approach.

The outline of statistical mechanics is as follows:

- 1) Enumerate the quantum mechanical states of a system. We use the results of quantum mechanics to find all of the "micro-states" of a system.
- 2) Evaluate the statistical properties of the system. Which states are accessible? What is the average of a property (e.g. pressure, magnetization, energy, etc.) over all of the accessible micro-states?
- 3) Determine the macroscopic thermodynamic state of the system, and understand how it interacts with other macroscopic systems.

We discussed the solutions to a number of simple quantum problems. The key concepts to take away from this discussion are the facts that **the bound energy eigenstates of the systems are discrete** – they are typically labeled by one or more integers, and the fact that **the degeneracy or multiplicity of each state grows quickly with excitation number**. The systems included:

- a) Particle of mass m in an infinite square well of width L. 1D version has energy eigenvalues $E_n=n^2\pi^2\hbar^2/(2mL^2)$, where n=1,2,3,... is the quantum number. In a 3D infinite cubical well of side L the energy eigenvalues are also discrete: $E_{n_x,n_y,n_z}=(n_x^2+n_y^2+n_z^2)\pi^2\hbar^2/(2mL^2)$, where $n_x=1,2,3,...,n_y=1,2,3,...$, and $n_z=1,2,3,...$ are the three independent quantum numbers.
- b) The Hydrogen atom has discrete energy eigenvalues given by $E_n = -me^4/(8h^2\varepsilon_0^2n^2)$, where m is the electron mass, e is the electronic charge, h is Planck's constant, ε_0 is the permittivity of free space and n=1,2,3,... is called the principal quantum number. There are in fact three quantum numbers that label the solutions of the Schrodinger equation for the (unperturbed) Hydrogen atom: n, l and m. Degeneracy means that two or more distinct quantum states (labeled by different sets of quantum numbers) have the same energy. The degeneracy of the unperturbed hydrogen atom increases as $g(n) = n^2$.
- c) A mass m on a spring with spring constant k is a harmonic oscillator. The 1D version has discrete energy eigenstates with energies $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$, where $\omega = \sqrt{k/m}$. The 3D version has discrete energy eigenvalues $E_{n_x,n_y,n_z} = (n_x + n_y + n_z + 3/2)\hbar\omega$, where $n_x = 1, 2, 3, ..., n_y = 1, 2, 3, ...$, and $n_z = 1, 2, 3, ...$ are the three independent quantum numbers. Often this is written as $E_n = (n + 3/2)\hbar\omega$, where $n = n_x + n_y + n_z$. It can be shown that the 3D harmonic oscillator states have multiplicity or degeneracy of g(n) = (n+1)(n+2)/2.
- d) Consider a small circular loop of wire carrying a current I. Such a current loop generates a magnetic moment $\overrightarrow{m}=I\overrightarrow{a}$, where $\overrightarrow{a}=A\widehat{n}$ is the vector area (Griffiths Electrodynamics, p. 244) and A is the area of the loop and \widehat{n} is the unit vector normal to the plane containing the loop, with a direction given by the right hand rule for the sense of current flow in the loop. If an external magnetic field \overrightarrow{B} is applied to the loop, a torque is exerted on the loop trying to align the direction of \overrightarrow{m} with \overrightarrow{B} . This interaction can be summarized with a classical

potential energy $U=-\overrightarrow{m}\cdot\overrightarrow{B}$. The aligned configuration has the lowest (most negative) energy. Classically this energy can have any value because \overrightarrow{m} can have any direction relative to \overrightarrow{B} . An electron has an intrinsic magnetic moment associated with it's spin. However in the quantum mechanics of the electron there are only two possible values of $\overrightarrow{m}\cdot\overrightarrow{B}$, namely $U=+m_eB$ or $U=-m_eB$, where $m_e=e\hbar/2m$ is the Bohr magneton. This arises from a quantum mechanical property of the electron termed a "two-valuedness not describable classically" by Wolfgang Pauli. The electron acts as if it has a small current loop and magnetic moment, and the orientation of this moment with respect to any magnetic field direction has only one of two possible projections, called "up" or "down" depending on whether its projection on \overrightarrow{B} is either positive or negative. We will use this quantum spin/magnetic moment property of the electron to begin our study of statistical mechanics.