561 Fall 2005 Lecture 12

Broken Symmetry Transitions, Order Parameters: Mean field theory of phase transitions

Anderson, Basic Notions in Condensed Matter Physics", General discussions in Ch. 2; See also p. 96-104.
Pines and Nozieres, Quantum Liquids, Vol 1.
Kittel, "Intro. to Solid State Physics", p. 284 (Peierls Instability)
N. Goldefeld, "Phase Transitions".

1. What is Broken Symmetry? Order Parameter?

- Spontaneous Symmetry Breaking is a collective effect in which the ground state (or the state of lowest free energy) has lower symmetry than the hamiltonian. For example, the hamiltonian describing nuclei and electrons is translation invariant, rotational invariant, time-reversal invariant.
  - A crystal with a definite orientation in space in an anisotropic state. The ground state excitations of the crystal are not isotropic. There is symmetry under finite crystal translations instead of the continuous translation symmetry.
  - A magnetic with a given direction of the magnetization has broken rotational symmetry and time reversal symmetry
- The order parameter describes the new order, for the above examples:
  - The density of the crystal $\rho(r)$ which is periodic with discrete translations $r \to r + R$
  - The magnetization which has a magnitude and direction
- If the order parameter breaks a continuous symmetry (as those above) there is always a "Goldstone mode" an excitation with energy that vanishes in the limit of slowly varying small variations of the order parameter. For the above examples:
  - Acoustic phonons with $\omega \to 0$ as the wavevector $k \to 0$
  - Spin waves (magnons) with $\omega \to 0$ as the wavevector $k \to 0$
- The breaking of symmetry in a macroscopic state of condensed matter, is a phase transition to a new phase
- When this occur the ground state changes. The new state cannot be described as a perturbation on the old state.
- The approach to the transition can be studied by perturbation theory. At a second order phase transition the linear response diverges for applied external fields, and the system becomes unstable to the spontaneous development of finite order parameter in the absence of external fields. For the above examples:
  - Crystallization is usually first-order, with no divergence of linear response, and a discontinuous change

- Ferromagnetic magnetization is often second order, with the magnetic susceptibility diverging at the onset of magnetization

2. Mean field theory of transition: generalized RPA

- Consider the response of an observable to an external perturbation just as we considered in linear response theory. For example, consider a density ρ of particles which interacts with an external field V_{ext} with an internal interaction V treated in mean field approximation. If we consider a homogeneous case for simplicity then each Fourier component q can be treated separately and each particle feels a total potential $V_{tot}(q) = V_{ext}(q) + V(q)\langle\delta\rho(q)\rangle$, where $\langle\delta\rho(q)\rangle$ is the average change in density. In linear response:

$$\begin{aligned} \langle\delta\rho(q)\rangle &\equiv \chi^0(q)V_{tot}(q) && (1)\\ &= \chi^0(q)[V_{ext}(q) + V(q)\langle\delta\rho(q)\rangle] && (2)\\ &\equiv \chi(q)V_{ext}(q) && (3) \end{aligned}$$

or

$$\chi(q) = \frac{\chi^0(q)}{1 - V(q)\chi^0(q)} \tag{4}$$

(Note that with this definition, we expect $\chi^0 < 0$ and $\chi < 0$ for a stable system.)

- Example: Spin susceptibility and Ferromagnetic susceptibility. This is favored by exchange which is an attractive interaction between electrons of the same spin.

  In Fermi Liquid Theory the average spin-dependent interaction is given by the parameter $f_{a,l=0}$ or $F_{a,l=0} = f_{a,l=0}N(E_F)$, where $N(E_F)$ is the density of states at the Fermi energy.

  The non-interacting susceptibility is just $\chi^0_{spin} = -N(E_F)$, which leads to an effective susceptibility including the effects of interactions. For attractive interactions, this is considered in a homework problem where you are asked to find the parameter $f_{a,l=0}$ or $F_{a,l=0}$ for which there is an instability to ferromagnetism. The susceptibility has the same form as equation 4 and as the Stoner expression for magnetic susceptibility

$$\chi(q) = \frac{\chi^0(q)}{1 - IN(E_F)}, \tag{5}$$

  where I is the Stoner enhancement parameter, which is widely used in the theory of magnetism in solids.

3. Peierls Instability in a 1-D electron system

- Consider simple 1-D electron band which filled to a Fermi energy E_F and Fermi momentum k_F. For simplicity assume a free electron dispersion $\epsilon(k) = k^2/2m$.

- Let there be a perturbation $U(x) = A\Delta cos(qx)$, due to a phonon of amplitude Δ and wavevector q.
- If the wavevector is $q = 2k_F$ there is maximum effect upon the electrons and the resulting dispersion has a gap at E_F. Since this lowers the energy of filled states, it lowers the total electron energy.
- The change in total energy of the system is the change in the electron energy (negative) plus a positive distortion energy $E_{elastic} = \frac{1}{4}C\Delta^2$.
- It is straightforward to show that the total energy is always lowered in this case, with the magnitude of the gap given by $|A\Delta| = E_{gap} = 4We^{-\frac{1}{N(E_F)V}}$, where $W = \hbar^2 k_F^2/2m$ is the band width, $N(E_F) = 2m/\pi\hbar^2 k_F$ is the density of states in one dimension, and $V = aA^2/C$ is an effective electron-electron interaction.
- The resulting variation in electron density at wavevector $q = 2k_F$ is a charge density wave. If the cause is a phonon at this wavevector (as in the Peierls model) the lattice also has a density wave. This is observable by x-ray scattering. Either the electron density of the lattice wave can be considered an "order parameter"
- The reason for the exponential form is the same as in the Kondo effect and superconductivity – the log singularity that comes from the sharp cutoff in the electron occupation at the Fermi energy.
- Commensurate vs. incommensurate. If q is rational fraction of a reciprocal lattice vector, density wave is locked in the lattice. Leads to insulator in 1-D. If q is irrational, can lead to "sliding charge density wave".
- The Peierls-type instability an occur in higher dimension only in very special cases. Note: this is very different from superconductivity, which has a different order parameter, occurs in any dimension, and leads to very different effects.

4. Effects of Temperature

- Temperature broadens the change in the occupation at the Fermi energy and reduces the effect
- Log singularity for $T = 0$ gives Peierls instability.
- At high temperature the instability disappears and the homogeneous undistorted system is stable
- See hand-written notes for discussion of the finite T solution
- Example of mean field theory of phase transition as a function of T