Lecture 1 — Introduction

Quantum mechanics – describes matter at the atomic level and below.

Things that we see around us consist of a huge number of atoms $\sim 10^{23}$.
Even though individual atoms obey quantum mechanics it is impossible to describe macroscopic collections of ~~atoms from "first principles" i.e. by solving~~ microscopic particles "from first principles", i.e. by solving a many-particle Schrödinger equation.

Macroscopic systems obey entirely different laws that follow, but are not derivable from quantum mechanics.

Statistical physics or many-body physics describes macroscopic matter, i.e. systems consisting of macroscopic number of quantum particles.

Statistical physics I – basics of statistical physics, ~~[illegible] macroscopic~~ theory of ideal gases.

Statistical physics II – theory of phases and phase transitions.

One of the most fundamental facts in physics: macroscopic matter exists in different phases.

Examples :

1. Solid - liquid - gas.
2. Ferromagnet - Paramagnet.
3. Superconductor - normal metal or insulator.
4. Metal - Insulator.
5. Superfluid - normal liquid.

Phases of matter are distinguished by certain robust macroscopic properties, which are either present or not.

Examples :

1. Solid - has rigidity to shear deformation.
   Liquid - does not have rigidity to shear deformation.
2. Liquid - has a well-defined interface
   Gas - does not have a well-defined interface
3. Ferromagnet - has macroscopic magnetization in the absence of external field.

   Paramagnet - does not have macroscopic magnetization.
4. Superconductor - has zero resistance and expels magnetic field (Meissner effect)
   Normal metal - finite resistance and no Meissner effect.

Fundamental idea, due to Landau:
macroscopic properties, distinguishing different phases of matter arise as a consequence of <u>ordering</u>.

<u>Examples</u>:

1. Rigidity of a solid is a consequence of ordering of atoms in a crystal lattice. (not always true: in 2D a solid can have a finite rigidity but no perfect crystalline order – the order in this case is more subtle – topological).

2. Macroscopic magnetization of a ferromagnet is a consequence of alignment of atomic magnetic moments.

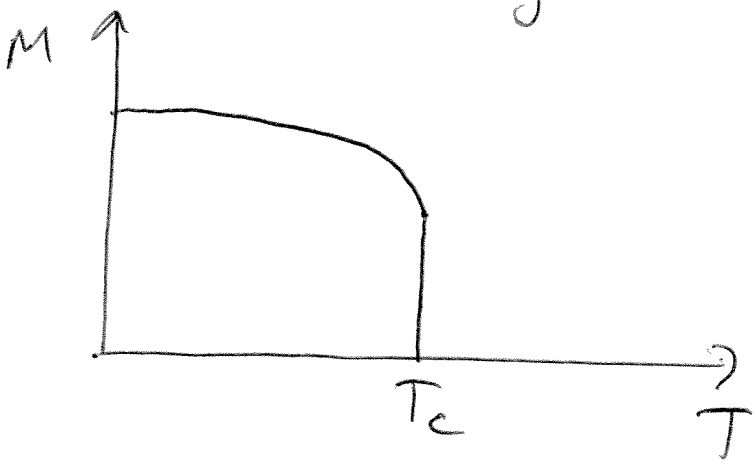
3. Superconductivity is due to phase coherence of electron pairs.

The degree of ordering can be quantified by an order parameter – a physical quantity which is zero in one phase and nonzero in the other.

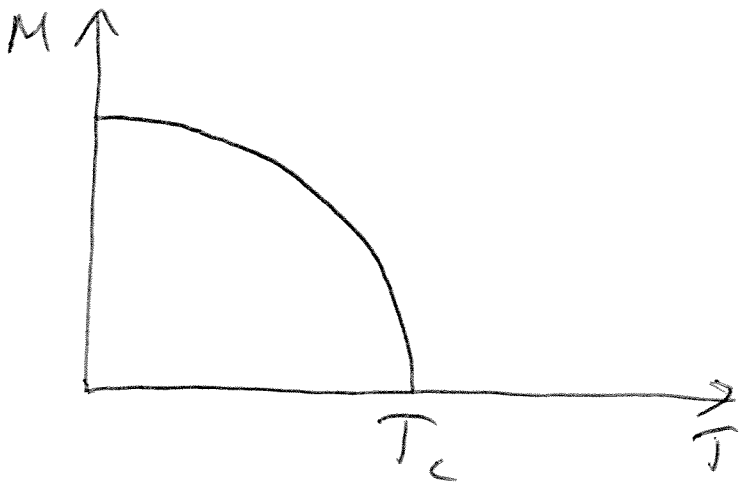
<u>Examples</u>:

