PH325: Advanced Statistical Mechics

Chapter 1: Models, Scales, Symmetries

We have seen in the introductory discussion that phases and phase transitions are ubiquitous in physics. Further, we have seen that in a given phase transition only some key degrees of freedom of the constituent objects are involved. Keeping in mind these points, and drawing on the vast experience, insights and brilliancies of our predecessors, we follow the path laid out by them in studying the phyics of phases and phase transitions. This is by constructing some well thought out models that capture the crucial physics.

What is really a "model"? A model is a "minimal" description of a system

of intents, that allows us in a realistic fashion ask and answer questions related to the system. Ideally, a model (or theory) must not only "explain" but "predict".

Construction of a model involves identifying three key things

① The "arena" – { continuum/lattice
{ spatial dimension

② The key degrees of freedom
– { phase space
{ Hilbert space

③ The Hamiltonian → This denotes the "energetics" and even "dynamics".

A system definition will require its symmetries and the understanding of [redacted] scales. (Scales mean the intrinsic energy scales, extrinsic scales (such as temperature) – broadly called as coupling constants).

This then allows us to proceed with the calculation. Let us discuss these things a bit further.

The arena is usually either a continuum (L^d) or lattice (L^d) in d dimens., where L^d is the volume (. ~~vacuo~~ for the lattice). If we have a lattice, we have to specify its structure, such as simple cubic (in 3d) or triangular (in 2d). We will find that the structe of the lattice can have a big say in what finally happens. ~~Adeep~~

The second part is identify the key degrees of freedom (dof). At each point in the "arena" we associate a degree of freedom. The dof can by any kind of quantity, number, vector, tensor, matrix, complex number, grassmann variables ~~used~~ etc, in other words whatever

You can think of (or not!) this defines us the phase space, configuration space, or Hilbert space. Ω. We shall use these phrases interchangably.

The third part requires writing down a Hamiltonian for the set of degrees of freedom in our arena. A key steps in the process is the identification of the symmetries of our system. This is where our "physical experience" is used. (indeed, we have already used this in the identification of the degrees of freedom, but now we need this even more!)

What do we mean by symmetry of our system?

Crudely; it is the set of things which we can do to the system with out "changing" any physics.

Let be a bit abstract cabout this. Let Ω be the space of configurations. Let x be one configuration

Let U be a symmetry operation. Then $x' = Ux$ is a new configuration. x' and x are said to be "symmetry related". We ask what is the relation between $\mathcal{H}(x)$ (the Hamiltonian defined as a function of the configuration), $\mathcal{H}(x')$? If it turns out that $\mathcal{H}(x') = \mathcal{H}(x)$ $\forall x$, then U is a symmetry of our system. This way of defining the symmetry is the "Schrödinger picture". We can also view it in the "Heisenberg way": we say if $H' = U^{+} H U$ is invariant, ie $H' = H$., then U is a symmetry of our system.

Usually there are many Us that are symmetries of our system. In fact, symmetries can be described by a parameter $a \to$ we write $U(a)$. If a is a continuous parameter, we call this a continuous symmetry while if a is a discrete parameter, we call this a discrete symmetry (sit tight, we will see concrete examples). Further, the symmetries usually come in different varieties and form groups (in the mathematical sense).

Once we identify the symmetries of the system, we can write down the Hamiltonian. The usual trick is to put down terms (such as kinetic energy, potential energy, interaction energy) such that the total ~~system~~ has the necessary symmetry. In fact, in practice, each term (except perhaps what are called a source terms) have the symmetry required. Let us call each of these terms $H(x) = \sum_i \mathcal{H}_i(x)$, i runs over all "terms". Now associated with each $\mathcal{H}_i(x)$ there may be some characteristic scales (usually energy scales). The set of all such ~~scales~~ quantities form the intrinsic coupling constants of the system. Note that there can be energy scales that are not apparent in the Hamiltonian (such as the lattice spacing).

Once we are done identify our system, (arena, dofs, Hamiltonian), we can study what the system looks like when we change some "external" parameters such as temperature or chemical potential or pressure.

We will ~~not~~ usually use the canonical / grand canonical ensemble. and this will introduce new scales such as temperature or chemical potential. Just keep in mind that the distinction between intrinsic and extrinsic scale (such as temperature) is completely artificial. (You will realize this later).

Now the Gibbs distribution

$$\rho(x) = \frac{e^{-\beta \mathcal{H}(x)}}{Z}$$

defines the probability distribution.

$$\langle O \rangle = \int dx \, \rho(x) \, O(x)$$

where O is some observable.

Now $\rho(x)$ describes the state of our system kept (by us) in a given condition of temperature etc. It is the answer to the problem!

~~But~~ It is natural to now ask: How do I know that my system is expected to show

Different phases and phase transitions behind the phases. Suppose I know about state (i.e. ρ is given), how do I know if I am in one phase or the other?

This naturally raises the question of what a phase is. We will not worry about this immediately and take an intuitive idea of a phase for granted.

