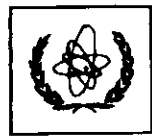




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INTERNATIONAL ATOMIC ENERGY AGENCY  
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**SMR.959 - 11**

**MINIWORKSHOP ON STRONG ELECTRON CORRELATIONS**  
**"Disorder and Interaction in Quantum Systems**  
**and Their Classical Analogs"**

**(1 - 19 July 1996)**

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**"Spin Order in (Some) Quantum Magnets**  
**with Quenched Disorder"**

**Ravin Bhatt**  
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**Dept. of Electrical Engineering**  
**Princeton, NJ 08544-5263**  
**U.S.A.**

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***These are preliminary lecture notes, intended only for distribution to participants.***



# THE ANTIFERROMAGNETIC N.N. SPIN- $\frac{1}{2}$ CHAIN (HEISENBERG)

$$H = \sum_i J (\vec{S}_i \cdot \vec{S}_{i+1}) \quad J > 0$$

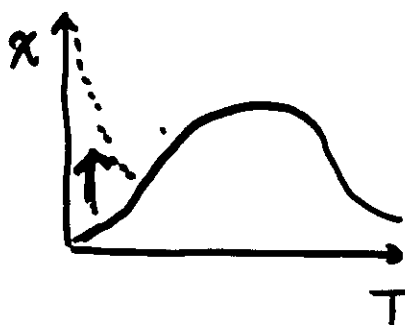
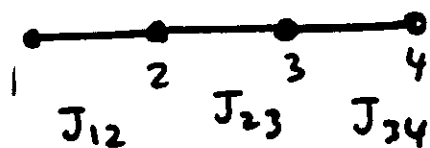
Bethe ansatz soln. Power law correlations.  
(Critical)

Random bonds  $J \rightarrow J_i (> 0) P(J)$

Studied by Dasgupta & Ma (79), Jozsa & Hirsch (80)  
Bondeson & Son (80), Bhatt & Lee (81) ... etc

$\Rightarrow$  Divergent susceptibility at low  $T$ , for  
arbitrarily weak disorder  $x$

Physics:

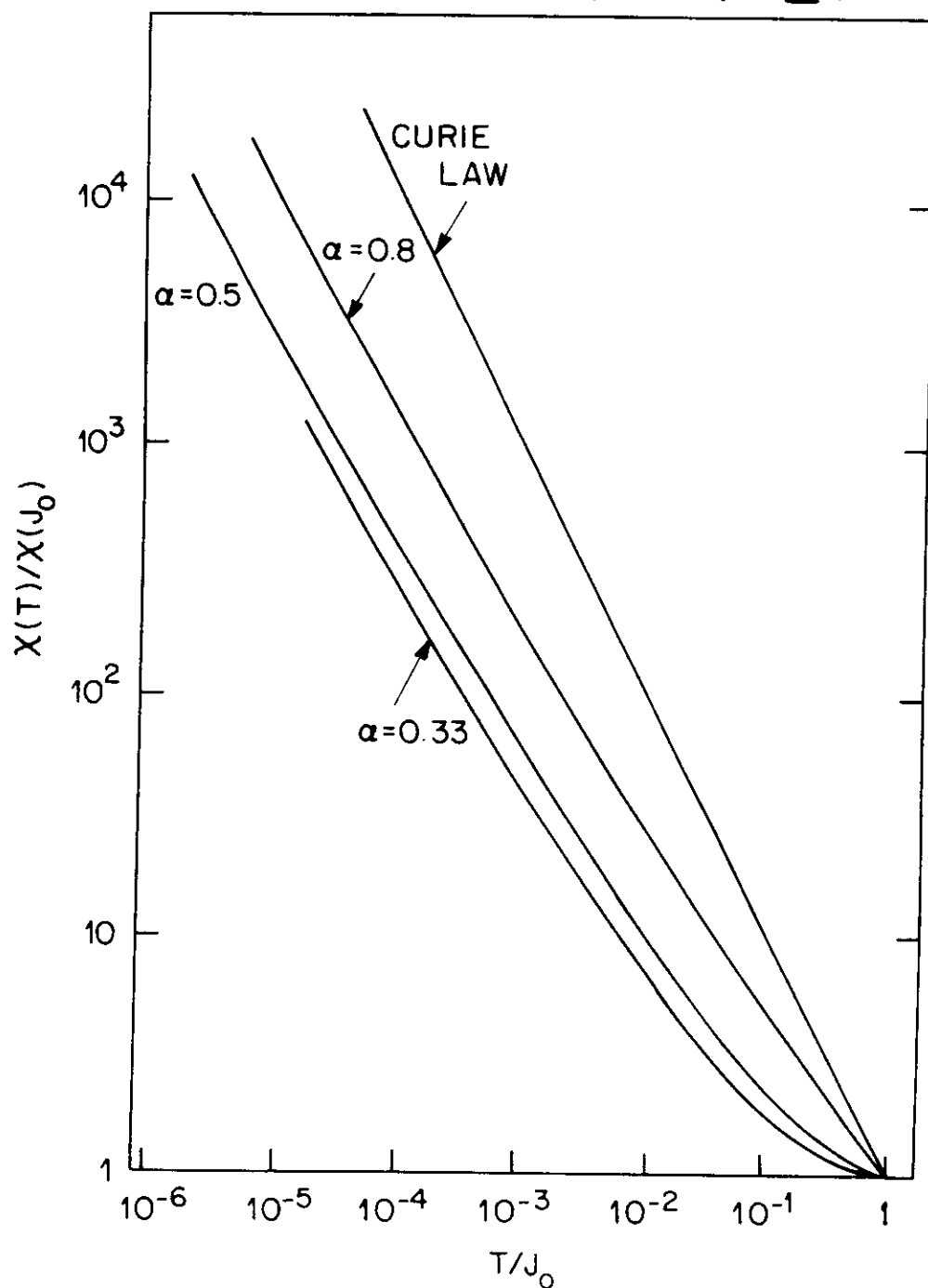


If  $J_{23} \gg J_{12}, J_{34}$ , low energy excitation structure  $\equiv \uparrow \tilde{J}_{14}$

$$\tilde{J}_{14} = \frac{J_{12} J_{34}}{2J_{23}} \quad (\text{very small})$$

$\downarrow$   
 $\bullet \dots \bullet$   
 $1 \quad \tilde{J}_{14} \quad 4$

Bhatt & Lee, J. Appl. Phys 52, 1703 (81)

