

## Lecture 3: Conceptual overview

In the last lecture, we reminded ourselves that the statistical approach to macroscopic systems is not just a technical tool that allows us to apply the laws of classical and quantum mechanics to large systems—instead, it represents a *conceptual advance* since many concepts like heat and temperature which are well-motivated by everyday experience cannot even be defined in a precise scientific way using just the equations of motion of classical and quantum mechanics. Instead, these properties are given a precise characterization starting from Gibb’s statistical approach which says that a system can be in any allowed state with a particular equilibrium probability.

Now, does this mean that one can replace the equations of motion of Newton and Schrodinger by the probability distribution of Gibbs, and simply “turn the crank” to back out all the physics of macroscopic systems? Even a moment’s reflection should convince you that this cannot be the case. Consider the following phenomenological facts, again drawn from everyday experience:

- Matter exists in several different phases:

For instance, water exists in several different crystalline ice phases, a liquid phase, and gaseous phases. Likewise some metals exist in both a low temperature ferromagnetic phase and a higher temperature paramagnetic phase. Others become superconducting at very low temperatures. Helium exists as a gas, ordinary liquid, superfluid, and at higher pressures, even a so-called “supersolid” phase, although the last has not been fully confirmed as there is some disagreement between different experimental groups pursuing its study.

- These phases are separated by phase transitions, accessed by changing pressure, temperature, magnetic field etc.
- Some of these phases are “distinctly” different from other phases:

Atoms in a crystal have a very “ordered” arrangement. This is clearly not so in a liquid. Some phase transitions are “first order” with latent heat of phase change, like the familiar melting transition of ice. Other transitions, for instance, the transition of helium from an ordinary liquid to a superfluid, or the transition of water from its liquid to gaseous phase near the “critical end-point” of the liquid-gas transition,

are accompanied by large scale fluctuations which are at the root of the experimentally well-known phenomenon of “critical opalescence”

Faced with this list of phenomena, we must naturally ask: Where is all this “hiding” inside Gibb’s “master-formula”

$$Z = \sum_n \exp(-\beta E_n) ? \quad (1)$$

(here and henceforth in this course of lectures,  $\beta \equiv (k_B T)^{-1}$  unless I warn you that this is temporarily not the case).

Indeed, in the first few decades of the twentieth century, it was by no means clear even to experts whether phenomena such as phase transitions and critical end-points could be captured by Gibb’s statistical approach. This question motivated the study of simple lattice models of interacting many-body systems, starting with the thesis of Ising, who was a student of Lenz, who asked him to explore the question of phase transitions in a simple lattice model in which there are two states at each site. We now know this model as the “Ising model”. Ising was able to show that such a model, when treated using the principles of Statistical Mechanics, does not exhibit any phase transition phenomena in one spatial dimension. This was an important and correct negative result.

Perhaps influenced by the prevailing uncertainty about the ability of this statistical approach to describe things like phase transitions, Ising went ahead and also conjectured that the same is true in higher dimension, *i.e.* the Ising model, when treated using the Gibb’s statistical approach, does not exhibit a phase transition in any dimension. It was more than a decade later that Onsager explicitly solved for the properties of the two dimensional Ising model using the Gibb’s approach and demonstrated that the statistical approach *does indeed predict* a sharp phase transition, but *only in the limit of infinite volume*.

Why were these questions difficult to answer before the work of Onsager? The answer is that the phenomena we have just described do not emerge in an “automatic” manner from the formalism of Gibbs without introducing some new ways of thinking and another layer of new concepts, which are needed to think about these macroscopic phenomena. In this lecture, we will try to provide a preview of these new ideas, which will be fleshed out in considerable detail in the rest of this course.

Consider then, the phenomenon of crystallization of a liquid. What is the distinction between water in its liquid phase, and a block of ice? At an intuitive level, one might say that water flows and assumes the shape of its container, while ice is rigid. Digging slightly deeper, we would ask: What is it that allows water to flow, but requires that ice be rigid? After all, both are made of the same water molecules, so why the distinction? The answer comes from a study of the internal arrangement of water molecules in ice: Water molecules in ice (and there are actually many different ice-phases of water, but that is a matter of detail that need not concern us here) are arranged in a regular array. On the other hand, the positions of water molecules in liquid water bear no particular relationship with each other.