To get an idea of <u>how to describe a phase</u>, we look at a magnet. Above T_c, the system is paramagnetic and there is no magnetic moment - the spins are not <u>ordered</u>. However, below T_c the story is entirely different. The spins form a "well organized" array and we obtain a nonzero magnetization.

The first thing you notice is that the magnetized <u>state</u> does not have the symmetry of the system (In this case the spin rotation symmetry). In other words if ρ_m is the magnetized state $U^{-1}\rho_m U$ is <u>not</u> equal to ρ_m!

But this is rather puzzling! We say that

$$\rho \sim e^{-\beta \mathcal{H}}$$

It has the $\mathcal{H}$ symmetry but ρ does not! which is rather contradictory. No alarm! Indeed, there is more to this.

To see whether ρ describes an "ordered phase" we have to do something more. Take our system and apply a symmetry breaking field.

$$H_B = \mathcal{H} - BS$$

where S is a physical quality that couples to the magnetic field.

Now

$$\rho_B(x) \sim e^{-\beta(\mathcal{H}(x) - BS(x))}$$

Note that the $-BS$ term breaks the symmetry of the system $\mathcal{H}$ - deliberately!

Now comes the key:

We obtain:

$$\rho = \lim_{B \to 0} \lim_{V \to \infty} \rho_B \qquad (V = L^d)$$

If we now find that

$$U^{-1} \rho U \neq \rho$$

then we say that ρ describes a broken symmetry state.

Note that the order of limits in the above equation is CRUCIAL!

For example

$$\tilde{\rho} = \lim_{V \to \infty} \lim_{B \to 0} \rho_B$$

will always repeat the symmetry.

i.e., $U^{\dagger} \tilde{\rho} U = \tilde{\rho}$.

In other words ρ and $\tilde{\rho}$ defined in the two equations can be different!

This is tantamount to the famous statement found in books that "true" phase transitions occur only in the thermodynamic limit, or statement like, only in the thermodynamic limit does the free energy have singularities. Rather than explore the formal formulations of these statements, we will learn by example.

So the overall strategy is clear:

(0) Identify the problem of interest

(1) Define the model.

(2) obtain $\rho = \lim_{B\to 0} \lim_{V\to\infty} \rho_B$.

This is one way of obtaining a phase diagram.

Admittedly, this stuff is all quite "abstract". The best thing one can do now is to put down some specific models and study them.

1. Interacting particles

This model can be used to study ~~Ideal~~ Imperfect gases, liquids and solids. We think of the simplest (mass m) structureless particles such as Argon atoms. We will also restrict ourselves to classical mechanics.

(A) Identify the "arena".

We think of a box of volume V in d dimensions with periodic boundary conditions $V = L^d$. A particle leaving the box will enter it back from the other side.

B) The degrees of freedom. We "label" the particles $i = 1, \ldots, N$, ($n_0 = N/V$ is the density which is fixed)

$$x = \{\vec{r}_i, \vec{p}_i\}$$ (positions and momenta of all particles)

and

Ω = the set of all possible x.

C). What is the Hamiltonian of the system. Let us find out the symmetries of our system to begin with.

① Translation ② Rotation ③ Time reversal.

We can now put down terms (based on "experience") in the Hamiltonian.

$$\mathcal{H}(x) = \underbrace{\sum_{i=1}^{} \frac{p_i^2}{2m}}_{\text{Kinetic}} + \underbrace{\frac{1}{2} \sum_{i \neq j}^{} V(|\vec{r}_i - \vec{r}_j|)}_{\text{Potential or Interaction}}.$$

Note that each term respects the symmetries. Let us see this explicitly.

Let $T(\vec{a})$ be a translation operator.

Note that $T(\vec{a})$, $\forall \vec{a}$ form an Abelian group (show this).

$$T(\vec{a})\, x = \{\vec{p}_i, \vec{r}_i + \vec{a}\} = x'.$$

Note $\mathcal{H}(x') = \mathcal{H}(x)$

Since we can see that $R(\theta,\varphi)$ (rotation defined by Euler angles) $SO(3)$ group leaves the ~~Hamiltonian~~ system unchanged.

Time reversal has Θ

$$\Theta x = \{-\vec{p}_i, \vec{r}_i\}$$

also leaves the system invariant. Note that time reversal is a <u>discrete</u> group $\{1, \Theta\}$ such that $\Theta^2 = 1$

(This is <u>not</u> generically true, particularly with fermion and spin $-1/2$ particles).

We have now a complete model once we specify the interaction potential V. We now specify external conditions such as temperature $T(1/\beta)$ and a chemical potential μ.