1. Magnetization M for paramagnet – ferromagnet pair.
2. Shear modulus for solid – liquid.
3. Macroscopic wavefunction for superconductor.

Transitions between different phases can be first or second order.
At a first order phase transition the order parameter changes discontinuously:



At a second order phase transition the order parameter changes continuously:



In this class we will focus almost exclusively on second order phase transitions.

Phase transitions can also be classified into classical or thermodynamic and quantum.
Classical phase transitions occur as temperature is varied.
Quantum phase transitions occur at $T=0$ as some parameter in the Hamiltonian is varied.

We will start with classical phase transitions.

We will develop the theory of phase transitions starting from a concrete microscopic model of interacting "particles".
The simplest such model is the <u>Ising model</u>:

$$\mathcal{H} = -\frac{1}{2} \sum_{ij} J_{ij} \sigma_i \sigma_j$$

Here i label the sites of d-dimensional hypercubic lattice, $J_{ij} > 0$ and $\sigma_i = \pm 1$.

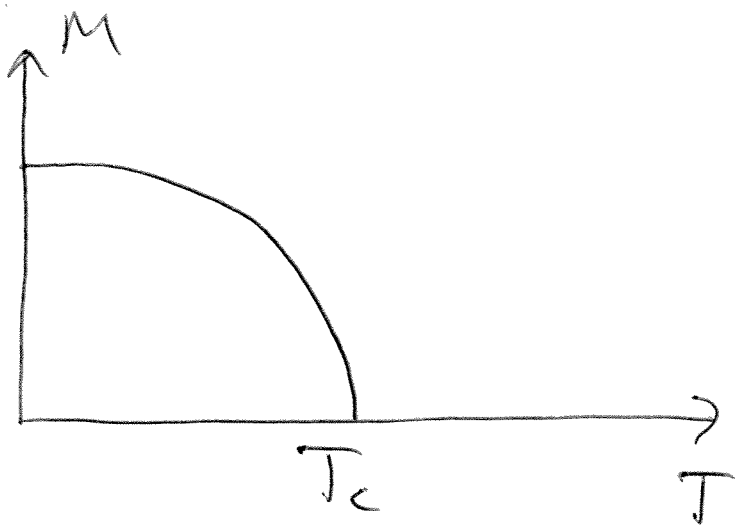
σ_i can represent z-component of atomic magnetic moment, in which case Ising model is a model of ferromagnetism; σ_i can also represent the presence $(+1)$ or absence (-1) of a particle at a given site — in this case this is a simple model of interacting particles. It turns out that a lot of phase transitions observed in nature are related to Ising model, we will see why later.

Ising model has two phases — ferromagnetic and paramagnetic.

They are distinguished by the following order parameter:

$M = \langle \sigma_i \rangle$ — macroscopic magnetization per site.

$\langle \ \rangle$ denote thermodynamic average.



$T < T_c$ - ferromagnetic phase, $M \neq 0$.

$T > T_c$ - paramagnetic phase, $M = 0$.

<u>Spontaneous symmetry breaking</u>

Note that the Ising model Hamiltonian is invariant under the following transformation:

$$\sigma_i \to -\sigma_i \quad \forall i.$$

This means that there are two ferromagnetic states: one with $M > 0$ and the other with $M < 0$. Due to the above symmetry of the Hamiltonian these states have the same free energy and are equally probable. However, in a ferromagnetic state M has a definite sign $\Rightarrow$ the symmetry of the Hamiltonian is <u>spontaneously broken.</u>

Existence of a nonzero order parameter is often (but not always) related to spontaneously broken symmetry: the phase with zero order parameter

(disordered phase) has full symmetry of the Hamiltonian, while in the ordered phase this symmetry is spontaneously broken, i.e. ordered phase is less symmetric.