This regular arrangement of molecules breaks a symmetry of the underlying equations of motion, namely the symmetry of translations in three dimensional space. To understand this symmetry breaking better, we can assume that the positions of all other water molecules are fixed once the “first” water-molecule decides where it will sit. But since all points in space are equivalent, there is an infinite choice of positions for this “first molecule”. These choices are connected by translational symmetry. This translational symmetry, at least in idealized experiments, is broken “spontaneously”. In other words, no external force tells the water molecules which of the symmetry equivalent set of positions they should choose.

This notion of spontaneous symmetry breaking is at the heart of our present day understanding of a large class of phase transitions in which it is possible to make a sharp symmetry distinction between the high and low temperature phases.

In such cases, the two phases are distinguished by the presence of “long-range order” which is present in one phase and absent in the other—in our example above, this long-range order is simply the statement that the relative position of two far away water-molecules is fixed in the crystalline ice phase, but not in the liquid water phase.

The notion of an “order parameter” provides a sharp characterization of the presence of long-range order, and the spontaneous breaking of symmetry. In the case of a crystal, the order parameter is the Fourier component of the mass density at wavevectors corresponding to the reciprocal lattice vectors of the crystal lattice (familiar from your elementary solid state physics course).

Whenever a continuous symmetry is broken and there is long-range order, there is an associated “rigidity” property that goes hand in hand with this symmetry breaking. In the case of a crystal, this rigidity corresponds closely

to our intuitive, colloquial usage of the term, as well as to the notion of a “rigid body” in solid mechanics. In other examples like a ferromagnet or a superfluid, it is a generalization of the notion of rigidity familiar from solid mechanics.

To illustrate this, let us consider the example of an insulating antiferromagnet made up of localized magnetic moments (spins) with anti-aligning interactions on a bipartite lattice (whereby every spin points anti-parallel to its neighbours). In the low temperature phase, the magnetic moments thus spontaneously choose a common axis  $\vec{n}$  so that each  $A$  sublattice spin points along this axis, which all its  $B$  sublattice neighbours point antiparallel to this axis. This spontaneously breaks the symmetry of simultaneous rotation of all the spins in tandem in spin space.

This symmetry breaking is associated with long-range order of the spins: two  $A$ -sublattice spins point in the same direction even if they are located very far away from each other. This long-range order can be characterized by a non-zero value for the order parameter, which, in this case, is the antiferromagnetic order parameter  $\vec{m}$  defined as

$$\vec{m} = \sum_{\vec{r}} \eta(\vec{r}) \langle \vec{S}(\vec{r}) \rangle \quad (2)$$

where  $\eta(\vec{r})$  is  $+1$  ( $-1$ ) for  $\vec{r}$  belonging to the  $A$  sublattice ( $B$  sublattice).

As in the case of crystal formation, the spontaneous breaking of symmetry is accompanied by the development of rigidity. In the case of the antiferromagnet, the rigidity has to do with the fact that a gradient  $\nabla \vec{m}$  in the order parameter costs nonzero energy per unit volume—the net energy cost is then proportional to

$$\Delta E \sim \rho_n \int d^d x (\nabla \vec{m})^2. \quad (3)$$

Here  $\rho_n$  is the rigidity or stiffness parameter.

Whenever a continuous symmetry (such as the symmetry of translations or the symmetry of rotations in spin space) is spontaneously broken by the establishment of long-range order, one always has “gapless” elementary excitations which cost arbitrarily low energy to produce if the wavelength associated with the excitation is allowed to become arbitrarily long.

These excitations are similar to the “Goldstone modes” familiar to particle physicists. The reason for their existence is quite simple and general.

Since the symmetry that is spontaneously broken is a continuous symmetry, *there is no energy cost* to performing a global symmetry operation that rotates all the spins of the system, and thereby rotates the order parameter  $\vec{m}$  rigidly. Upon doing so, one obtains a new state that is symmetry equivalent to the original state. Now, one can *introduce a small and very slow spatial dependence* in  $\vec{m}$  by performing slightly different rotations at different points in space. Clearly, the energy cost for making this excitation goes to zero as the wavelength of the spatial dependence goes to infinity. And therefore, there are gapless low energy modes whose excitation energy goes to zero as their wavelength goes to infinity.