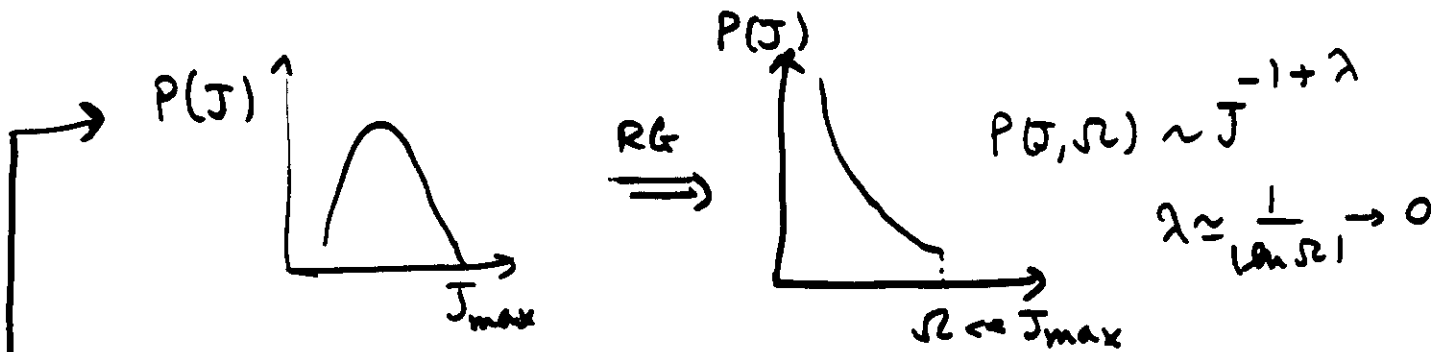


Similar results obtained by Dasgupta & Ma,  
and by Jose and Hirsch.

R.G. procedure generates weak bonds

$P(J)$  broad on logarithmic scale

$$(\ln \tilde{J}_{14} = \ln J_{12} + \ln J_{34} - \ln J_{23} - \ln L)$$



⇒ Random Singlet or Valence-Bond-Glass Phase



Thermodynamics : Decimate till  $\Omega \sim T$

$$N_{\text{spins}} \sim \frac{1}{\ln^2 T}$$

$$\chi \sim \frac{1}{T |\ln^2 T|} ; C \sim \frac{1}{|\ln^3 T|} \quad \text{universal}$$

Detailed analysis by Fisher (94)

$$\langle \vec{S}_i \cdot \vec{S}_j \rangle \sim \frac{1}{|i-j|^2} \quad \text{universal}$$

Experiments on  $(\text{TCNE})_2$ , NMP TCNE, Acridinium-TCNE etc  
 $\chi \sim T^{-\alpha}$   $\alpha$  dependent on sample (0.6-0.8)

# ANALOG IN THREE DIMENSIONS

Doped semiconductors in dilute limit

Localized, hydrogenic bound states, with Bohr radius  $\gg$  lattice constant.  
 $\sim 30 \text{ \AA}$   $\sim \text{\AA}$

For  $n \ll n_c (\sim a_B^{-3})$ , effective Heisenberg Hamiltonian (for uncompensated case),

$$H = \sum_{i,j} J(\vec{R}_{ij}) \vec{S}_i \cdot \vec{S}_j$$

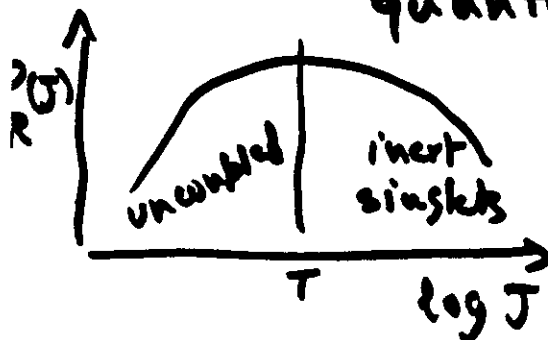
with  $J(\vec{R}) \sim \exp(-2R/a_B)$ , and ANTIFERRO.  
 $\uparrow$   
Short range

Physics (Bhatt + Lee) —

Decimate strongly coupled pair, generate effective couplings for low T

Results: Broad distribution of  $J$ , remains broad, can calculate thermodynamic quantities perturbatively

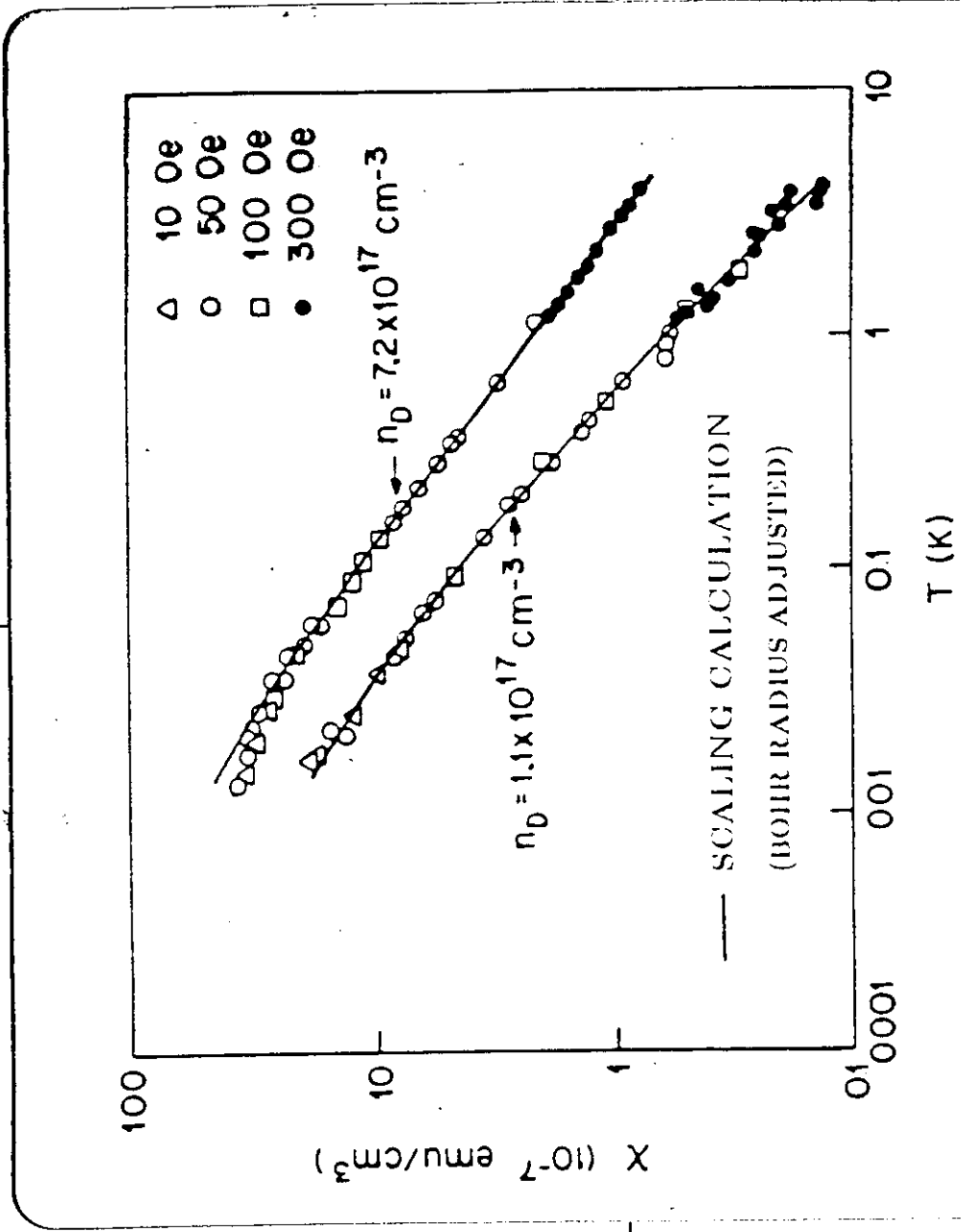
Renormalized distribution of pairs (Random Singlet)



