

Quantum Statistics (Please see alternate derivation in reading)

→ Ensembles + Partition Functions in Stat. Mech.

Want to understand how to find average properties of a system

- Imagine that we average over an ensemble of identical systems. That's a lot like QM expectation value.

- But we can consider different ways the system can interact with the environment

+ A closed system (meaning E conserved, particle # N conserved) = micro canonical ensemble

+ System exchanges energy with heat bath = canonical ensemble

+ System exchanges energy + particles with heat bath = grand canonical ensemble

- The probability of a system (from the ensemble) to be in state i is

+ $P = e^{-E_i/kT} / Z$, $Z = \sum_i e^{-E_i/kT}$ = partition function
in canonical ensemble. \uparrow Boltzmann factor

+ $P = e^{-(E_i - \mu N_i)/kT} / \mathcal{Z}$, $\mathcal{Z} = \sum_i e^{-(E_i - \mu N_i)/kT}$ = grand partition

+ k = Boltzmann's constant, T = temperature, μ = chemical potential.

kT is related to average energy, μ to average particle number.

Use units with $k=1$.

- Calculate averages from partition functions

+ Canonical $\langle E \rangle = \frac{1}{Z} \sum E_i e^{-E_i/T} = -\frac{1}{Z} \frac{dZ}{d(1/T)} = T^2 \frac{d \ln Z}{dT}$

+ Grand canonical

$\langle N \rangle = \frac{1}{\mathcal{Z}} \sum N_i e^{-(E_i - \mu N_i)/T} = \frac{1}{\mathcal{Z}} \frac{d\mathcal{Z}}{d\mu} = T \frac{d \ln \mathcal{Z}}{d\mu}$

+ Ensembles equivalent in large systems with small fluctuations $\langle SE^2 \rangle$, $\langle \delta N^2 \rangle$, ...

- Quantum Distribution Functions

- Consider many indistinguishable particles that don't interact
 - + Each particle just fills a 1-particle state j w/energy ϵ_j
 - + The many-particle state is specified by # n_j of particles in each single particle state (since they're identical)

$$E = \sum_j n_j \epsilon_j, \quad N = \sum_j n_j \quad \text{for each many particle state.}$$

- The grand partition function becomes (of whole system)

$$\mathcal{Z} = \sum_{\{n_j\}} e^{-(E-\mu N)/T} = \sum_{\{n_j\}} \exp\left[-\sum_j n_j (\epsilon_j - \mu)/T\right]$$
$$= \left(\sum_{n_1} e^{-n_1(\epsilon_1 - \mu)/T}\right) \left(\sum_{n_2} e^{-n_2(\epsilon_2 - \mu)/T}\right) \dots$$

• Bose-Einstein Distribution

- + Any number of bosons can be in any given 1-particle state so n_j runs from 0 to ∞ .

- + Each sum is geometric series $\mathcal{Z} = \left(\frac{1}{1 - e^{-(\epsilon_j - \mu)/T}}\right) \dots$

- + The Bose-Einstein distribution

$$f(\epsilon, \mu, T) \equiv \langle n_j \rangle = -T \frac{d \ln \mathcal{Z}}{d \epsilon_j} = \frac{e^{-(\epsilon - \mu)/T}}{1 - e^{-(\epsilon - \mu)/T}} = \frac{1}{e^{(\epsilon - \mu)/T} - 1}$$

- + The Planck law can be written as $E f(\epsilon, \mu=0, T) \times (\# \text{ states w/energy } \epsilon)$.

• Fermi-Dirac Distribution

- + Each single fermion state has only 0 or 1 particles due to antisymmetry

- + Then $\mathcal{Z} = (1 + e^{-(\epsilon_j - \mu)/T}) \dots$

- + The Fermi-Dirac Distribution is $f(\epsilon, \mu, T) = \langle n_j \rangle = \frac{1}{e^{(\epsilon - \mu)/T} + 1}$

- + As $T \rightarrow 0$, exponential is 0 if $\epsilon < \mu$, ∞ if $\epsilon > \mu$

$$\text{so } f(\epsilon, \mu, T=0) = \Theta(\mu - \epsilon)$$

That's just what happens in a free-electron (Fermi) gas if $\mu = E_F$.

- See HW for more.