This brings us to the final and most subtle aspect of spontaneous symmetry breaking: Namely, how do we reconcile

$$\vec{m} \neq 0 \tag{4}$$

with

$$\vec{m} = \text{Tr} \sum_i \eta(r) \vec{S}(r) e^{-\beta H} \tag{5}$$

when  $H$  is symmetric under a global spin flip  $\vec{S}(r) \rightarrow -\vec{S}(r)$  which sends  $\vec{m}$  to  $-\vec{m}$ , and therefore seems to imply

$$\vec{m} = 0 \tag{6}$$

The answer follows if we ask: Once the system has settled into an equilibrium state with order parameter  $\vec{m}$ , how long does it take to reorient the order parameter vector to point in a different direction? If this time is very large, then the statistical prescription for calculating  $\vec{m}$  from the Gibbs distribution is not appropriate, since it assumes in effect that the system has had time to explore all available states on time scales less than the experimental timescale.

What is it that actually prevents the order parameter from exploring on the experimental timescale all the symmetry related choices available to it? For instance, what prevents the antiferromagnetic order parameter  $\vec{m}$  from rotating to point in a different direction in spin space on the time scale of a neutron scattering experiment? It is this question that goes to the heart of the matter, and the answer to it is actually quite simple: The point is that the order parameter *does rotate*, but on a timescale that *diverges* with the size of the system.

This is in effect due to the fact that the order parameter is, in a certain well-defined sense which we make precise below, a “heavy” “classical” variable with very slow dynamics. How does this actually come about? The answer is obvious if we ask the corresponding question for the case of a crystal. Assuming a perfectly rigid crystal, in which the relative positions of all the molecules in the crystal is fixed, the only remaining low energy degree of freedom is the center of mass coordinate  $q_{CM}$ . The conjugate variable is of course  $P_{tot}$ , the total momentum of the crystal as a whole. Thus, a system that has spontaneously broken translational symmetry to form a crystal will have a “tower” of very low energy states corresponding to the center of mass degree of freedom. The corresponding effective Hamiltonian is

$$H_{eff} = \frac{P_{tot}^2}{2M_{tot}} \quad (7)$$

The ground state is of course the state with  $P_{tot} = 0$ , *i.e.* the state whose wavefunction  $\Psi(q_{CM})$  is uniformly spread out over all space. A system in this state corresponds to the crystal order parameter sampling all its symmetry equivalent values without prejudice. However, since the mass  $M_{tot}$  goes to infinity in the thermodynamic limit, a *wavepacket* localized at a particular location  $q_{CM} = r_0$  with a spread of  $\delta r$ , will remain stable over a time-scale  $\delta t \sim \hbar/\delta E$ , where the spread in energy  $\delta E$  can be estimated as

$$\delta E \sim \frac{\hbar^2}{2M_{tot}(\delta r)^2} \quad (8)$$

This gives

$$\delta t \sim \frac{2M_{tot}(\delta r)^2}{\hbar} \quad (9)$$

The main thing to notice in this formula is that the time over which the wavepacket remains stable, *i.e.* the time over which the order parameter remains well-defined, scales with the *total mass* of the system, which means it diverges in the thermodynamic limit of infinite volume and constant finite density.

This is the key point. Quite generally, the order parameter variable has its own dynamics, which, in a finite system allows it to explore all symmetry equivalent choices—in other words, there is no spontaneous symmetry breaking, and no sharp phase transition in finite volume. However, as the system

volume becomes large, this dynamics slows down because the corresponding degree of freedom becomes “heavy” and “classical”—in other words, there is always some analog of  $M_{tot}$  which diverges in the thermodynamic limit, leading to the possibility that the symmetry broken state has infinite lifetime in this limit.

All of this will be quite explicitly demonstrated in the examples we take up later in the course, and I suggest you come back and re-read this chapter midway through the course—this will allow you to correlate what you have learnt, with the general comments made here.