Define

$$\mathcal{H}(x) = H(x) - \mu N$$

N is the number of particles

$$Z = \text{tr}\, e^{-\beta \mathcal{H}} \equiv \int dx\, e^{-\beta \mathcal{H}(x)}$$

$$= Z_{ideal}\, Z_{int}$$

$Z_{ideal}(\beta, \mu, V)$ is the partition function of a classical ideal gas while Z_{int} is the interacting contribution to the partition function (Note that such splitting up is generically not possible if we are dealing with quantum mechanics)

$$Z_{int} = \int \Pi d\vec{r}_i\; e^{-\frac{\beta}{2} \sum_{i \neq j} \phi(|\vec{r}_i - \vec{r}_j|)}$$

* This looks like a discrete problem, in that there are ~~a fixed number of particles~~ discrete sums. But note that we can convert this problem to a "field theory" The trick is to define a function which depends on $\vec{r}$ (the spatial coordinate)

Define a function

$$n(\vec{r}) = \sum_i' \delta(\vec{r} - \vec{r}_i)$$

to obtain

$$\mathcal{H}_u = \sum_{ij}' u(|\vec{r}_i - \vec{r}_j|) = \int d\vec{r}\, d\vec{r}'\, n(\vec{r})\, u(|\vec{r}-\vec{r}'|)\, n(\vec{r}')$$

Thus

$$Z_{ex} = \int \mathcal{D}[n(\vec{r})]\; e^{-\frac{\beta}{2}\int d\vec{r}\, d\vec{r}'\, n(\vec{r})\, u(|\vec{r}-\vec{r}'|)\, n(\vec{r}')}$$

Note that the integral on the right hand side is a functional integral.

Note that $Z = Z_{ideal}\, Z_u$.

Nothing interesting happens with Z_{ideal}.

So we can in fact redefine our problem a little bit. We say that our configuration space is given by set of all density functions $n(\vec{r})$. (This allows us many techniques of field theory to be used. More on this later.) Note that $(x \equiv n(\vec{r}))$

$$T(\vec{a})\, x = n(\vec{r}+\vec{a}).$$

With this we can easily see that $\mathcal{H}_u$ is translation invariant.

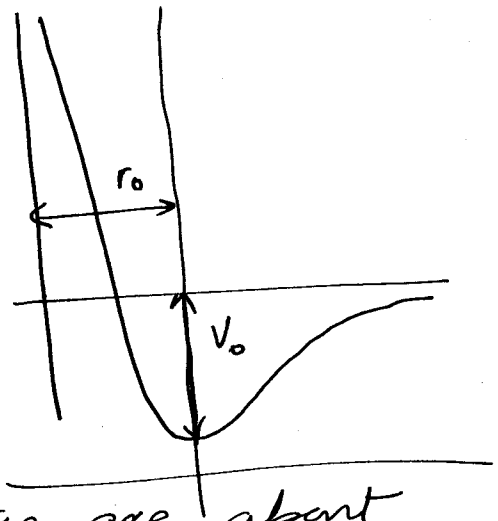
If we work in the grand canonical ensemble we have

$$\frac{1}{V}\int d\vec{r}\, \langle n(\vec{r}) \rangle = n_0$$ which then

delermis the chemical potential.

Let us now consider states of this system. To see the physics, we have to understand the scales in the system. For this we need to specify the potential of interaction $u(r)$.

A typical potential is of Lennard-Jones type and is specified by a couple of scales r_0 and V_0.



Now ~~let us~~ we see that there are about four scales in the problem. T - kinetic energy, r_0, V_0 and n_0 (density of particles).

Let us stay in 3D. If we now assume that $T \ll V_0$ and $r_0 \simeq n_0^{-1/3}$, then we expect that the atoms will form

a crystalline solid. How do we describe the state of the system? Where the atoms have formed a solid. Here the atoms arrange themselves in a lattice (such a bcc) with lattice point $\vec{R}_i$ (Let us work at zero temperature). Then

$$x = \{\vec{0}, \vec{R}_i\}$$

and are standing still in space at $\vec{R}_i$. In terms of the density the state is described by $x = n_s(\vec{r}) = \sum_i \delta(\vec{r} - \vec{R}_i)$

The probability distribution is a functional

$$\delta\text{-function} \qquad S = \delta[n - n_s].$$

We immediately see that

$$T(\vec{a})\, x = n_s(\vec{r}+\vec{a}) \neq n_s(\vec{r})$$

and consequently

$$T^{\dagger}(a)\, S\, T \quad \text{is also not translationally}$$

invariant. Thus this state of the system does not have the symmetry of the Hamiltonian! This is an example of a state with broken symmetry.

Note that in a gaseous state the translational symmetry is preserved. In a solid, where the atoms are arranged regularly, translational symmetry is broken. We know that gas and solid are different phases. We pick up on first clue to describing phases. Phases may possess different symmetries! In other words symmetry can be used to describe phases. Note that the converse is not true, i.e., if two phases have same symmetry they are the same. — this statement is FALSE (why?).

2. Ising Model.

The Ising Model will be the work horse for this course. It can describe many physical phenomena as uniaxial magnets (both ferro and antiferro), order-disorder transition (such as β-brass), liquid-gas transition, etc. (Yes, you should be surprised by this! What has a magnet got to do with liquid-gas transition?)