SEQUENCE NO. \_\_\_\_\_

TOP  
DO NOT AFFIX OVERLAYS ALONG THIS SURFACE

NOTES:



Data: K. Andres et al, Phys Rev B 24, 244 (81)  
Theory: Bhatt & Lee, PRL 48, 344 (82)

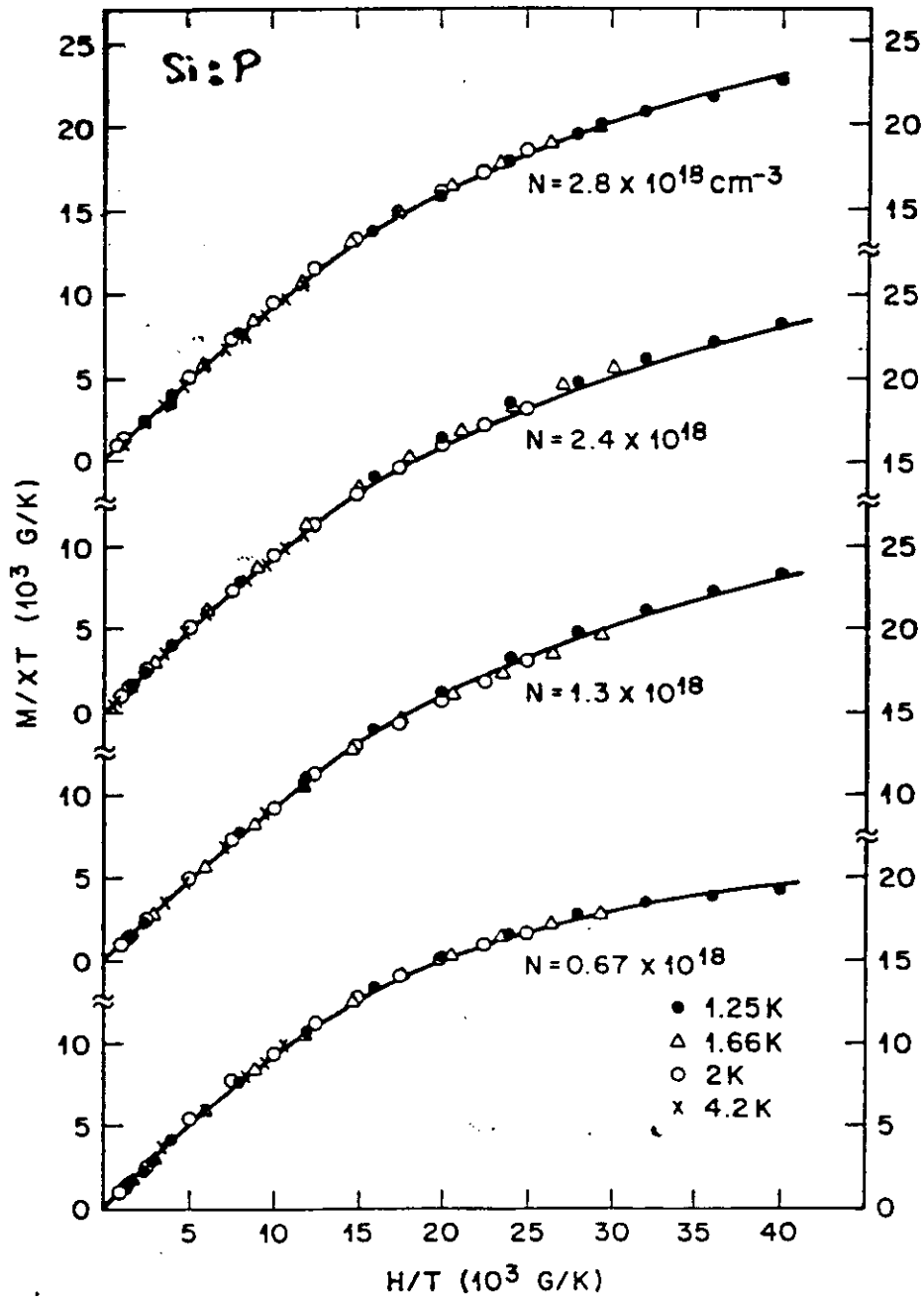




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VG. NO. \_\_\_\_\_

Sarachik et al (CCNY) + R.N.B. (Bell)



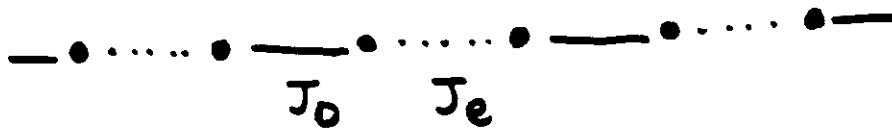
Sarachik et. al., Phys. Rev. B 34, 387 (1986)

$$M/XT = f_{\alpha}(H/T)$$

## II. GAPPED SPIN CHAINS

- SPIN - 1 AF CHAIN (Haldane 83)

- DIMERIZED SPIN- $\frac{1}{2}$  CHAIN



- (nn + nnn) SPIN- $\frac{1}{2}$  CHAIN (Majumdar-Ghosh) 1969

$$\mathcal{H} = J \sum_i (\vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{2} \vec{S}_i \cdot \vec{S}_{i+2})$$

SPONTANEOUSLY DIMERIZED GROUND STATE



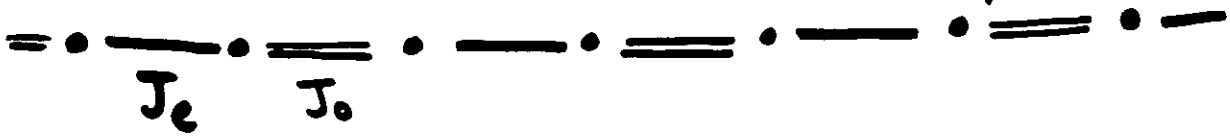
### ADD RANDOMNESS:

Naive Expectation: Models have gaps, no effect at low  $T$  for small randomness, then Random Singlet Phase at high randomness.

