

06/01/25

Lecture 1

Stat. Mech: Calculating the bulk properties of a large system in equilibrium from microscopic information about it.

Input: Energies due to interactions

Output: Thermodynamic quantities & correlation functions

Example

$$H_{\text{Ising}} = -\frac{1}{2} \sum_{i,j} J_{ij} S_i S_j - h \sum_i S_i$$

↓	↑	↓	↑	↑	↓	↑	↓	↑
↑	↓	↓	↑	↓	↓	↑	↓	↓
↓	↑	↑	↓	↓	↑	↓	↓	↑
↑	↓	↑	↓	↓	↓	↓	↑	↓
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↓	↓	↑	↓	↑	↓	↑	↓	↑

$C: \{S_i\} \Rightarrow$ Configuration of Spin lattice

Probability of that configuration 'C' exists is $\text{Prob}(C)$

one type of $\text{prob}(C) = \frac{e^{-\beta H}}{Z}$

Z = Partition function

$$\langle A \rangle = \sum_C \text{Prob}(C) A(C)$$

↓

Ensemble Average value of any quantity 'A'

Correlation function b/w spins in Site 'i' & 'j' is $\langle S_i S_j \rangle$

Main aim of any thermodynamic Calculation is getting the eqⁿ of

State $\leftarrow \rho \rightarrow \rho(P, T)$

Hydrodynamic density Pressure temperature

Magnetodynamics : $M(h, T)$

↓ External mag. field

Magnetization

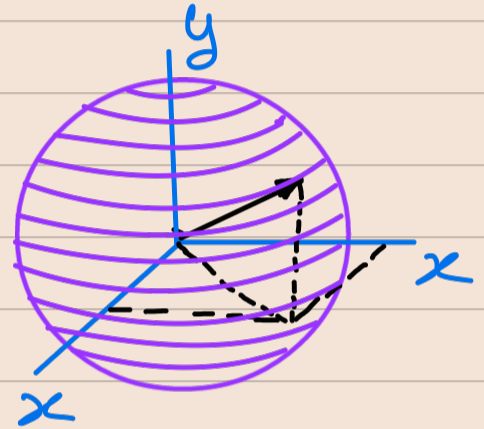
Thermodynamic limit : $\begin{cases} N \rightarrow \text{large } (\infty) \\ V \rightarrow \text{large } (\infty) \\ \frac{N}{V} \rightarrow \text{finite} \end{cases}$

A Model Magnet

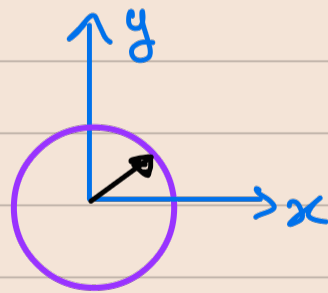
d : Spatial dimension of System

n : Spin dimensions

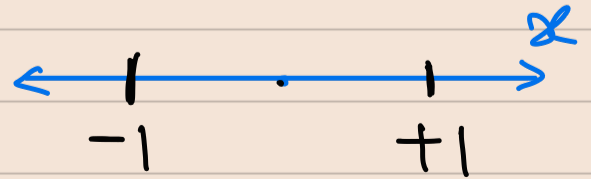
$n: 3 \rightarrow$ Heisenberg Spin



$n: 2 \rightarrow$ X-Y Spin



$n: 1 \rightarrow$ Ising Spin
($S_i = \pm 1$)



Spin Systems

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↑	↓	↓	↑	↓	↓	↑	↓	↓
↓	↑	↑	↓	↓	↑	↓	↓	↑
↑	↓	↑	↓	↓	↓	↓	↑	↓
↓	↑	↑	↓	↑	↑	↓	↓	↓
↓	↓	↑	↓	↑	↓	↑	↓	↑