The Ising model was suggested to Ising as a thesis problem by his advisor Lenz some time in the 1920s. Very soon many prominent physicists realized the power of this model in the conceptual foundation of statistical physics. The model as studied by Ising was meant to study magnetic phenomena and associated phase transitions.

The standard example of an Ising magnet is $LiHoF_4$ which is a tetragonal crystal. The Ho^{3+} ions have a magnetic moment which interacts with others via dipolar coupling. The spin of an ion is a quantum mechanical entity. In the case of Ho^{3+} ions, there a very strong ~~[illegible]~~ anisotropy in the crystal that make the spin point only standing the $\pm\frac{1}{2}$ direction of the tetragonal ~~[illegible]~~ plat. Thus the only allowed

states are $|\uparrow\rangle$ or $|\downarrow\rangle$ at each site.
This is what we want to model — and this is the Ising model. Let us discuss this within the frame work of our formulation.

1. Arena. The arena of the Ising model is a lattice. We will, for most part, take a hypercubic lattice in d dimension. The lattice parameter of the lattice is 'a'. We will consider a lattice of volume $V = L^d$ with N sites, $N = \frac{V}{a^d}$. The volume of the unit cell is a^d, and the Brillouin zone of the lattice is $\left[-\frac{\pi}{a}, \frac{\pi}{a}\right]^d$.

(2) Degrees of freedom.
As was discussed above, there is a strong uniaxial constraint in the magnets that we are interested in. This means that the degree of freedom at a site is the spin in the $|\uparrow\rangle$ state or $|\downarrow\rangle$ state. We can therefore represent this by a number $s_i = \pm 1$

+1 stands for $|\uparrow\rangle$ and -1 for $|\downarrow\rangle$.

A configuration $x = \{s_i\}$ where s_i is the set of all spin values on the sites.

Ω the configuration space is the set of all x, which has 2^N entries.

(3) Hamiltonian

To write out a Hamiltonian we need to identify the symmetries.

There are the usual symmetries like ① lattice translation, ② lattice rotation (point group) symmetry etc.

The most important symmetry, in addition to the above, is the internal symmetry.

The key thing is that the system is such that the spin always likes to align along the $+z$ direction or $|\uparrow\rangle$ is completely "equivalent" to the $|\downarrow\rangle$ direction (spin points in the $-z$ direction.

We now now take a configuration $x = \{s_i\}$ and define a symmetry operation F - the flip operation.

$$x' = Fx = \{\bar{s}_i\}$$

where. $\bar{s}_i = -s_i$

We see two things ① F is a symmetry operation $\Omega \to \Omega$ under the action of F ② ~~Every state~~ No configuration x is mapped on to itself.. ~~NOT OK~~

We demand that F be a symmetry of the system. Actually consider another "symmetry" which is doing nothing (you must be pretty familiar with this), call this symmetry I ; $Ix = x$!

Now we have two symmetry operators I and F. We can show that they form a group with the multiplication.

$Z_2 = \{I, F\}$

*	I	F
I	I	F
F	F	I

Note $F^2 = I$. and thus we see that we get a group. This is the famous Z_2 group. We thus demand that the model we write down has the Z_2 Symmetry!

We now want to write a model which has the Z_2 symmetry. and Here is the Ising model.

$$H^{Ferro}_{Ising} = -J \sum_{\langle ij \rangle} S_i S_j$$

$\langle ij \rangle$ runs over all nearest neighbour bonds (and of them in our system). that one $J > 0$, is a coupling constant. This is called the Ferro Ising model. If $J < 0$, it is conventionally written as

$$H^{Af}_{Ising} = |J| \sum_{\langle ij \rangle} S_i S_j .$$

In other words J is always chosen positive which the over all sign decides weather the model is ferro(-) or Anti ferro(+).

One can begin to wonder if this is "just" a discrete model. Actually we can put down the Ising model as a field theory on a continues arena.

Define the Fourier tranform of S_i as $S_i = \frac{1}{\sqrt{N}} \sum_{\vec{k}} s(\vec{k})\, e^{i \vec{k} \cdot \vec{R}_i}$

where $\vec{k} = \frac{\pi}{L}(\frac{m_1}{L} \cdots \frac{m_d}{L})$ $m_i = -\frac{N}{2}+1, \cdots 0, \cdots \frac{N}{2}$

We see that (in the thermodynamic limit)

$$H^F_{Ising} = \frac{V}{(2\pi)^d} \int_{BZ} d^dk \; f(\vec{k}) \, |S(k)|^2 \qquad f(\vec{k}) = -\sum_i^d \cos(k_i)$$

(We have used the fact that S_i is a real function and $S^*(k) = S(-k)$ For those of who are perceptive: This Hamiltonian appears to be "quadratic" in the field $S(k)$ and looks like a non interacting problem. Where then does the interesting physics come from?)