• Magnetism

Understanding different types of magnetism is a major problem still

- Models:

• We've seen how to solve the Hamiltonian $H = -J \vec{S}^{(1)} \cdot \vec{S}^{(2)}$

+ Now imagine a (magnetic) solid is a lattice of ions, each carrying some spin (due to electrons) of total spin S .

+ So we can model all pairs of ions as having interacting spins

$$H = -\frac{1}{2} \sum_{ij} J_{ij} \vec{S}^{(i)} \cdot \vec{S}^{(j)} - \sum_i \gamma \vec{S}^{(i)} \cdot \vec{B}$$

Heisenberg Hamiltonian

+ Note: the interactions are not due to the magnetic field of one dipole on the dipole of the other spin. Too small!

Instead, it's due to a combination of exchange + Coulomb forces.

• A simplified version uses only z -components

$$H = -\frac{1}{2} \sum_{ij} J_{ij} S_z^{(i)} S_z^{(j)} - \gamma \sum_i S_z^{(i)} B_z$$

(all operators now commute)

This is the Ising Model. Still, can't be solved exactly except for simple geometries in 1D or 2D. (Very hard!)

- • A little interpretation + more comments:

+ If $J_{ij} > 0$, spins want to line up. This is ferromagnetic.

The Heisenberg model ground state is all spins equal.

+ If $J_{ij} < 0$, you get anti-ferromagnetism. "Alternating" reversed spins is not an eigenstate of Heisenberg! (but is of Ising)

A great deal of current research is on "frustrated" anti-ferromagnets, which are prevented by geometry from alternating spins.

+ The external magnetic field \vec{B} can overwhelm the interactions, leading to alignment. $\vec{B} = 0$ case is interesting.

- Heisenberg Model with $\vec{B} = 0$. (Ferromagnetic)

• We can't generally solve it but will use the "mean field approximation". This is pretty poor but at least easy + qualitatively correct. Set $\vec{B} = 0$.

+ Focus on a single spin. $H_i = -\vec{S}^{(i)} \cdot \left(\sum_{j \neq i} J_{ij} \vec{S}^{(j)} \right)$

Let's call $\sum_{j \neq i} J_{ij} \vec{S}^{(j)} \equiv \gamma \vec{B}_{\text{MFT}}$

+ \vec{B}_{MFT} is an ugly operator, but let's replace each $\gamma \vec{S}^{(i)}$ by the thermal average value (see HW)

$$\langle \gamma \vec{S}^{(i)} \rangle = \gamma_s B_s(\gamma B_z / T) \quad (*)$$

where B_z = field experienced by spin j and $B_s(x) \equiv$ Brillouin function.

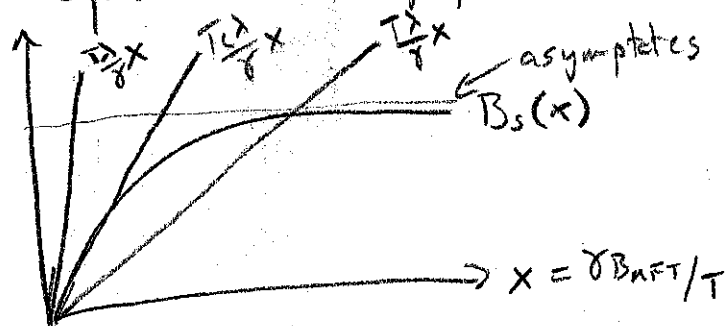
+ But each spin is the same on average, so replace B_z in (*) by B_{MFT} ! Then

$$H_i = -\vec{S}^{(i)} \cdot \vec{B}_{\text{MFT}} \Rightarrow \langle \gamma \vec{S}^{(i)} \rangle \equiv \lambda \vec{B}_{\text{MFT}} = \gamma_s B_s\left(\frac{\lambda B_{\text{MFT}}}{T}\right)$$

$\lambda =$ proportionality constant

• What are features of the solution?

+ Transcendental equation. Solve graphically



+ There is only a solution when the slope of the RHS is less than the slope of $B_s(x)$ at $x=0$. This leads to a critical temperature T_c (Curie temperature) below which the ferromagnet magnetizes spontaneously - phase transition.

+ Can analyze behavior near T_c , domains + domain walls, etc.