PHYS 460 - LECTURE 22

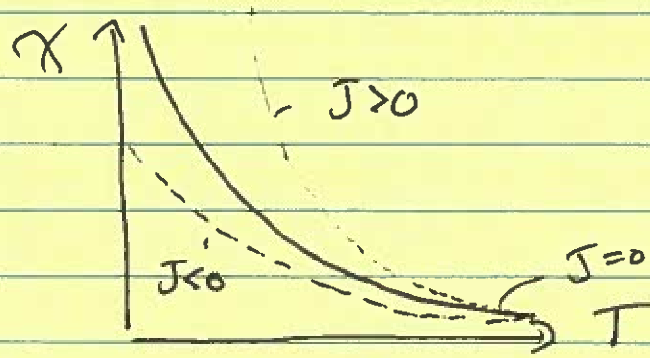
THE LAST THING WE DISCUSSED WAS INTERACTIONS BETWEEN LOCAL SPINS IN MATERIALS, WHICH I ARGUED WAS CAPTURED BY THE "HEISENBERG HAMILTONIAN"

$$\mathcal{H} = -\frac{1}{2}\sum_{\langle i,j\rangle}' J\,\vec{S}_i\cdot\vec{S}_j + g\mu_B\sum_i' \vec{B}\cdot\vec{S}_i$$

nearest neighbors

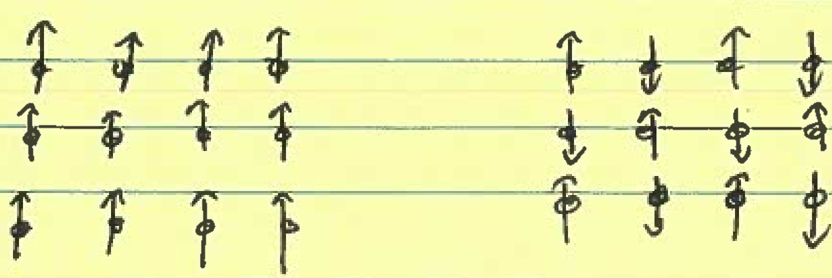
THE ORIGIN OF THESE INTERACTION IS THE EXCHANGE MECHANISM, AND TELLS US THAT NEIGHBORING SPINS LIKE TO ALIGN (IF $J>0$) OR ANTI-ALIGN (IF $J<0$).

THIS WILL CLEARLY HAVE CONSEQUENCES, FOR EXAMPLE, THERE IS NOW AN ADDITIONAL BENEFIT FOR SPINS TO ALIGN WITH FIELD FOR $J>0$ AND COST FOR $J<0$, AFFECTING THE BALANCE BETWEEN ENERGY AND ENTROPY $\longrightarrow$ MAGNETIZATION EVOLVES AS SO



AND AT $T=0$, SPINS WILL SPONTANEOUSLY CHOOSE DIRECTIONS $\rightarrow$ "ORDER"

$T=0$



TREATING THE FULL N SPIN PROBLEM EXACTLY IS NOT A SIMPLE MATTER, IT TURNS OUT (AT LEAST MUCH HARDER THAN THE INDEPENDENT SPIN MODEL)

ONE APPROXIMATION WHICH IS OFTEN MADE TO GET A BASIC IDEA OF WHAT HAPPENS COMPRISES A SERIES OF CALCULATIONS KNOWN AS "MEAN FIELD THEORY". HERE IS THE BASIC IDEA:

FOCUS ON 1 SPIN

↓

ASSUME THE EFFECT OF ALL SPINS CAN BE CAPTURED BY THE AVERAGE (MEAN) FIELD INDUCED AT THE SITE OF THAT SPIN

↓

ASSUME THAT ALL SPINS SEE THE SAME AVERAGE FIELD

↓

ENFORCE SELF-CONSISTENCY

↓

SOLVE

THIS STRATEGY NEGLECTS A LOT OF STUFF (e.g. QUANTUM FLUCTUATES), BUT USUALLY REPRODUCES GENERAL BEHAVIORS.

THIS IS BEST SEEN THROUGH AN EXAMPLE.

THE FERROMAGNETIS $S=\frac{1}{2}$ ISING MODEL

CONSIDER THE ABOVE HAMILTONIAN APPLIED TO A BUNCH OF $S=\frac{1}{2}$ SPINS. IF $\vec{B}=B\hat{z}$, THERE ARE ONLY TWO SPIN POSSIBILITIES FOR EACH SITE $S_z=\frac{1}{2}$ OR $S_z=-\frac{1}{2}$ (THE "ISING MODEL").