A Spin is a degree of freedom for a quantum particle & is an intrinsic property. Spin transforms like Angular momentum & hence it is a vectorial quantity. Spin operator is $\vec{\hat{S}} = (\hat{S}_x, \hat{S}_y, \hat{S}_z)$ & the square of magnitude of Spin is

$$\hat{S}^2 = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2$$

The Spin operators obey the Commutation relations given by

$$[\hat{S}_\alpha, \hat{S}_\beta] = i\hbar \epsilon_{\alpha\beta\gamma} \hat{S}_\gamma$$

$$[\alpha, \beta, \gamma = (x, y, z)]$$

$$\& [\hat{S}^2, \hat{S}_z] = 0$$

Every spin is associated with a quantum number 's' that can take values like $(s = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots)$

The particles whose spin number is Integral are called Bosons & those with half-Integral spins are called Fermions.

The eigen value of $\hat{S}^2$ is given by $\hbar^2 s(s+1)$ & is $2s+1$ fold degenerate. Since $\hat{S}_z$ commutes with $\hat{S}^2$ we can label

the eigen states togetherly.

For a given 's', the $\hat{S}_z$ has eigen values of $m_s \hbar$.

where $m_s = s, s-1, \dots, 1-s, s$

Thus a quantum particle with spin number 's' has states denoted as $|s, m_s\rangle$

$$\hat{S}^2 |s, m_s\rangle = \hbar^2 s(s+1) |s, m_s\rangle$$

$$\& \hat{S}_z |s, m_s\rangle = m_s \hbar |s, m_s\rangle$$

The most studied spin systems have particles with $s = \frac{1}{2}$.

with states

$$|\frac{1}{2}, \frac{1}{2}\rangle \equiv |\uparrow\rangle : \text{up-spin}$$

$$|\frac{1}{2}, -\frac{1}{2}\rangle \equiv |\downarrow\rangle : \text{down-spin}$$

If there are ' N ' particles all with spin number $\frac{1}{2}$, then for an i^{th} particle we have a spin operator set $(\hat{S}_i^x, \hat{S}_i^y, \hat{S}_i^z)$ where the states of i^{th} particle can be labelled by $|\frac{1}{2}, m_{s_i}\rangle$ $m_{s_i} = \pm\frac{1}{2}$

Coupling of spins with external magnetic field $\vec{B}$

Consider a d -dimensional arrangement of spins in a lattice. Each spin has a Magnetic Spin-dipole moment given by $\vec{\mu}_i = \frac{e}{m_e} \hat{S}_i$ & it is an operator. In the presence of $\vec{B}_{\text{ext}}$.

The energy of interaction is given by,

$$\hat{H}_i = - \vec{\mu}_i \cdot \vec{B}_{\text{ext}}$$

(Per-particle)

But for N -particles it's interaction with external field is given by

$$\hat{H}_{\text{int.}} = - \sum_{i=1}^N \vec{\mu}_i \cdot \vec{B}_{\text{ext}}$$

Now for magnetic field in any arbitrary direction the interaction energy is

$$\hat{H}_{\text{int}} = - \sum_{i=1}^N \frac{e}{m_e} (\vec{S}_i \cdot \vec{B}_{\text{ext}})$$

Let $\vec{B}_{\text{ext}} = B \hat{n} \Rightarrow \vec{S}_i \cdot \vec{B}_{\text{ext}} = B (\vec{S}_i \cdot \hat{n})$

Eigen values of $\vec{S}_i \cdot \hat{n}$ is $\hbar m_{S_i}$
where $m_{S_i} = \pm \frac{1}{2}$.