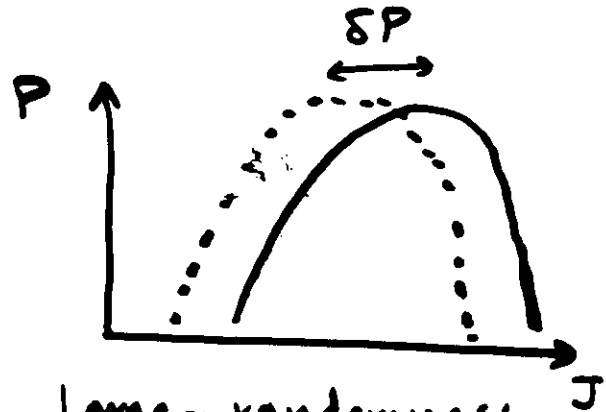
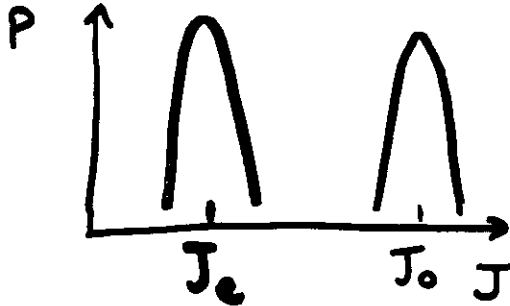
Cautions (Haldane): Non-trivial Topological Order.

# RANDOM DIMERIZED SPIN- $\frac{1}{2}$ CHAIN

[Hyman, Yang, Bhatt & Girvin  
PRL 76, 839(1996)]



Small Randomness - Gap remains  
(non-overlapping dist.)



Look at effect of  $\delta P$  on RG procedure

Large-randomness  
Overlapping distributions  
What happens?

$$\frac{d \delta P}{d |\ln b|} = + \delta P \Rightarrow \text{RELEVANT!}$$

Basically in RG procedure



the middle (large) bond more likely to be odd, leaving very weak even bond instead of two moderate even bonds.

$P_{\text{even}}$  scales to zero coupling faster than  $P_{\text{odd}}$ , leaving uncoupled dimers.

In the end, a soluble RANDOM DIMER model  
(dist. determined by initial dist.)

For small initial dimerization( $\delta$ ) can show

$$P_{\text{odd}}(T) \sim T^{-1+\gamma} \quad \gamma \propto \delta \ll 1$$

$$\chi(T) \sim T^{-1+\gamma}$$

$$C(T) \sim T^\gamma$$

$$\langle \vec{S}_i \cdot \vec{S}_j \rangle \sim e^{-|i-j|/\xi} \quad \xi \sim |\delta|^{-2}$$

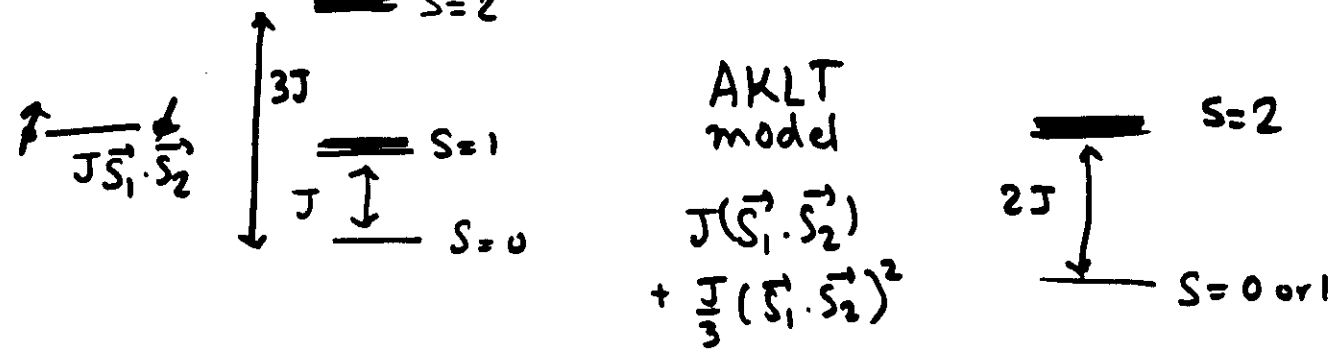
$$\Rightarrow \nu = 2 \left( = \frac{2}{d} \right)$$

distance from criticality

cf.  $\nu = \frac{2}{3}$  without randomness

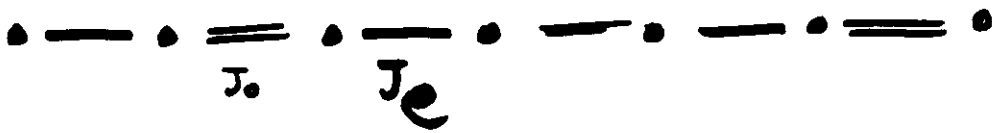
In random spin- $\frac{1}{2}$   
 $\langle \vec{S}_i \cdot \vec{S}_j \rangle \sim |i-j|^{-2}$   
 Uniform spin- $\frac{1}{2}$   
 $\langle \vec{S}_i \cdot \vec{S}_j \rangle \sim |i-j|^{-1/2}$

HOW ABOUT SPIN-1 CHAIN?



Can try to decimate  $S=2$  state. Looking at various cases, appears to be similar to dimerized spin- $\frac{1}{2}$  case

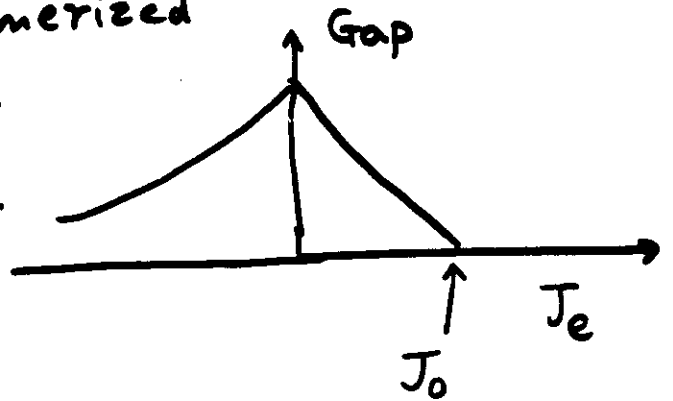
Reason for similarity - Same Phase  
(Hida 92)



$0 < J_e < J_0$  spin- $\frac{1}{2}$  dimerized

$J_e = 0$  trivial dimer

$J_e = -\infty$  spin-1 chain



Conjecture: Same results  
(numerical work underway).

