Statistical Physics 2006/7
Section 9: Phase Transitions and the Ising Model

9. 1. Review of Basic Phenomenology

A: Critical Point of a Fluid

Figure 1: **i)** Phase diagram for a fluid in the P–T plane. Note the 'vapour-pressure' curve which separates the liquid and gas phases and terminates at the critical point **ii)** Isotherms in the P–ρ plane. Note the emergence of a flat piece in the co-existence region when $T < T_c$ **iii)** Plot of $\rho(T)$ as we move along the co-existence curve. Note the emergence of two values ρ_l and ρ_g for $T < T_c$

- Along the vapour-pressure or co-existence curve in Figure 1 the gas and liquid coexist i.e. the fluid can exist in two different forms or phases characterised by different densities.
- The co-existence curve terminates at **the critical point** which has unique thermodynamic co-ordinates T_c, P_c, ρ_c where ρ is the density
- In Figure 2 the critical isotherm has zero slope at ρ_c, which means that the isothermal susceptibility, a response function defined by

$$\kappa_T = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T ,$$

  diverges at the critical point. In turn from the discussion of fluctuation-response in section 3, this implies that there are large scale fluctuations in the density.
- In the coexistence region the liguid and gas coexist and the fluid separates into a mixture of gas and liquid, which have densities ρ_l and ρ_g, with the required overall density ρ.

B: Critical Point of a Magnet

- A magnetic solid, made up of atoms with dipole moments, exhibits no global magnetisation at high T (in zero applied field). This is known as the *paramagnetic* phase.
- The interactions between dipoles, namely the quntum exchange interaction which tends to align the dipoles, become important at low T.
- For $T < T_c$ a global magnetisation emerges even in zero applied field i.e. the dipoles tend to line up in the same direction without the aid of an applied magnetic field. This is known as a *ferromagnetic* phase

Figure 2: **i)** Phase diagram for a magnetic system in the H–T plane where H is the applied magnetic field. The coexistence curve is along the $H = 0$ axis **ii)** Isotherms in the H–M plane where M is the global magnetisation. Note the emergence of a flat piece when $T < T_c$ **iii)** Plot of $M(T)$. Note the emergence of two non-zero values $\pm|M|$ for $T < T_c$

- For $T < T_c$ note the discontinuity in M as we cross the coexistence line i.e

$$\begin{cases} H = 0^+ & M > 0 \\ H = 0^- & M < 0 \end{cases}$$

- At T_C we have $M_c = H_c = 0$ which is due to the symmetry between the two ferromagnetic phases $\pm|M|$
- The critical isotherm has zero slope at $M = 0$ which implies that at T_c the response function diverges

$$\chi = \left.\frac{\partial M}{\partial H}\right|_{H=0} \to \infty$$

and there are large scale fluctuations in the magnetisation

C: Critical Point of a Binary Alloy

Finally we briefly mention a less familiar system exhibiting a phase transition

- There are equal concentrations of A and B type atoms arranged on a regular lattice.

- For $T > T_C$ we have the disordered phase where the atoms are arranged randomly on the lattice sites
- For $T < T_C$ an ordered state emerges where A and B atoms are concentrated on their own separate sublattices

There are countless other examples of phase transitions. However rather than attempting to catalogue each and every one, our aim is to unify the common features.

9. 2. Common Features

- **Co-existence Curve**: line separating two phases differing by macroscopic properties
- **Critical Point**: terminus of co-existence curve
- **Order Parameter** O: characterises the difference between the two phases.

  For example

  – Fluid $O \equiv \rho_l - \rho_g$ the density difference between the two phases

  – Magnet $O \equiv M$ the global magnetisation
- **Phase Transition**: qualitative change in macroscopic properties as some parameter e.g. T is varied

  Generally we have two types of phase transition

  – a *discontinuous* transition (often referred to as 'first order') exhibits a jump in O e.g. on crossing the co-existence curve

  – a *continuous* transition has $O \to$ zero (but in a nonanalytic way — see later) e.g. in the passage through the critical point. The transition is accompanied by divergence of response functions and accompanying large-scale fluctuations.

9. 3. Basic Model: The Ising Model

We now introduce the most widely studied model system in statistical physics

- We have N spins on a lattice, which we can take for simplicity to be a simple cubic lattice. The spins each occupy one lattice site i where $i = 1 \dots N$ and take values $S_i = \pm 1$ 'up' or 'down'.
- The Configurational Energy (often referred to as the 'Hamiltonian') is given by

$$E(\{S_i\}) = -h \sum_i S_i - J \sum_{<ij>} S_i S_j \tag{1}$$

  – Ist term: h is the 'field' i.e. the applied magnetic field. If S_i is aligned to the field it gives a lower energy contribution

– 2nd term: here, <> means nearest neighbour (n.n) pairs. The number of n.n. of a site is z, the co-ordination number of the lattice, and the total number of n.n. pairs is $Nz/2$. For example, on a simple cubic lattice $z = 6$

  $J > 0$ is the 'coupling constant' so if neighbouring spins S_i and S_j are aligned they give a lower contribution to the energy.

- The Partition Function

$$Z_c = \sum_{\{S_i = \pm 1\}} \mathrm{e}^{-\beta E(\{S_i\})} \qquad \beta = 1/kT \tag{2}$$

  The configurational sum (sometimes referred to as the 'trace') is explicitly

$$\sum_{\{S_i = \pm 1\}} = \sum_{S_1 = \pm 1} \sum_{S_2 = \pm 1} \cdots \sum_{S_N = \pm 1}$$

Why should we expect a phase transition? Recall from P3 that we can write the partition function as a sum over possible energies of the system

$$Z_c = \sum_E \Omega(E) \mathrm{e}^{-\beta E} = \sum_E \mathrm{e}^{-\beta F(E)} \tag{3}$$

where

$$F(E) = E - kT \ln \Omega(E) = E - TS \tag{4}$$

is the Helmholtz free energy and we have used the Boltzmann definition of the entropy. The equilibrium state is given by *minimising* F with respect to E. T sets the balance between minimising E and maximising S

At low T minimise E $\Rightarrow$ ground states $\uparrow\uparrow \ldots \uparrow\uparrow$ and $\downarrow\downarrow \ldots \downarrow\downarrow$ dominate

At high T maximise S $\Rightarrow$ disordered states $\uparrow\downarrow\downarrow \ldots \uparrow\downarrow\uparrow$ dominate

But we need to show that there is a phase transition between the two regimes rather than a smooth crossover.