$\Rightarrow$ Energy of interaction is given by

$$E_{\text{int}} = - \sum_{i=1}^N \left(\frac{e\hbar}{2m_e} \right) B S_i$$

where $S_i = \pm 1$. $\left(m_{S_i} = \frac{S_i}{2} \right)$

$$\mu_B = \frac{e\hbar}{2m} \text{ (Bohr magneton)}$$

$$\Rightarrow E_{\text{int}} = - \mu_B B \sum_{i=1}^N S_i$$

$$\text{Let } \epsilon h = \mu_B B$$

where ' ϵh ' corresponds to the energy of coupling of one spin with ext. field

$$\Rightarrow \boxed{E_{\text{int}} = -h \sum_{i=1}^N S_i}$$

The states of the system can be described by

$$|S_1, S_2, \dots, S_i, \dots, S_N\rangle$$

where S_i represents the spin state of i^{th} particle. $S_i = \underbrace{+1}_{\text{up spin}} \text{ or } \underbrace{-1}_{\text{down spin}}$

Note:

The Hilbert Space for the total Hamiltonian is now the tensor product of the Spin Space of each individual Spins at each lattice points.

$$\Rightarrow H = H_1 \otimes H_2 \otimes H_3 \dots \otimes H_i \dots \otimes H_n$$

Where H_i is the Spin Space of Spin at i^{th} site. The Spin state of i^{th} Spin is $|S_i\rangle$, which can be either $|1\rangle_i$ or $|-1\rangle_i$. Then the state of the entire lattice is given by $\underbrace{|S_1, S_2, S_3, \dots, S_i, \dots, S_n\rangle}_{\text{This state lives in}}$.

$$H = H_1 \otimes H_2 \otimes H_3 \dots \otimes H_i \dots \otimes H_n$$

Exchange Interaction

The exchange interaction between two spins $\hat{S}_i$ & $\hat{S}_j$ is given by,

$$\hat{H}_{e.x.} = - \sum_{\substack{i,j \\ i \neq j}} J_{ij} \hat{S}_i \cdot \hat{S}_j$$

This interaction is called as the Heisenberg interaction where exchange is considering all components of spin.

But in case of Ising spins, only one component of spin is considered.

Ising exchange hamiltonian is given by,

$$H_{ex.} = - \sum_{\substack{i,j \\ i \neq j}} J_{ij} S_i S_j$$

where $\underline{S_i = \{+1, -1\}}$

If the interaction energy J_{ij} is constant for all lattice site, then

$$H_{exchange} = -J \sum_{\substack{i,j \\ i \neq j}} S_i S_j$$

Heisenberg Model of Spins

$$\hat{H} = - \sum_{\substack{i,j \\ i \neq j}} J_{ij} \hat{\vec{S}}_i \cdot \hat{\vec{S}}_j - \sum_i \vec{h} \cdot \vec{S}_i$$

$(\vec{h} = \mu_B \vec{B})$

Ising Model of Spins

$$H = - \sum_{\substack{i,j \\ i < j}} J_{ij} S_i S_j - h \sum_i S_i$$

or

$$H = - \frac{1}{2} \sum_{\substack{i,j \\ i \neq j}} J_{ij} S_i S_j - h \sum_i S_i$$

factor of $\frac{1}{2}$ since the summation will repeat pair of particles.
 $i, j = \{1, 2, \dots, N_s\}$

$$\text{Magnetization, } m = \frac{1}{N} \frac{\partial H}{\partial h} = \frac{1}{N} \sum_i \langle S_i \rangle$$

$$m = \frac{1}{N_s} [\langle N_{\uparrow} \rangle - \langle N_{\downarrow} \rangle]$$

Correlation function (at site " i "
with a spin at " $i+\gamma$ ")

$$C_i(\gamma) = \langle S_i S_{i+\gamma} \rangle$$

$C_i(r)$ is related to joint prob. of spins S_i & S_{i+r} to be parallel.

$$\text{Joint prob} = \text{Prob}(S_i = \uparrow, S_{i+r} = \uparrow)$$

$$+ \text{Prob}(S_i = \downarrow, S_{i+r} = \downarrow)$$

they are mutually exclusive events
hence the prob. is added.