## TOPOLOGICAL ORDER (Haldane)

SPIN-1  $\langle \vec{S}_i \cdot \vec{S}_j \rangle \sim (-1)^{i-j} e^{-|i-j|/\xi}$

Structure + followed by 0's & -, not another +

+ - 00 + 00 - 000 + , + 000 +  
okay not okay

$$T_{ij} = \langle S_i^z \exp \left[ i\pi \sum_{i < k < j} S_k^z \right] S_j^z \rangle = \text{const} \left( -\frac{4}{9} \right)^{|i-j|}$$

DIMERIZED SPIN- $\frac{1}{2}$  eventual order

$$\langle \vec{S}_i \cdot \vec{S}_j \rangle = 0 \quad |i-j| \rightarrow \infty$$

$T_{ij} =$  non zero for  $i$  odd,  $j$  even  
zero otherwise. SURVIVES RANDOMNESS!

In Dimerized Spin- $\frac{1}{2}$  chain



$$\langle \vec{S}_i \cdot \vec{S}_j \rangle = 0 \quad \text{for } |i-j| > 1 \quad \delta = 0$$

$$T_{ij} = \langle S_i^z e^{i\pi \sum_{i < k < j} S_k^z} S_j^z \rangle$$

If  $i$  odd,  $j$  even

$$\begin{aligned} T_{ij} &= \langle S_i^z e^{i\pi S_{i+1}^z} e^{i\pi S_{j-1}^z} S_j^z \rangle \\ &= -4 \langle S_i^z S_{i+1}^z S_{j-1}^z S_j^z \rangle = -\frac{1}{4} \neq 0 \\ & \quad (T_{ij} = 0 \text{ otherwise}) \end{aligned}$$

With randomness

$$T = \lim_{|j-i| \rightarrow \infty} (\overline{T_{2i, 2j-1}} - \overline{T_{2i+1, 2j}})$$

$$\sim -|\delta|^{2\beta} \text{sign}(\delta) \quad \beta = 2$$

$\Rightarrow$  T order exists all throughout for dimerized chain

~~There is a spontaneous order~~

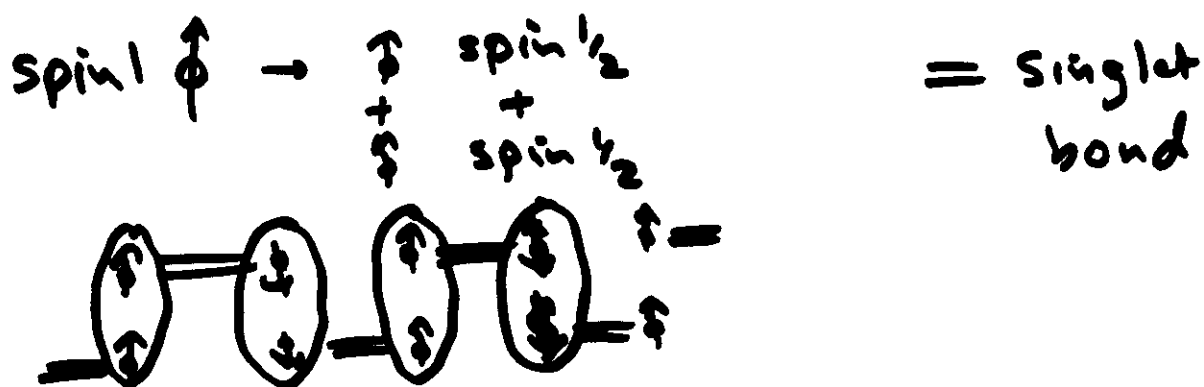
In SPIN-1 case, look at AKLT

model:

$$H = \sum_i J_i \left[ \vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3} (\vec{S}_i \cdot \vec{S}_{i+1})^2 \right]$$

$$J_i > 0$$

Ground state identical for all  $J_i$  configurations



Thermodynamics (at low T)  
also

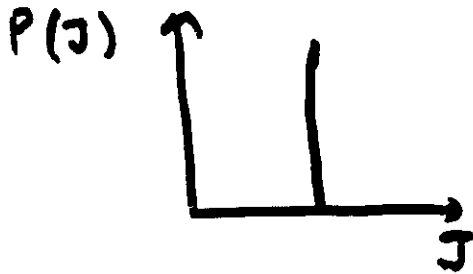
depends on  $P(J_i)$

but ground state order persists.  
↓  
topological

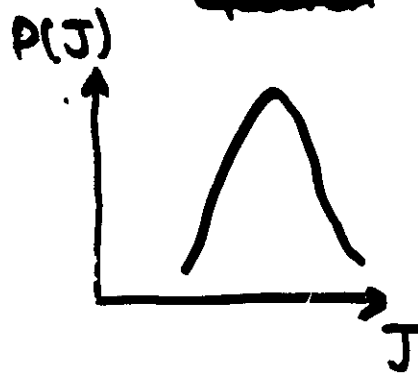
Is this generic ?

# SPIN-1 CHAIN

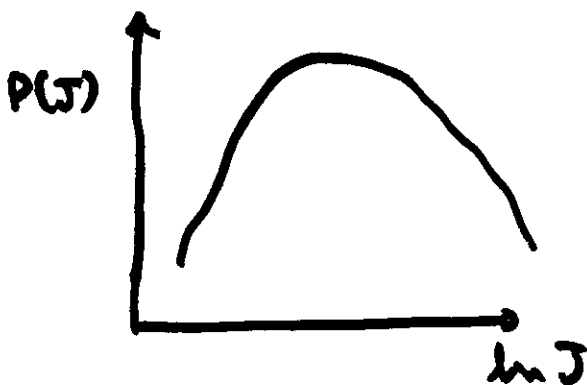
(Preliminary Results  
Haldane & Yang)



Haldane Gap  
Topological Order  
 $\chi(T) \rightarrow 0$  as  $T \rightarrow 0$   
exponentially



at a Critical width  
 $\chi(T) \rightarrow \infty$  as  $T \rightarrow 0$   
BUT Topological Order  
persists  
Non-universal low  $T$   
behaviour  $\chi(T) \sim T^{-\alpha}$   
varying  $\alpha$