We have now completely specified the problem. To see what physics emerges we now need to do

$$Z = \sum_{\{S_i\}}{}' \; e^{-\beta H_{Ising}(\{S_i\})}.$$

Note that for nearest neighbor interactions there is only one effective coupling constant, that is J/T.

Note that this, as was discussed, obtained with the symmetry breaking fixed ansatz. Let us do this more specifically.

$x = \{s_i\}$

~~$\rho_B(x) = \frac{e^{-\beta \mathcal{H}}}{Z_B}$~~

$\downarrow$ need

$$\mathcal{H}_B(x) = \mathcal{H}^{Ising} - h \sum_i s_i$$

$$\rho_B = \frac{e^{-\beta \mathcal{H}_B(x)}}{Z_B}$$

We need $\lim_{h \to 0} \lim_{N \to \infty} \rho_B(x) = \rho(x)$

This is a highly nontrival problem to evaluate $\rho(x)$. Infact much of this course will deal with ways of evaluting this reliably, albeit approximately.

Let us do something less ambitious. Let us look at just two sites numbers 1 and 2.

The Ising model is (Ferro). 1 — 2

$$H = -J s_1 s_2 - h(s_1 + s_2)$$

$$\Omega = \{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$$

x	$H(x)$
$\|\uparrow\uparrow\rangle$	$-J-h$
$\|\uparrow\downarrow\rangle$	J
$\|\downarrow\uparrow\rangle$	J
$\|\downarrow\downarrow\rangle$	$-J+h$.

Level structure

J ——————— $|\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle$ $(h>0)$

$-J+h$ ——————— $|\downarrow\downarrow\rangle$

$-J-h$ ——————— $|\uparrow\uparrow\rangle$

We see that for $T \ll h$ the configuration $|\uparrow\uparrow\rangle$ is the overwhelmingly most probable. We ask what is the state of the system defined by the following limit.

$$\rho(x) \quad \lim_{h\to 0} \lim_{T\to 0} \rho_B(x)$$

We see that $\rho(x) = \frac{1}{2}\delta(x-|\uparrow\uparrow\rangle)$.

So in a sense the state at $T=0$ obtained by the procedure above is $|\uparrow\uparrow\rangle$ state. But not that the $|\uparrow\uparrow\rangle$ state is not flip symmetric (no pure state is). Thus we see that the ground state has broken the symmetry of the flip Hamiltonian

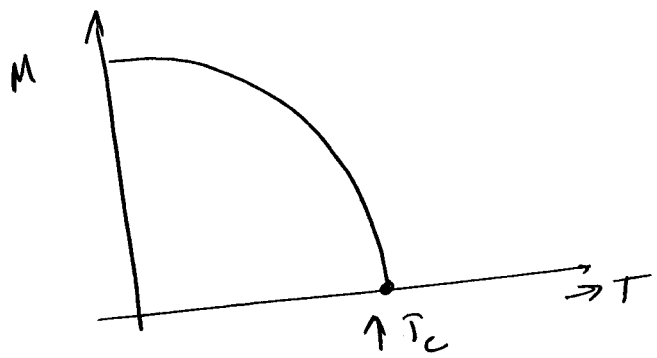
Now we see generically that if $Fx = x'$ and $\rho(x') \neq \rho(x)$ then we have

broken the Flip symmetry, i.e., the state described by $\rho(x)$ is a <u>broken symmetry</u> state.

Define $M = \left\langle \underbrace{\frac{1}{N}\sum_i^{\prime} S_i}_{M(x)} \right\rangle$

$$M = \sum_x^{\prime} \left(\frac{1}{N}\sum_i^{\prime} S_i\right) \rho(x)$$

In a broken symmetry state $M \neq 0$. Indeed we can use this to "describe a phase". We know that in a 3d system like Li Ito F_4, when the coupling constant is changed (Temperature is reduced) has a phase transition.



one reaches T_c, below which $\langle M \rangle \neq 0$.

Below T_c we have a broken symmetry phase while above T_c $\rho(x') = \rho(x)$ and hence $M = 0$. (This is because $M(x') = -M(x)$).

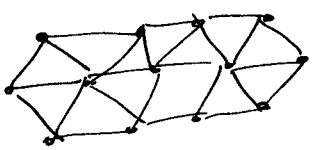
Let us now discuss the Ising antiferromagnet. Note that there is no "symmetry difference" between the F and AF cases. The key difference is the sign of the coupling constant. In many ways the AF system is quite interesting. A key point to be noted is that the lattice structure enters in a crucial way in the AF Ising model.

Let us understand this a little below.

A lattice is said to be bipartite if it can be "decomposed" into two sub lattices A & B such that sites of A sublattice has only B neighbors and vice versa.

Now we make a statement which you have to prove. Hypercubic lattices in d dimensions are bipartite.

Also give an example of a non-bipartite lattice.



The AF state is obtained by pulling say $|\uparrow\rangle$ on the A sublattice and $|\downarrow\rangle$ on the B sublattice.