THE FULL HAMILTONIAN REDUCES TO

$$\mathcal{H} = -\frac{1}{2}\sum_{\langle i,j\rangle} J S_z^i S_z^j + g\mu_B B \sum_i S_z^i$$

IF WE FOCUS ON A SINGLE SITE, i, THAT SPIN HAS

$$\mathcal{H}_i = \left(g\mu_B B - J\sum_j S_z^j\right) S_z^i$$

WHERE SUM IS OVER NEIGHBORS

FOR GIVEN S_z^j, THE ( ) JUST LOOKS LIKE AN EFFECTIVE ("MOLECULAR") FIELD

$$B_{eff}^i = B - \frac{J}{g\mu_B}\sum_j S_z^j$$

NOW THE MAIN PRINCIPLE OF MEAN FIELD THEORY IS THAT WE CAN REPLACE B_{eff}^i WITH IT'S AVERAGE VALUE ("MEAN FIELD") AND THIS VALUE WILL, ON AVERAGE, BE THE SAME FOR ALL SITES

$$B_{eff}^i \rightarrow \langle B_{eff} \rangle$$

THEN $\mathcal{H}_i = g\mu_B \langle B_{eff} \rangle S_z^i$, WHICH IS JUST THE LONE SPIN-$\frac{1}{2}$ HAMILTONIAN CONSIDERED LAST CLASS

USING THE SAME ANALYSIS

PARTITION FUNCTION

$$\rightarrow \quad Z_i = e^{-\frac{g\mu_B \langle B_{eff} \rangle}{k_B T}} + e^{\frac{g\mu_B \langle B_{eff} \rangle}{k_B T}}$$

$$\rightarrow \quad \langle S_z^i \rangle = -\frac{1}{2} \tanh\left(\frac{g\mu_B \langle B_{eff} \rangle}{2 k_B T} \right)$$

BUT IF WE ARE JUST AVERAGING, THERE IS NO REASON THAT $\langle S_z^i \rangle$ IS DIFFERENT ON ANY SITE, j

$$\Rightarrow \quad \langle B_{eff} \rangle = B - \frac{J}{g\mu_B} \sum_j' \langle S_z^j \rangle$$

$$= B - \frac{J}{g\mu_B} \sum_j' \langle S_z \rangle$$

$$= B - \frac{J}{g\mu_B} z \langle S_z \rangle$$

WHERE z = # NEAREST NEIGHBORS ("COORDINATION NUMBER")

THE ONLY THING LEFT TO DO IS ENFORCE SELF - CONSISTENCY

$$\langle S_z^i \rangle = -\frac{1}{2} \tanh\left(\frac{g\mu_B B - Jz\langle S_z^i \rangle}{2k_B T}\right)$$

~~WHICH~~ THIS EQUATION DOESN'T HAVE A CLOSED FORM SOLUTION, BUT CAN BE SOLVED NUMERICALLY, ONCE $\langle S_z \rangle$ IS FOUND, IT CAN BE ASSOCIATED WITH A MEAN MOMENT $\mu_s = -g\mu_B \langle S_z \rangle$ PER SITE AND NET MAGNETIZATION

$$M = -gN\mu_B \langle S_z \rangle$$

SOLVING THE TRANSCENDENTAL EQUATION COMES DOWN TO FINDING THE INTERSECTION OF A STRAIGHT LINE (LHS OF EQ) WITH A HYPERBOLIC TANGENT (RHS OF EQ) THAT VARIES WITH TEMPERATURE. AS I STATED, IT CANNOT BE SOLVED ANALYTICALLY, BE YOU CAN EASILY NOTE SOME GENERAL ~~SEE~~ FEATURES

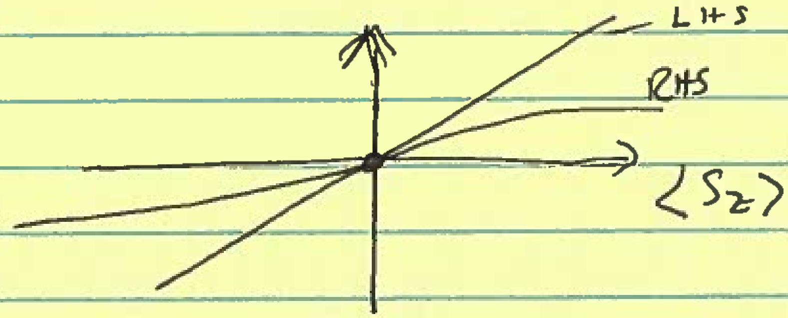
CONSIDER (FOR NOW) THE $B=0$ CASE

THEN

$$\langle S_z \rangle = +\frac{1}{2} \tanh\left(\frac{Jz\langle S_z \rangle}{2k_B T}\right)$$

