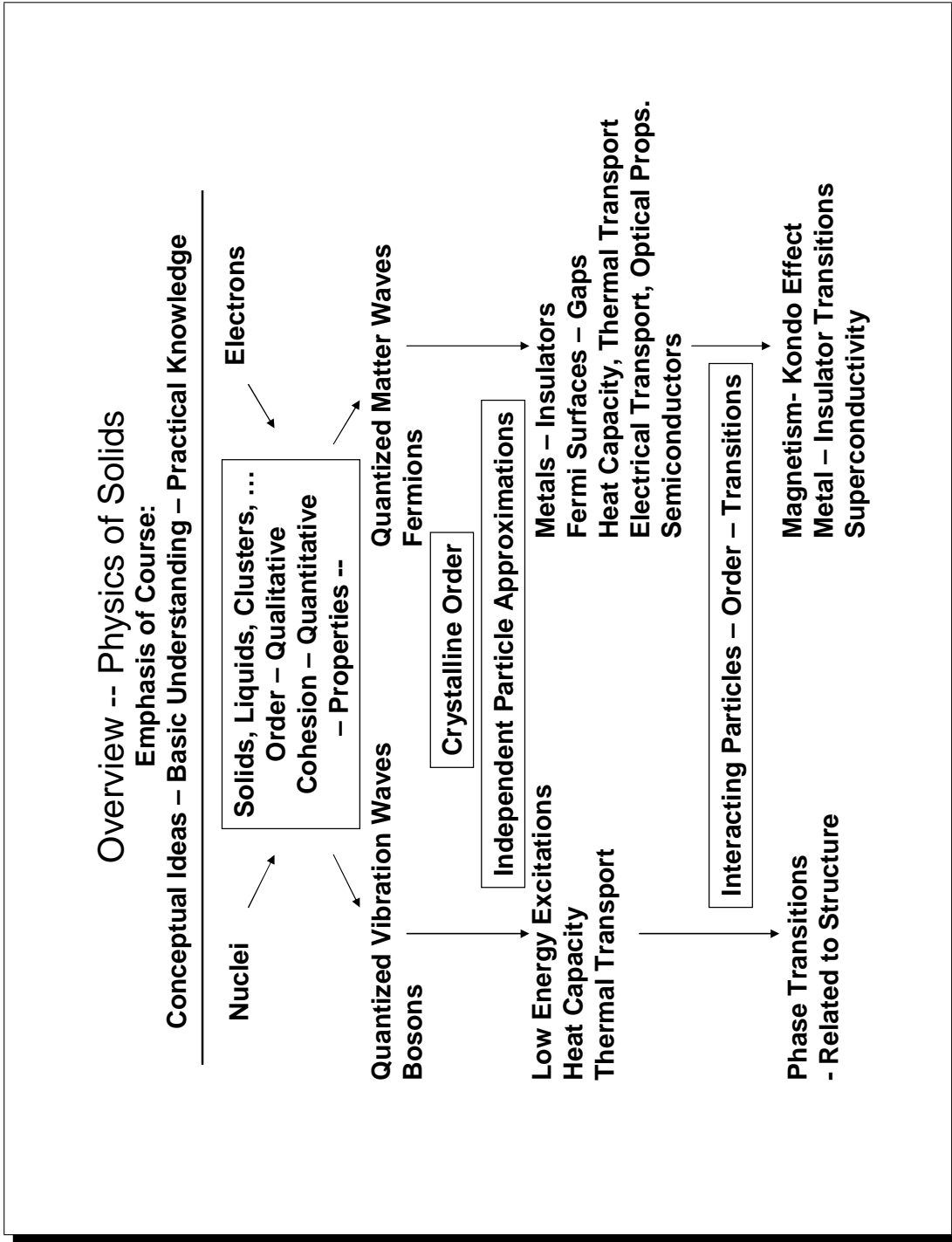**489 S 04 Lecture 1**

Overview of Course

1. Outline of course - Calendar on Web

2. Overview of properties of condensed matter - Mainly within independent-particle pictures

3. Beyond the independent-particle approximations: Strong Interactions and Collective Phenomena

   (Article *More is Different* by P. W. Anderson.)

4. Background: Review of Statistical Mechanics (Basic formulas - many derivations and developments for specific cases will be be part of course later.)

Overview -- Physics of Solids
Emphasis of Course:
Conceptual Ideas – Basic Understanding – Practical Knowledge

Nuclei

Electrons

Solids, Liquids, Clusters, …
Order – Qualitative
Cohesion – Quantitative
– Properties --

Quantized Vibration Waves
Bosons

Quantized Matter Waves
Fermions

Crystalline Order

Independent Particle Approximations

Low Energy Excitations
Heat Capacity
Thermal Transport

Metals – Insulators
Fermi Surfaces – Gaps
Heat Capacity, Thermal Transport
Electrical Transport, Optical Props.
Semiconductors

Interacting Particles – Order – Transitions

Phase Transitions
- Related to Structure

Magnetism- Kondo Effect
Metal – Insulator Transitions
Superconductivity

Selected Review of Statistical Mechanics

1. Sources: Feynman, Ch. 1; A & M, p. 40-42, 426-8,452-4; Mihaly and Martin, Ch. 6 and related sections; Kittel, Ch 5, App. D; Reif, Ch. 9.1-9.8.

2. Fundamental Law of Statistical Mechanics: (Feynman, Ch. 1; Reif, Ch. 9; A & M, p. 426 footnote)

   (a) For a general interacting system of N bodies , classical or quantum, let the the *exact* states of the N-body system be labelled by m.

   (b) If the system is in equilibrium with a temperature T, the probability the system is in state m with energy E_m is given by:
   $P(E_m) = \exp(-\beta E_m)/Z$, where $\beta = \frac{1}{k_B T}$.