$$\text{Joint Prob} = \left\langle \frac{(1+S_i)}{2} \frac{(1+S_{i+r})}{2} \right\rangle$$

$$+ \left\langle \left(\frac{1-S_i}{2}\right) \left(\frac{1-S_{i+r}}{2}\right) \right\rangle$$

$$= \left\langle \frac{1}{4} \left[\begin{aligned} &1 + S_i + S_{i+r} + S_i S_{i+r} \\ &+ 1 - S_i - S_{i+r} + S_i S_{i+r} \end{aligned} \right] \right\rangle$$

$$\text{Joint prob.} = \frac{1}{2} \left[1 + \langle S_i S_{i+r} \rangle \right]$$

$$\text{Thus } \langle S_i S_j \rangle = 2(\text{Joint Prob.}) - 1$$

General Prescription to Solve

Such problems is get the indicator function & then take its average.

$$\text{Prob}(\mathcal{E}) = \sum_C \text{Prob}(C) \cdot I[\mathcal{E}(C)]$$

$$I[\mathcal{E}(C)] = \begin{cases} 1, & \mathcal{E}(C) \text{ is full filled in } C \\ 0, & \mathcal{E}(C) \text{ is not full filled in } C \end{cases}$$

→ Covariance

$$G_i(\tau) = \left\langle (S_i - \langle S_i \rangle) (S_{i+\tau} - \langle S_{i+\tau} \rangle) \right\rangle$$

$$G_i(\tau) = \langle S_i S_{i+\tau} \rangle - \langle S_i \rangle \langle S_{i+\tau} \rangle$$

It gives the information of Scattering Cross-Section.

$S_i - \langle S_i \rangle \Rightarrow$ Mean average error or fluctuations.

& they are Causes of Scattering.

- Homework: Find $\langle S_i S_j S_k \rangle$ & its connection with joint prob. of $\uparrow\uparrow\uparrow$ & $\downarrow\downarrow\downarrow$.
- Study $\rightarrow$ Magnetism by P. Fazekas
 $\rightarrow$ " " Coey

Ordered Phases in 1D Ising Model

Ferro & Anti Ferromagnets

$$H = - \frac{J}{2} \sum_{i,j} S_i S_j$$

If $J < 0 \Rightarrow S_i S_j$ are usually parallel (Ferromagnets)

$J < 0 \Rightarrow S_i S_j$ are anti-parallel. (Anti-ferromagnets)

- Home work: Find $\langle S_i S_j S_k \rangle$ & its connection with joint prob. of $\uparrow\uparrow\uparrow$ & $\downarrow\downarrow\downarrow$.

$$\text{Joint prob} = \text{Prob}(S_i = \uparrow, S_j = \uparrow, S_k = \uparrow) + \text{Prob}(S_i = \downarrow, S_j = \downarrow, S_k = \downarrow)$$

$$= \left\langle \left(\frac{1+S_i}{2} \right) \left(\frac{1+S_j}{2} \right) \left(\frac{1+S_k}{2} \right) \right\rangle + \left\langle \left(\frac{1-S_i}{2} \right) \left(\frac{1-S_j}{2} \right) \left(\frac{1-S_k}{2} \right) \right\rangle$$

$$= \frac{1}{8} \left\langle 1 + S_i + S_j + S_k + S_i S_j + S_i S_k + S_j S_k + S_i S_j S_k \right\rangle + \frac{1}{8} \left\langle 1 - S_i - S_j - S_k + S_i S_j + S_j S_k + S_i S_k - S_i S_j S_k \right\rangle$$

$$= \frac{1}{4} \left\langle 1 + S_i S_j + S_i S_k + S_j S_k \right\rangle$$

- Homework: Find $\langle S_i S_j \rangle$ & its connection with joint prob. of $\uparrow\downarrow \neq \downarrow\uparrow$