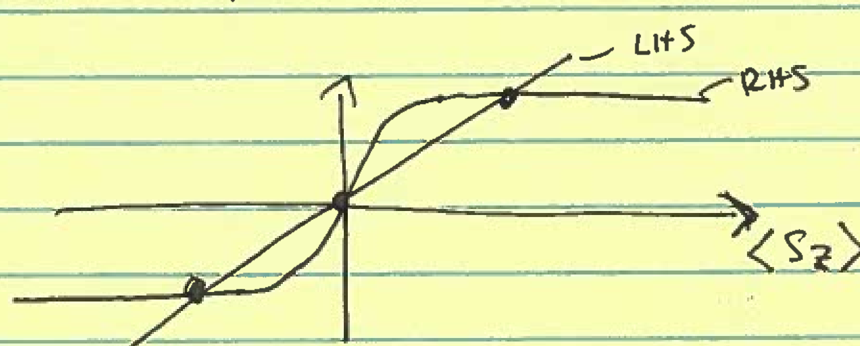
WHERE I HAVE USED $\tanh(-x) = -\tanh(x)$

FOR HIGH TEMPERATURES $k_B T \gg J z \langle S_z \rangle$, THE RHS OF THE EQ IS "FLAT" AND THE TWO SIDES PLOTTED TOGETHER LOOK AS SO



CLEARLY THIS IS ONLY ONE INTERCEPTION AT $\langle S_z \rangle = 0$ $\Rightarrow$ THE SPINS AVERAGE TO ZERO, WHICH IS CONSISTENT WITH THEM BEING RANDOMIZED AT HIGH T (GO ENTROPY!)

THE SITUATION CHANGES AS T GETS SMALLER. THE SLOPE OF THE tanh BECOMES LARGER AND LARGER UNTIL, BELOW SOME CRITICAL TEMPERATURE (T_c), YOU START ENCOUNTERING A SITUATION THAT LOOKS LIKE

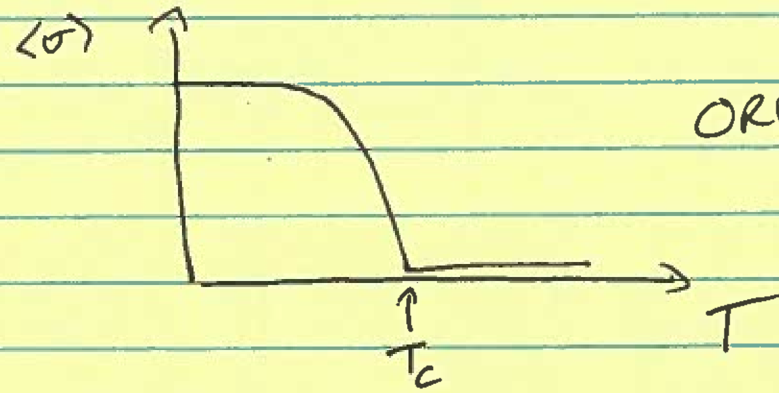


NOW THERE ARE THREE SOLUTIONS:

$\langle S_z \rangle$, WHICH CAN BE SHOWN TO BE UNSTABLE

AND $\langle S_z \rangle = \pm \sigma(T)$

THUS THE SYSTEM EVOLVES WITH TEMPERATURE FROM $\langle\sigma\rangle = 0$ TO SOME FINITE VALUE



ORDER!

WHETHER $\langle S_z\rangle = +\sigma$ OR $-\sigma$ IS CHOSEN SPONTANEOUSLY (SOME FLUCTUATION) OR IS DICTATED BY SOME SMALL ENVIRONMENTAL BIAS (A SMALL FIELD)

FOR FERROMAGNETS, THE CRITICAL TEMPERATURE T_c IS OFTEN CALLED THE "CURIE TEMPERATURE"

THIS TEMPERATURE IS PRECISELY WHEN THE TWO CURVES ARE TANGENTIAL

USING THE EXPANSION

$$\tanh\left(\frac{Jz\langle S_z\rangle}{2k_BT}\right) \approx \frac{Jz\langle S_z\rangle}{2k_BT}$$

WE CAN THUS FIND T_c BY SETTING SLOPES OF LHS & RHS EQUAL

$$1 = \frac{1}{2}\left(\frac{Jz}{2k_BT_c}\right)$$

$$k_BT_c = \frac{Jz}{4}$$

ORDER HAPPENS SUDDENLY, AT A T_c PROPORTIONAL TO J

THIS WAS A $B=0$ RESULT: YOU GET A NON-ZERO NET MAGNETIZATION AT LOW TEMPS SPONTANEOUSLY
$\longrightarrow$ THE VERY DEFINITION OF FERROMAGNET