The key point to be noted is that the order parameter is no longer $\langle M(x) \rangle$ but $M_A(x)$

$$M_A(x) = \frac{1}{N} \sum_i' (-1)^{\alpha(i)} S_i$$

where $\alpha(i) = \begin{cases} 0 & \text{if } i \text{ is in } A \\ 1 & \text{if } i \text{ is in } B \end{cases}$

The ~~ordered~~ state has to be obtained by a symmetry breaking field that is the staggered field

$$\mathcal{H}_B(x) = \mathcal{H}_{Ising}^{AF}(x) - h_s M_A(x)$$

$$\rho_B(x) = \frac{e^{-\beta \mathcal{H}_B(x)}}{Z}.$$

The order parameter is

$M_A = \langle M_A(x) \rangle$ and is nonzero below the Néel temperature.

The AF model on a non-bipartite lattice is frustrated. You will see what this means in a homework.

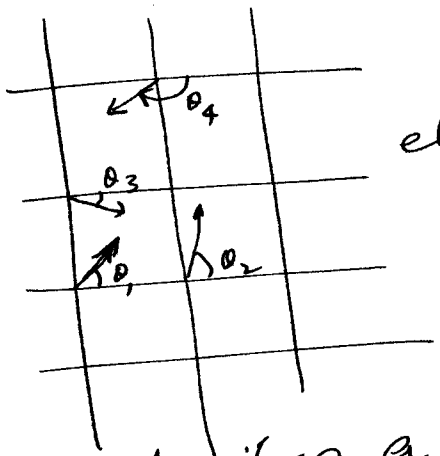
The X-Y model.

The X-Y model is used to study the physics of easy plane magnets (as opposed to the Ising, which is is easy axis), and superconductors.

Arena :- We will chose the simple cubic lattice in d-dimensions. as the arena. Note that we can define this also on more complicated Lattices.

Degrees of freedom :- At each site of the hypercubic lattice we have a vector of fixed length which has two components. This is what makes it "easy plane". There is a plane in "spin-space" if you want to imagine a magnetic problem. Note Now a two component fixed length vector can be denoted by an angle θ

from the fixed "x-axis" of spin space.
Thus we can describe the configuration of this system by a set of angles θ_i at each site $x = \{\theta_i\}$.



etc.

Why this describes a superconductor should be puzzling to you!

Hamiltonian.

We demand the system has rotational symmetry about the "z-axis" in spin-space. O(2) rotation or SO(2)

Rotation by angle α means that ~~each vector is rotated by~~ the vector at every site is rotated by an angle α. $R(\alpha)\, x = x' = \{\theta_i + \alpha\}$.

Note that if $|\theta_i + \alpha| > 2\pi$, we take modulo

Now $\mathcal{H}(x) = -J \sum'_{\langle ij \rangle} \cos(\theta_i - \theta_j)$.

Note that In addition to the lattice symmetries, $\mathcal{H}$ is symmetric under $O(2)$ rotations

$$H(x') = H(x).$$

Note that this is the first time we are seeing an internal symmetry that is continuous.

In the Hamiltonian H_{XY}, if J is +ve we call this the Ferro XY model (which is what is usually discussed). If $J < 0$, then it the anti-ferro XY model. (this is important in cuprates as shown at IISc recently).

What is the ground state of the XY (Ferro) model?

Well take all spins to point along the "x axis" i.e, $\{\theta_i = 0\}$.

Note that this ~~state~~ the ground state is not ~~not~~ $O(2)$ invariant, and provides yet another example of a broken symmetry state.

One can define an order parameter as

$$M(x) = \frac{1}{N} \sum_i' e^{i\theta_i}$$

Why this strange definition? This comes that $\theta_i = \theta_i + 2\pi$ are identified with each other. Note that

$M = \langle M(x) \rangle$ in our $\{\theta_i = 0\}$ grand state, is $M = 1$.

But if $\{\theta_i = \theta_0\} \neq 1$ $(\theta_0 = 0)$

$M = \langle M(x) \rangle = e^{i\theta_0}$

which is diffent from 1 and denotes the spin all point in the θ_0 direction.

We will see later in this course that there is immensely rich physics in this model.

Heisenberg Model. (Classical)

This is the "canonical" model for magnetism. Here there are no constrains on the spins to point in specific direction in space (unlike the Ising or the XY models).

Arena: The arena is the hypercubic d-dimsnal lattice. (We can also consdr this on other lattices)

Dofs.: The degrees of freedom at each lattic siti is a spin vector (3 components) $\vec{S}_i$ with $|\vec{S}_i| = 1$

Hamiltonian:-

Symmetris:- Usual symmetri (traslation, pint grup etc).

Inlenal symmetry $O(3)$ → Rotatins.

The $O(3)$ grup is ~~described~~ ~~fabricated~~ ~~by~~ R scomist of all 3×3 matrins suchat $R^T R = I$.