Let's add a uniform "magnetic field" B to the Ising model Hamiltonian:

$$H = -\frac{1}{2}\sum_{ij} J_{ij}\sigma_i\sigma_j - B\sum_i \sigma_i$$

Let's assume that the system is finite - the lattice has a total of N sites.
Assume that N is large. In this case:

$$\frac{1}{N}\sum_i \sigma_i \approx M.$$

Then:

$$H = -\frac{1}{2}\sum_{ij} J_{ij}\sigma_i\sigma_j - BNM.$$

B clearly breaks the $M \to -M$ symmetry of the Ising model.

If $B > 0$ the state with $M > 0$ will be preferred.

Consider relative probability for the system to be in a state with $M > 0$ vs in a state with $M < 0$ at some temperature T.

$$\frac{P_{M<0}}{P_{M>0}} = \frac{e^{-\frac{NBM}{T}}}{e^{\frac{NBM}{T}}} = e^{-\frac{2NBM}{T}}$$

Throughout this class I will use units in which $k_B = 1$, i.e. the temperature has dimensions of energy.

Now consider the limit $B \to 0+$, taken at fixed N.

Obviously $\frac{P_{M<0}}{P_{M>0}} \longrightarrow 1$, i.e. $M \to 0$ as $B \to 0+$ at fixed N.

On the other hand, if we take the limit $N \to \infty$ (thermodynamic limit) first and only after that take the limit $B \to 0+$, we will have:

$$\frac{P_{M<0}}{P_{M>0}} \longrightarrow 0$$ — the system will remain in the $M>0$ state even in the limit $B \to 0$ — spontaneous symmetry breaking.

This shows that spontaneous symmetry breaking and therefore sharp distinction between phases are only possible in the thermodynamic limit.

Mean-field theory

We want to develop a description of the ferromagnet paramagnet transition in the Ising model, preferably a description that can be generalized to other models.

In 1D the Ising model can be easily solved exactly by the transfer matrix method (first done by Ising). It turns out that in this case there is no phase transition: $M=1$ at $T=0$, but $M=0$ for all $T>0$.

In 2D there is also an exact solution due to L. Onsager. From this solution it follows that there is a phase transition at nonzero T. This solution however, is quite complicated and is specific to the 2D Ising model it can't be generalized even to the same model in 3D.

An exact solution for 3D Ising model has not yet been found and probably doesn't exist. There is a relation between 3D Ising model and certain type of string theory.

We want to develop a universal framework for the description of phase transitions. The first step towards such a description is mean-field theory.

We can write σ_i as:

$$\sigma_i = \sigma_i - \langle \sigma_i \rangle + \langle \sigma_i \rangle = \sigma_i - M + M$$

Substitute this into the Hamiltonian:

$$\sigma_i \sigma_j = (\sigma_i - M + M)(\sigma_j - M + M) =$$
$$= (\sigma_i - M)(\sigma_j - M) + (\sigma_i - M)\cdot M + (\sigma_j - M)\cdot M +$$
$$+ M^2 = (\sigma_i - M)\cdot(\sigma_j - M) + M\cdot(\sigma_i + \sigma_j) - M^2$$

Assume that fluctuations about the mean value are small $\Rightarrow$ can neglect $(\sigma_i - M)\cdot(\sigma_j - M)$ term.
At this point, there is no justification for this, will discuss justification later.

The Hamiltonian becomes:

$$\mathcal{H} = -\frac{1}{2}\sum_{ij} J_{ij} M (\sigma_i + \sigma_j) + \frac{1}{2}\sum_{ij} J_{ij} M^2$$

let $J = \sum_j J_{ij}$ – doesn't depend on i if the Hamiltonian is translationally invariant.

Assume that J is finite – we will only consider such cases.
This means that J_{ij} has to decrease fast enough with the separation between the sites.