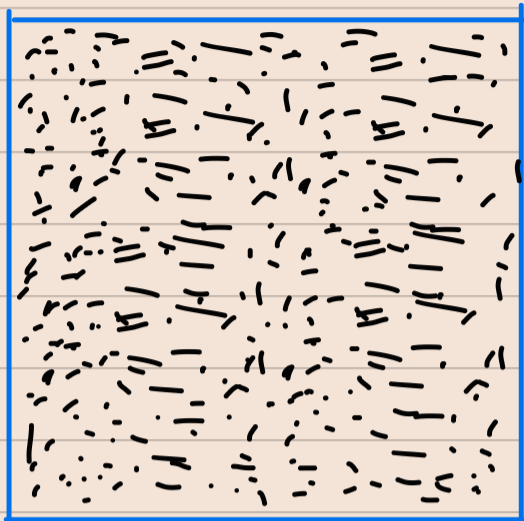
$$\begin{aligned}
 \text{Joint Prob} &= P(S_i = \uparrow, S_j = \downarrow) \\
 &\quad + P(S_i = \downarrow, S_j = \uparrow) \\
 &= \left\langle \left(\frac{1+S_i}{2} \right) \left(\frac{1-S_j}{2} \right) \right\rangle + \left\langle \left(\frac{1-S_i}{2} \right) \left(\frac{1+S_j}{2} \right) \right\rangle \\
 &= \frac{1}{4} \left[(1 - S_i S_j + S_i - S_j) + (1 - S_i S_j - S_i - S_j) \right] \\
 &= \frac{1}{4} \langle (2 - 2 S_i S_j) \rangle \\
 &= \frac{1}{2} (1 - \langle S_i S_j \rangle)
 \end{aligned}$$

$$\Rightarrow \langle S_i S_j \rangle = 1 - 2 J_{(\uparrow\downarrow + \downarrow\uparrow)}$$

$$\text{Also } \langle S_i S_j \rangle = 2 J_{(\uparrow\uparrow + \downarrow\downarrow)} - 1$$

$$\Rightarrow \boxed{J_{\uparrow\uparrow + \downarrow\downarrow} + J_{\uparrow\downarrow + \downarrow\uparrow} = 1}$$

Simple Fluid



$$E = \sum_k \frac{p_k^2}{2m} + \frac{1}{2} \sum_{i,j} V(\vec{r}_i - \vec{r}_j) - \mu N$$

find $C(r, r') = \langle n(r) n(r') \rangle$

$n(r) d^3r$ is the number of particles in a volume d^3r centered at a distance " r " from the origin.

one way is $n(r) = \sum_k \delta(\vec{r} - \vec{r}_k)$

(lattice gas model)

This is for a lattice of particles at positions $\vec{r}_k$

($k = 1, 2, \dots, N$)

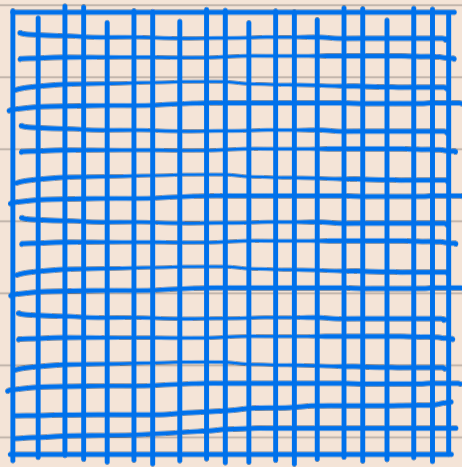
Joint Probability

$$P_{\text{joint}}(A, B) = P(A) P_{\text{cond}}(A|B)$$

$$\langle \underbrace{n(x_0) n(x_0 + r)}_{\text{for liquids}} \rangle = \sum_C P_{\text{prob}}(C) n_i(x) n_{i+r}(C)$$

Lattice Gas Model

$n_i \Rightarrow$ number
of particles
in i^{th} cell



discretize
the space
to cells &
find the
values. $n_i, \bar{n}_i$

$\bar{n}_i \Rightarrow$ no. of
holes.

treat $n_i = 1$ as up spin

$n_i = 0$ as down spin

$$n_i = 0 \Rightarrow \bar{n}_i = 1, \quad n_i = 1 \Rightarrow \bar{n}_i = 0.$$

$$n_i = \frac{1 + S_i}{2}, \quad S_i = 2n_i - 1$$

$$\bar{n}_i = \frac{1 - S_i}{2}$$

perform all
calculations as
we did in Ising model