WE CAN STILL EXPLORE THE REGIME $T>T_c$ THOUGH TO FIND THE GENERAL $\chi(T)$.
CONSIDER NOW THE FULL SELF CONSISTENCY EQUATION (WITHOUT SETTING $B=0$)

$$\langle S_z \rangle = -\frac{1}{2}\tanh\left(\frac{g\mu_B B - Jz\langle S_z\rangle}{2k_BT}\right)$$

AT HIGH T, THERE IS NO SPONTANEOUS $\langle S_z\rangle$ (WE JUST SAW) AND ANY $\langle S_z\rangle$ IS THUS A RESPONSE TO B. FOR SMALL B THEN, $\langle S_z\rangle$ IS SMALL

$$\Rightarrow \langle S_z \rangle = -\frac{1}{2}\tanh\left(\frac{g\mu_B B - Jz\langle S_z\rangle}{2k_BT}\right)$$

$$\simeq -\frac{1}{2}\left(\frac{g\mu_B B - Jz\langle S_z\rangle}{2k_BT}\right)$$

$$4k_BT\langle S_z\rangle = Jz\langle S_z\rangle - g\mu_B B$$

$$\langle S_z\rangle = \frac{g\mu_B B}{Jz - 4k_BT} = -\frac{g\mu_B B}{4k_B(T-T_c)}$$

THEN $M = -n g \mu_B \langle S_z \rangle$

$$\chi = \frac{\mu_0 n g^2 \mu_B^2}{4 k_B (T - T_c)}$$

IF YOU RECALL

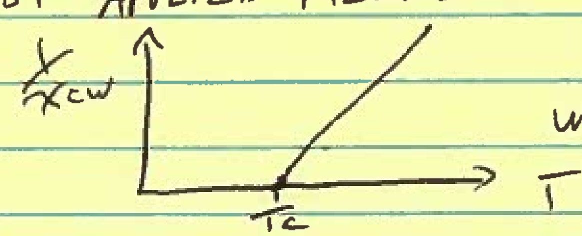
$$\chi_{CURIE} = \frac{\mu_0 n \tilde{g}^2 \mu_B^2 J(J+1)}{3 k_B T}$$

$$= \frac{\mu_0 n g^2 \mu_B^2}{4 k_B T} \quad \text{FOR } J = S = \tfrac{1}{2}$$

$$\Rightarrow \boxed{\chi_{CW} = \frac{\chi_{CURIE}}{(1 - T_c/T)}} \quad \text{"CURIE-WEISS LAW"}$$

THE RESULT IS EXACTLY AS WE EXPECTED FROM BASIC ENERGY CONSIDERATIONS: MAGNETIZATION AT ALL TEMPS ~~BE~~ IS A BIT HIGHER DUE TO ENERGY GAIN FROM EXCHANGE.

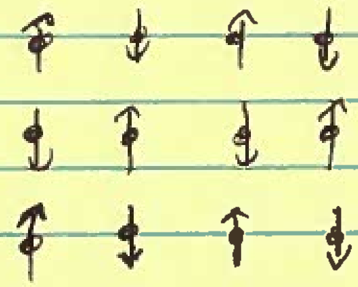
IN FACT, WE SEE THAT $\chi(T)$ DIVERGES AS $T \to T_c$, WHICH MAKES SENSE. AS SPINS APPROACH TEMPERATURES WHERE THEY WANT TO ALIGN SPONTANEOUSLY, THEY WILL BE INFINITELY SUSCEPTIBLE TO SUGGESTIONS TO ALIGN BY APPLIED FIELDS



THIS IS A COMMON WAY OF MEASURING J

EXTENSION TO THE AF ($J<0$) CASE

MARGINALLY MORE COMPLEX IS THE CASE $J<0$. IF, AS WE MIGHT GUESS, THE PREFERRED STATE LOOKS LIKE SO



THEN NOT ALL SPINS ARE EQUIVALENT. (WE HAVE BROKEN DISCRETE TRANSLATIONAL SYMMETRY OF THE LATTICE.) SOME SPINS WILL HAVE OPPOSITE $\langle S_z \rangle$ THAN OTHERS, AND THUS OPPOSITE $\langle B_{eff} \rangle$.

WE CAN GET AROUND THIS BY CONSIDERING "STAGGERED" MAGNETIZATION, WHERE WE SEPARATE THE LATTICE INTO 2 SUBLATTICES, AND ASSUME 2nd LATTICE IS EXACTLY OPPOSITE THE 1st LATTICE

$$m_{staggered} = -g\mu_B\left(\langle S_z\rangle_1 - \langle S_z\rangle_2\right)$$

THIS GIVES THE RESULT

$$\chi_{CW} = \frac{\chi_{CURIE}}{1 + T_c/T}$$

YOU WILL DO THIS ON HW 6.