& going with pairwise interactin, we see that

$$\mathcal{H}^{\text{Ferro}}_{\text{Hensby}} = -J \sum_{\langle ij \rangle}{}^{1} \vec{S}_i \cdot \vec{S}_j$$

desribs the Ferro Heisenberg

and $$\mathcal{H}^{\text{AF}}_{\text{Hensby}} = J \sum_{\langle ij \rangle}{}^{1} \vec{S}_i \cdot \vec{S}_j .$$

(J is the exchange energy, and is taken positiv).

For the Ferrocase, one can define an order parameter

$$\vec{M} = \left\langle \frac{1}{N} \sum_i \vec{S}_i \right\rangle = \langle \vec{M}(x) \rangle$$

(note that this is a vector). Message is that the order parameter can be any type of quantity number, complex number, vector etc.

Note that if $\vec{M} \neq \vec{0}$, then the state breaks $O(3)$ symmetry.

For the Antiferro case on a bipartite lattice $\vec{M}_s(x) = \left\langle \frac{1}{N} \sum_i (-1)^{\alpha(i)} \vec{S}_i \right\rangle$

and $\vec{M}_s = \langle \vec{M}_s(x) \rangle$

Heisenberg Model (Quantum)

The arena for this model is again the d-dimensional hypercubic lattice.

Dofs. At each site there is a 2D Hilbert space spanned by $|\uparrow\rangle_i$ and $|\downarrow\rangle_i$, ie, at any site the state can be $\alpha_i |\uparrow\rangle_i + \beta_i |\downarrow\rangle_i$ $|\alpha_i|^2 + |\beta_i|^2 = 1$.

Hamiltonian. We would like to endow (as the natural symmetry) spin rotation invariance to this system. ie, the system is invariant under SU(2) rotation. We can now intuit the Hamiltonian as

$$H^{F,AF}_{QHamm} = \mp J \sum_{\langle ij \rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j$$

Where $\vec{\sigma}_i$ are the vector of Pauli spin 1/2 operators (which can be represented by Pauli matrices). $[\sigma_{i\alpha}, \sigma_{j\beta}] = i\delta_{ij} \varepsilon_{\alpha\beta\gamma} \sigma_{i\gamma}$

This is a quantum mechanical problem (it has intrinsic dynamics) [Note that the Ising, XY and Classical Heisenberg all do not have any intrinsic dynamics]

One can again define

$$\vec{M}(x) = \langle x | \frac{1}{N} \sum_i \vec{\sigma}_i | x \rangle$$ (Quantum average)

and $\vec{M} = \langle \vec{M}(x) \rangle$ ↑ Thermal average

is the order parameter for the Ferro QHM.

Similarly $\vec{M}_s(x) = \langle x | \frac{1}{N} \sum_i (-1)^{\alpha(i)} \vec{\sigma}_i | x \rangle$ for the AF case.

Classical O(n) model

Now that we have seen Ising, XY and Heisenberg models, we get carried away and define general models with d-hypercube as our arena.

The dofs are n-component vectors $\vec{\phi}(i)$ such that $|\vec{\phi}(i)|^2 = 1$ at each site $x = \{\phi_i\}$.

The Hamiltonian is obtained by

$$\mathcal{H}_n^{F,AF} = \mp J \sum_{\langle ij \rangle}' \vec{\phi}_i \cdot \vec{\phi}_j.$$

One can again define an order parameter ele

$$\vec{M}(x) = N^{-1} \sum_i' \vec{\phi}_i$$

$$\Rightarrow \vec{M} = \langle \vec{M}(x) \rangle.$$ If $\vec{M} \neq 0$ then O(n) symmetry will be broken.

We have now seen a whole range of models. We have seen that the order parameter characterizes a state of broken symmetry and can help describe a phase.

Response functions : Linear Response

We now know that symmetry is a invaluable tool used to characterize phases (states). Another way to ~~see~~ is to "probe" the system and look at its response. For example a solid phase ~~de~~ responds very differently to shear stresses as opposed to a fluid phase — this is the origin of the statement that "fluids take up the shape of the container"!

We will now study responses of the system. Consider some observable A such that in our ~~[illegible]~~ undisturbed state denoted by ρ_0, the expectation value of A is $A_0 = \text{tr}\,\rho_0 A = \int dx\, \rho_0(x) A(x)$.

$$\rho_0(x) = \frac{e^{-\beta \mathcal{H}(x)}}{Z}$$ where $\mathcal{H}$ is the Hamiltonian of our system.

We now "pinch" the system (like apply a weak magnetic field to the Ising model)

The "pinching" can be modeled by a "force" f coupling to some "operator" B.

Now $\mathcal{H}_f = \mathcal{H} - f B$

(f: force; B: operator)

Then we now ask, what is the "response" of our system, i.e., this will for example change the $\langle A \rangle$.