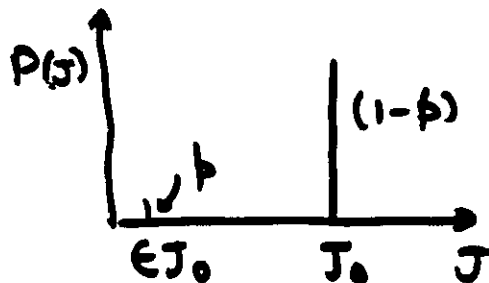
still broader  
 $P(J)$

Random Singlet Phase  
Topological order destroyed  
 $\chi(T) \rightarrow \infty$  as  $T \rightarrow 0$   
 $\sim (T \ln^2 \frac{1}{T})^{-1}$   
Universal low  $T$  behaviour  
as in  $\text{Spin-1/2}$

# SPIN-1 chain with "diluted" bonds

$$P(J) = p \delta(J - \epsilon J_0) + (1-p) \delta(J - J_0)$$

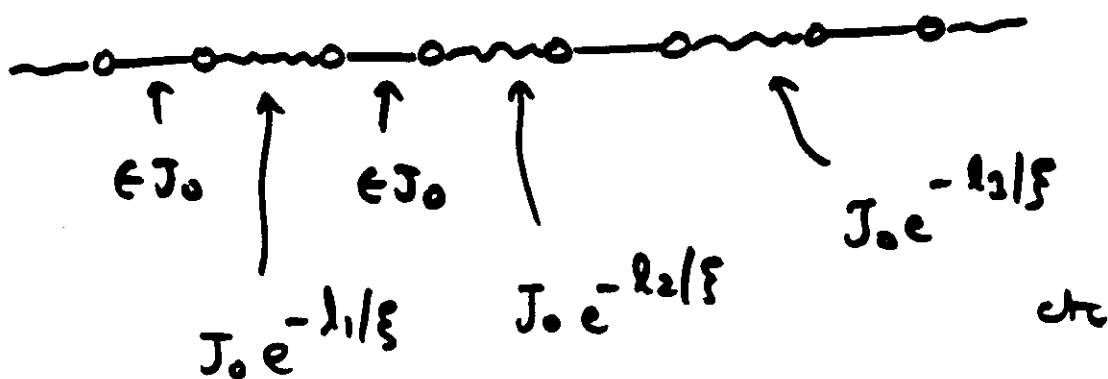
Goes to "Griffiths" phase  
rightaway?



$$\epsilon J_0 \ll J_0$$

$\Rightarrow$

- $\circ$  - spin 1
- $\circ$  - spin  $-\frac{1}{2}$



$\Rightarrow$  like dimerized spin- $1/2$  case

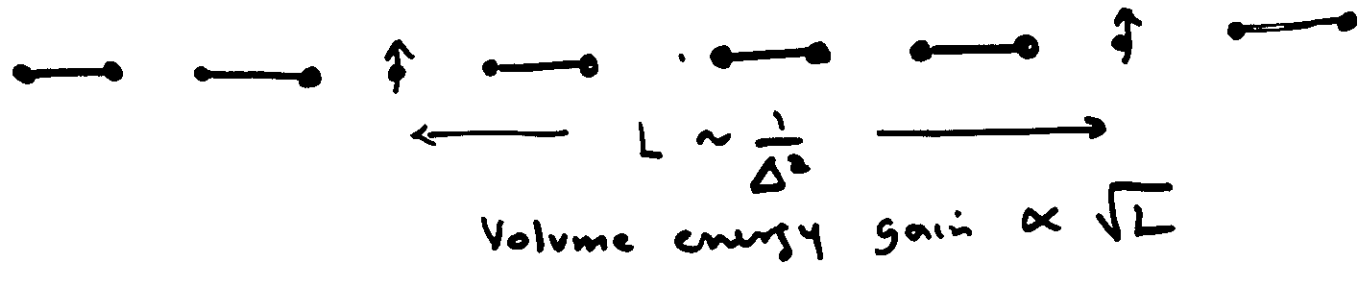
always in Griffiths phase  $\chi(T) \sim T^{-\alpha}$

MAJUMDAR-GHOSH MODEL  $H = \sum J (S_i \cdot S_{i+1} + \frac{1}{2} S_i^z \cdot S_{i+2}^z)$

Spontaneous Dimerization - two ground states



With randomness, for arbitrarily weak  $\Delta$ ,  
 create unpaired spins (topological solitons) in regions  
 between two phases



$\Rightarrow$  UNSTABLE AGAINST WEAK RANDOMNESS

$$\chi \sim \frac{\Delta^2}{T |\ln^2 T|}$$

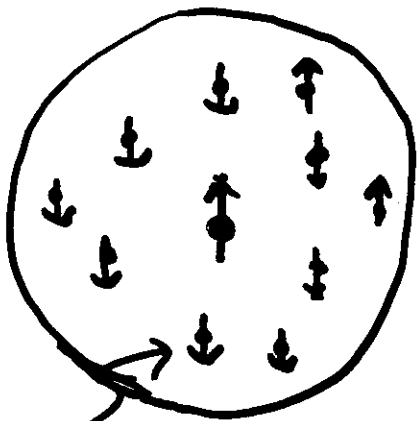
TOPOLOGICAL ORDER DESTROYED, IMMEDIATELY.

# SINGLE MAGNETIC POLARON

Donor Electron - Bohr radius  $\sim 20 \text{ \AA}$   
 Binding Energy  $\sim 20 \text{ meV}$

Scale of A-F. interaction with Mn  
 $\sim 20 \text{ K} \sim 2 \text{ meV}$

Assume Small Mn conc. (neglect Mn-Mn int.)

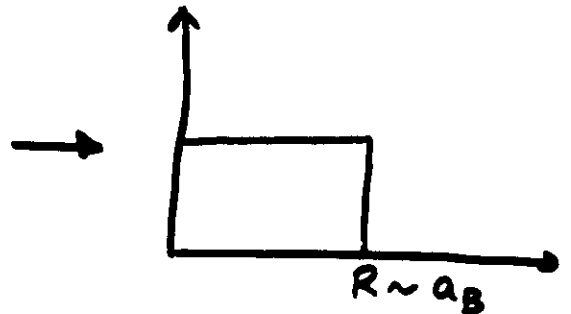
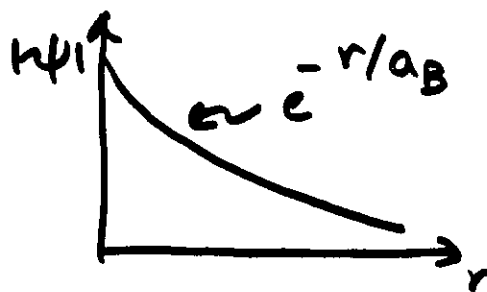