   (c) Z = partition function $Z = \sum_m \exp(-\beta E_m)$.

   (d) Since $Z = \exp(-\beta F)$, where F is the Helmholz Free Energy also given below, $P(E_m) = \exp(-\beta(E_m - F))$

   (e) The expectation value of any quantum mechanical operator for a physical variable is:
   $\langle O \rangle = \frac{1}{Z} \sum_m \langle m|O|m \rangle \exp(-\beta E_m)$, where $|m\rangle$ denotes an eigenstate of the hamiltonian.

3. Thermodynamic quantities

   (a) Internal Energy $U = -\frac{dlnZ}{d\beta}$, which follows directly from the expressions above.

   (b) For condensed matter it is important to use *intensive* quantities like energy density $u = \frac{U}{V}$ where V is the volume, which are independent of the volume V in the limit of large volume.

   (c) One can also specify that the system is in the presence of externally applied pressure and is in equilibrium with a reservoir that can supply particles at energy the chemical potential μ. (The energy may also depend upon the magnetization M and external field H, etc.)
   Then a change in U is given by:
   Change in $U(S, V, N)$: $dU = TdS - PdV + \mu dN + \ldots$

   (d) Set of thermodynamic potentials derived by Legendre Transformations of the variables:

   - Energy: U
     Enthalpy: $H = U + PV$
     Helmholz Free Energy: $F = U - TS = -k_B T lnZ$
     Gibbs Free Energy: $G = H - TS$
     Grand Canonical Potential: $\Omega = U - TS - \mu N$
   - Change in $U(S, V, N)$: $dU = +TdS - PdV + \mu dN + \ldots$
     Change in $H(S, P, N)$: $dF = +TdS + VdP + \mu dN + \ldots$
     Change in $F(T, V, N)$: $dF = -SdT - PdV + \mu dN + \ldots$
     Change in $G(S, P, N)$: $dF = -SdT + VdP + \mu dN + \ldots$

Change in $\Omega(S, P, N)$: $d\Omega = -SdT - PdV - Nd\mu + \ldots$
where $\ldots$ indicates possible dependence upon other variables like stress/strain, magnetization/field, etc.

(e) Heat Capacity: $C_v \equiv \frac{dQ}{dT}|_V, N = T\frac{\partial S}{\partial T}|_V, N$; and specific heat $c_v = \frac{C_v}{V}$

4. Non-interacting particles

5. Define the possible energies of one particle to be ϵ_i. A state m of a system of N particles is defined by specifying the one-particle state i of each one of the N particles. Many relations can be defined independent of the statistics of the particles (Fermions, Bosons, distinguishable) which are considered below. In all cases, the total energy is $E_m = \sum_i n_i \epsilon_i$, where n_i is the number of particles in the one-particle state i.

   (a) Mean occupation of single particle state: $< n_i > = -\frac{1}{\beta}\frac{\partial lnZ}{\partial \epsilon_i}$

   (b) Total energy density: $u = -\frac{1}{V}\sum < n_i > \epsilon_i$

   (c) For each of the cases below, calculation of the distribution depends upon whether or not the number of particles is conserved. The constraint of conservation of number of particles introduces a difficulty counting the states. A convenient way to treat this case is by introducing μ = chemical potential, which is the energy of particles in a reservoir, to avoid the difficulty of constraining particle number.

6. Classical Statistics (A & M, p. 426-8)

   (a) Equipartition: For any system with kinetic energy quadratic in the velocity of each particle and potential energy quadratic in the position of each particle, the average energy is $\frac{1}{2}k_BT$ for each degree of freedom

   (b) For ideal gas of particles in 3 dimensions: $C_v = \frac{3}{2}Nk_B$

   (c) For ideal harmonic oscillators in 3 dimensions: $C_v = 3Nk_B$

7. Particles obeying Bose-Einstein statistics

   (a) Bose-Einstein distribution: $< n_i > = \frac{1}{\exp(\beta(\epsilon_i - \mu)) - 1}$

   (b) If particle number is not conserved, Planck Distribution: $< n_i > = \frac{1}{\exp(\beta\epsilon_i) - 1}$

8. Particles obeying Fermi Statistics

   (a) Fermi-Dirac distribution: $< n_i > = \frac{1}{\exp(\beta(\epsilon_i - \mu)) + 1}$

   (b) Chemical potential μ at T=0 is called the Fermi energy E_F.

9. Expressions for a continuum of states

   (a) $n(\epsilon) = \frac{1}{\exp(\beta(\epsilon_i - \mu)) \pm 1}$

   (b) In large system with many states, states near the chemical potential that dominate the properties at low temperature.

10. Interacting Particles

(a) For interacting particles, one must treat the full interacting system and the above simple formulas *do not in general apply.*

(b) For localized states, particle interactions are often crucial: for example, consider the hydrogen atom, where the first electron is bound by 1 Ryd, but a second electron is barely bound.

(c) Example in homework problem.

(d) In condensed matter, the non-interacting approximation is often a good (even excellent) approximation, but interactions can make *quantitative* or *qualitative* changes.

11. Collective Behavior due to interactions - treated later in course

(a) Interactions can lead to qualitative effects: phase transitions, new types of order.

(b) Nevertheless, the first step is a "mean field approximation" in which the system is treated as a collection of non-interacting system with each particle moving in an "effective potential" due to the other particles. The result may be only quantitative changes or qualitative changes in which the order of the system changes. This is sufficient to describe many important problems like many phase transformations, superconductivity, etc.

(c) The most difficult cases - where a "mean field approximation" is not adequate - are beyond the scope of this course.