The response then is

$$A_f - A_0 = \langle A \rangle_f - \langle A \rangle_0 = A^r$$

Now $$\langle A \rangle_f = \frac{\sum_x e^{-\beta \mathcal{H}_f(x)} A(x)}{\underbrace{\sum_x' e^{-\beta \mathcal{H}_f(x)}}_{Z_f}}$$

Now we expect for "not to severe pinching", weak fields

$$Z_f = \sum_x' e^{-\beta (\mathcal{H}(x) - f B(x))}$$

$$\approx \sum_x' e^{-\beta \mathcal{H}(x)} (1 + \beta B(x)) f$$

$$\approx Z_0 (1 + \beta \langle B(x) \rangle_0 f)$$

The numerator is

$$\simeq \sum_{x'}^{1} e^{-\beta \mathcal{H}_s(x)} \left(A(x) + \beta A(x) B(x)\right)$$

$$\simeq Z_0 \left(\langle A(x) \rangle_0 + \beta \langle A(x) B(x) \rangle_0 \right)$$

$$\Rightarrow \langle A \rangle_f = \langle A \rangle_0 + \beta \left[\langle A(x) B(x) \rangle - \langle A(x) \rangle_0 \langle B(x) \rangle_0 \right]$$

$$\Rightarrow A^r = \frac{1}{T} \underbrace{\langle \delta A(x) \, \delta B(x) \rangle_0 f}$$

expectation value of the correlation function of fluctuation.

$$A^r = \chi_{AB} f$$

$$\chi_{AB} = \frac{1}{T} \langle \delta A(x) \, \delta B(x) \rangle_0 = \frac{1}{T} \langle \delta A \delta B \rangle_0$$

(Note that our derivation is valid only in classical mechanics)

Let us now discuss an example of this and what more better system than the Ising model.

I have an Ising model

$$\mathcal{H}_{Is} = -J \sum_{\langle ij \rangle} S_i \cdot S_j \,, \quad P_0 = \frac{e^{-\beta \mathcal{H}_I}}{Z}$$

I apply a magnetic field, h_j, at just one site j and ask what is the change in the magnetization at site i

Thus $A(x) = S_i \qquad B(x) = S_j$

applying the formula we find.

$$\mathcal{H}_f = \mathcal{H}_{Is} - h_j S_j$$

$$m_i^r = \langle S_i \rangle_f - \langle S_i \rangle_0 = \chi_{ij} h_j$$

$$\chi_{ij} = \frac{1}{T} \langle \delta S_i \, \delta S_j \rangle_0$$

$$\delta S_i = S_i - \langle S_i \rangle_0$$

Since I am in linear response regime

Even if I had a lattice dependent magnetic field, $\{h_j\}$, I have

$$m_i^r = \sum_j \chi_{ij} h_j \,!$$

which is a nice result!

Let us analyze this

$$\chi_{ij} = \frac{1}{T} \langle \delta S_i \, \delta S_j \rangle_0$$

We see that magnetization change at site i due to an applied magnetic field is related to how the fluctuations (in equilibrium), all these sites are correlated! This is actually an example of a more general result which we will see later in this course.

Let us now consider the case where the P_0 state does not break translational symmetry. Then we expect $\chi_{ij} = \chi(R_i - R_j)$.

We can now expand this in Fourier series

$$\chi(\vec{R}_i - \vec{R}_j) = \frac{1}{N} \sum_{\vec{q}} \chi(\vec{q}) \, e^{i \vec{q} \cdot (\vec{R}_i - \vec{R}_j)}.$$

We see that

$$\chi(\vec{q}) = \frac{1}{T} \frac{1}{N} \langle \delta S^*(\vec{q}) \, \delta S(\vec{q}) \rangle_0$$

We have used $\delta S^*(\vec{q}) = \delta S(-\vec{q})$ and

$$\delta S_i = \frac{1}{N}\sum_q e^{i\vec{q}\cdot\vec{R}_i}\,\delta S(q).$$

Let us go back to our formula

$$\chi_{ij} = \frac{1}{T}\langle \delta S_i\, \delta S_j\rangle.$$

Suppose $J=0$, then what do we expect? Clearly what we have is

χ_{ij} has a δ_{ij} structure since each spin is independent. The average value $\langle S_i\rangle_0$ is also zero, Thus

$$\chi_{ij} = \delta_{ij}\frac{\langle S_i\rangle_0^2}{T} = \delta_{ij}\frac{1}{T}!$$

This is the Curie Law.

Note that (magnetic susceptibility for a uniform field $\chi(\vec{q}=0)$

$$= \frac{1}{T}\frac{1}{N}\langle \delta S(\vec{q}=0)\,\delta S(\vec{q}=0)\rangle_0$$

$$= \frac{1}{T}\frac{1}{N}\left\langle \left(\sum_i S_i\right)^2\right\rangle_0$$

$$= \frac{1}{T}\frac{1}{N}\,N = \frac{1}{T}$$ Curie Law!

Which is the well known

Hopefully you see that all this is simply a formal way of stating things.