Then we obtain:

$$\mathcal{H} = -MJ\sum_i \sigma_i + \frac{1}{2}NJM^2$$

Now we can calculate the free energy.

$$F = -T\ln Z, \quad Z\text{ - partition function.}$$

$$Z = \sum_{\{\sigma\}} e^{-\frac{\mathcal{H}}{T}} = \prod_{i=1}^{N} \sum_{\sigma_i=\pm 1} e^{-\frac{\mathcal{H}}{T}} =$$

$$= e^{-\frac{NJM^2}{2T}} \prod_{i=1}^{N} \sum_{\sigma_i=\pm 1} e^{\frac{MJ\sigma_i}{T}} =$$

$$= e^{-\frac{NJM^2}{2T}} \prod_{i=1}^{N} \left[e^{\frac{MJ}{T}} + e^{-\frac{MJ}{T}} \right] =$$

$$= e^{-\frac{NJM^2}{2T}} \left[2\cosh\left(\frac{MJ}{T}\right)\right]^N$$

Thus the free energy is equal to:

$$F = \frac{NJM^2}{2} - NT\ln\left[2\cosh\left(\frac{MJ}{T}\right)\right]$$

M can be found by minimizing F.

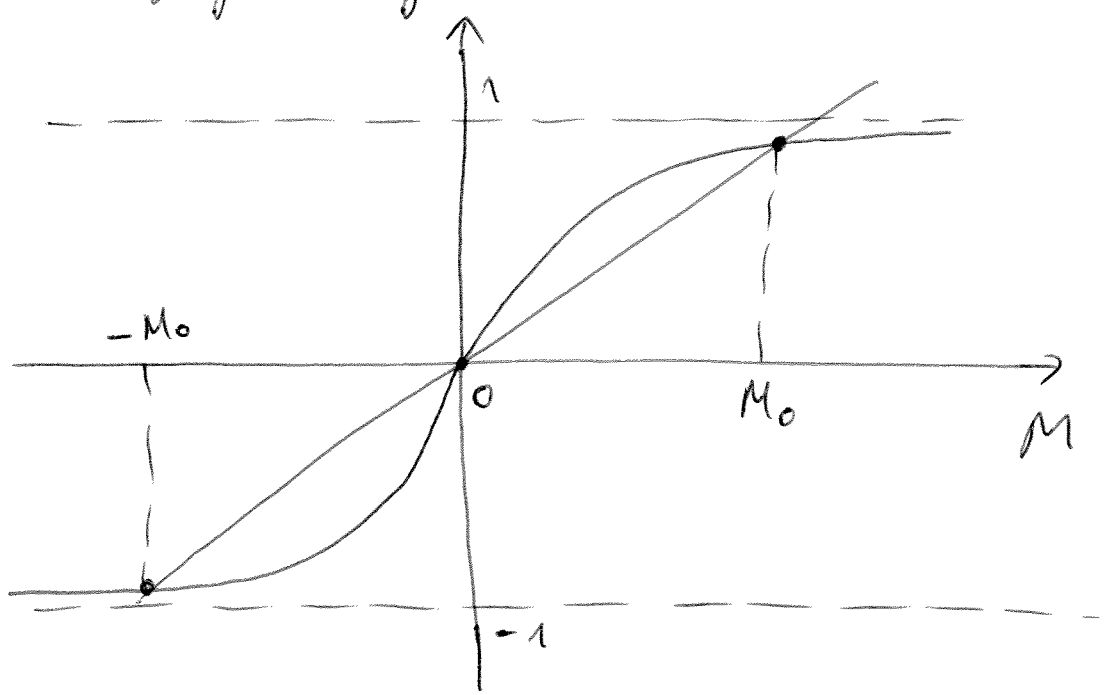
$$\frac{\partial F}{\partial M} = 0$$

$$\frac{\partial F}{\partial M} = NJM - JN\tanh\left(\frac{MJ}{T}\right) = 0$$

Thus we obtain a nonlinear equation for M:

$$M = \tanh\left(\frac{MJ}{T}\right)$$

Solve graphically.



The slope of $\tanh\left(\frac{MJ}{T}\right)$ is inversely proportional to T at small M. The transition happens when the slope becomes equal to 1.

Thus $T_c = J$.

$T > T_c$, the only solution is $M = 0$.

For $T < T_c$, there are two nontrivial solutions, $M = \pm M_0$. The system will spontaneously pick one of the solutions – spontaneously broken symmetry.