Typical #  
 of Mn in wavefn  
 $\sim 20 - 50$

$$\uparrow \vec{s} = 1/2 \quad \downarrow \vec{S}_i = 5/2$$

$$H = \alpha \sum_i (\vec{s} \cdot \vec{S}_i) |\psi_i|^2$$

$$\downarrow H_0 = K \sum_{|\vec{R}_i| < R} \vec{s} \cdot \vec{S}_i$$



## Justification of $H_0$ :

Feynman Variational Principle

$$F \leq F_0 + \langle H - H_0 \rangle$$

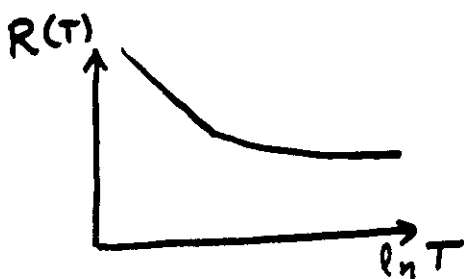
Use  $K$  and  $R$  as variational parameters  
minimize R.H.S. get "best"  $H_0(T)$ .

Result: High  $T$ , Mn spins all free,  
 $H_0$  tries to match wavefn. as best  
as it can.  $R = 1.16 a_B$ .  
 $K \sim .06 \alpha / a_B^3$

Low  $T$ : competition between entropy of  
free spins outside sphere, and energy  
gain due to exchange interaction within

$$\text{expect } \alpha |\Psi(R)|^2 \sim k_B T$$

$$\text{or } R \sim a_B \ln\left(\frac{T_0}{T}\right)$$

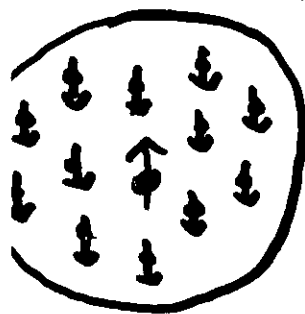


Reasonable.

Soln of  $H_0 = K \vec{a} \cdot \vec{S} \quad \vec{S} = \sum_i (\vec{S}_i)$

QM:  $H_0 = \frac{1}{2} K [(\vec{a} + \vec{S})^2 - \vec{a}^2 - \vec{S}^2]$

Eigenvalues of  $\vec{a} \cdot \vec{S} = S_{\pm} \frac{1}{2}$ , Energies



$$E_0 = -\frac{K}{2} (S+1) \quad + \quad \frac{K S}{2}$$

$(S - \frac{1}{2}) \qquad \qquad \qquad (S + \frac{1}{2})$

← Ground state

Classically ( $S$ ), with QM. ( $a$ )  $E_0 = \pm \frac{K S}{2}$

(can solve at all  $T$ ):

$$Z = 2 \int \dots \int d\Omega_1 \dots d\Omega_N \cosh(\gamma S)$$

$$S = \sqrt{(\sum_j \vec{S}_j)^2}$$

$$\gamma = \frac{\beta K}{2}$$

$$= 2 [F(\gamma)]^N \left[ 1 + \gamma \frac{N F'(\gamma)}{F(\gamma)} \right]$$

$$F(\gamma) = e^{5/2 \gamma} + e^{3/2 \gamma} + \dots + e^{-5/2 \gamma} \quad \leftarrow \quad 2\pi \int_{-1}^{+1} e^{-\gamma S_2} d\Omega$$

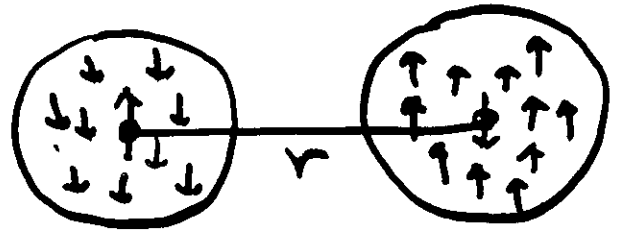
⇒ Can get all thermodynamic, magnetic quantities.

$$Z = 2 \int \mathcal{D}(S) \cosh(\gamma S) d^3 S$$

# TWO POLARONS

Include AF exchange between donor electron spins :  $J \vec{s}_1 \cdot \vec{s}_2$   $J(r) \sim e^{-2r/a_B}$

$$H = K(\vec{s}_1 \cdot \vec{S}_1 + \vec{s}_2 \cdot \vec{S}_2) + J \vec{s}_1 \cdot \vec{s}_2$$



( $J \ll K$ )

At low T,  $\vec{S}_\mu$  fully polarized, i.e.  $|\vec{S}_\mu| = S_{\max} = S$

$$E = -2 \cdot \frac{K(S+1)}{2} \pm \begin{cases} J/4 & \vec{s}_1, \vec{s}_2 \text{ parallel} \\ -3J/4 & \text{anti-} \end{cases}$$

$$\mu = 1, 2$$

$$\vec{S}_\mu \parallel \vec{s}_\mu$$

G-State  
 $\Rightarrow S_{\text{tot}} = 0$  at  $T=0$

With same classical approx for  $\vec{S}_\mu$ , can solve exactly, within fully polarized approx.

$$Z = \iint e^{\frac{\beta K}{2}(S_1 + S_2)} \delta(S_1) \delta(S_2) d^3 S_1 d^3 S_2$$

(allow for different angles bet.  $\vec{S}_1$  &  $\vec{S}_2$ )

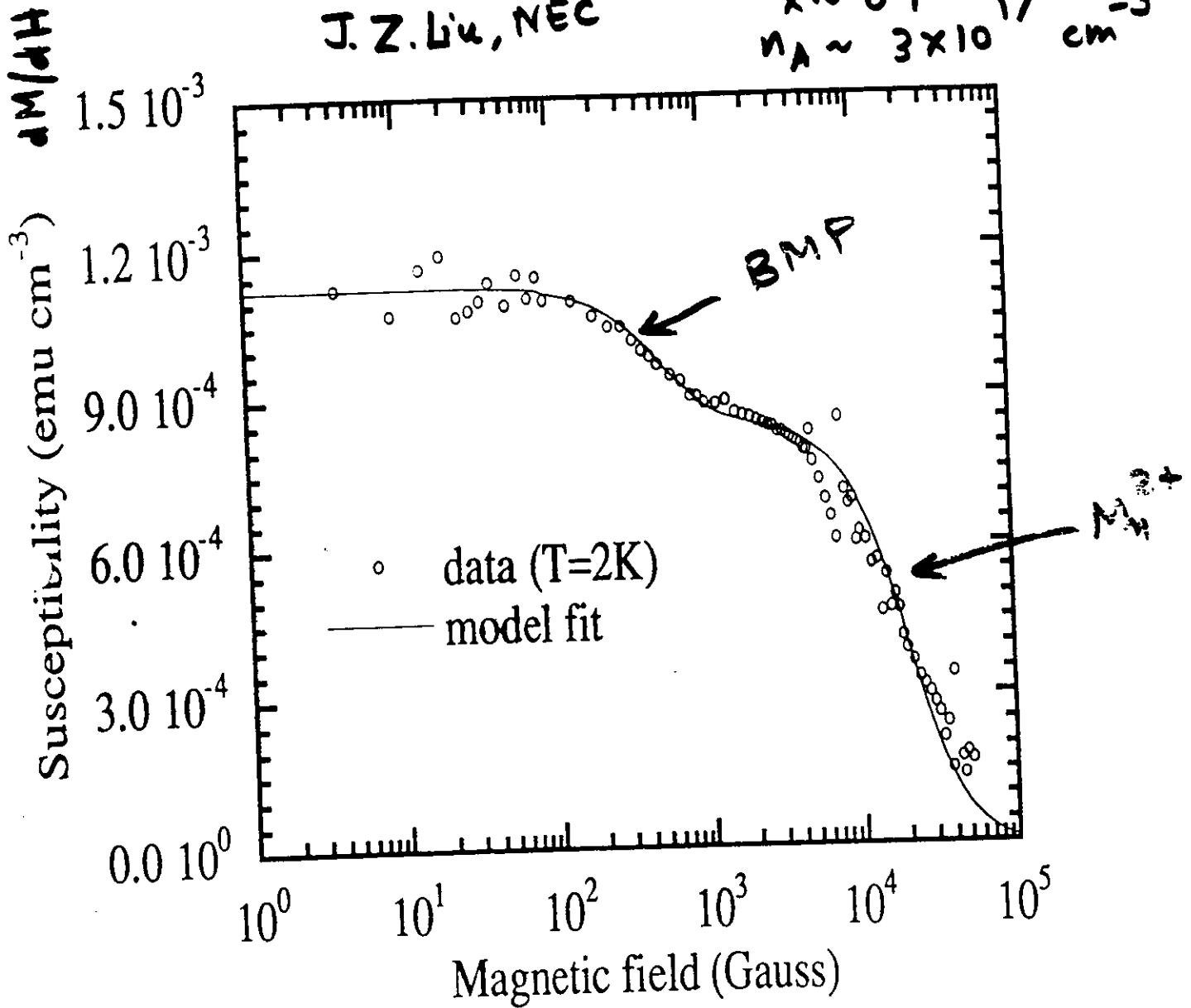
$$= \frac{1}{2} Z_1 Z_2 \frac{\sinh(\beta J/4)}{(\beta J/4)}$$

$$\Rightarrow \langle \cos \theta_{12} \rangle = - \left[ \coth \left( \frac{\beta J}{4} \right) - \frac{4}{\beta J} \right]$$

Exptl Data on p-type  
 $Zn_{1-x}Mn_xTe : P$

J. Z. Liu, NEC

$x \sim 0.1$   
 $n_A \sim 3 \times 10^{17} \text{ cm}^{-3}$

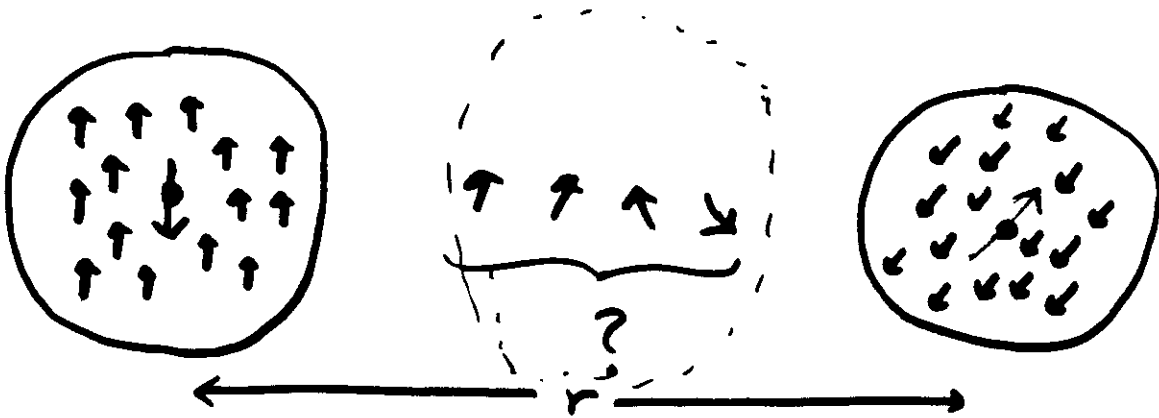


Because of separation of field scales, can analyse BMP & Mn separately. (Langevin / Brillouin fn. with effective interaction as Curie temp.)

Experimental Data  $\Rightarrow$  "Ferro magnetic interaction" between polarons, ie.

$$\chi \sim (T - T_0)^{-1} \text{ with } T_0 > 0.$$

$\rightarrow$  LEFT OUT INTERVENING  $M_n$  !



$$H = \alpha \sum_i (\vec{\delta}_1 \cdot \vec{S}_i |\psi_{1i}|^2 + \vec{\delta}_2 \cdot \vec{S}_i |\psi_{2i}|^2) + J \vec{\delta}_1 \cdot \vec{\delta}_2$$

$\downarrow$

$$H_0 = K \sum_{R_{i1} < R} \vec{\delta}_1 \cdot \vec{S}_i + K \sum_{R_{j2} < R} \vec{\delta}_2 \cdot \vec{S}_j + J \vec{\delta}_1 \cdot \vec{\delta}_2$$

$$+ K' \sum_{\text{inter.}} \vec{S}_k \cdot (\vec{\delta}_1 + \vec{\delta}_2)$$

For large  $r$ , expect  $K' \sim |\psi(\frac{r}{2})|^2 \sim e^{-r/a_B}$

$$\gg J \sim e^{-2r/a_B}$$

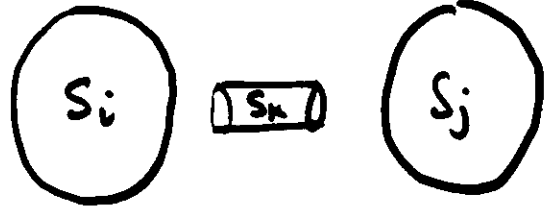
Q.M. can solve  $H_0$  with  $K'$  also. For

ground state,  $\sum_i S_i = S_{\max} = \sum_j S_j$ ,  $\sum_k S_k = S_{\max} = S'$

Two competing states

$$\vec{S}_1 + \vec{S}_2 = 0$$

$$E = -K(S+1) - \frac{3J}{4}$$

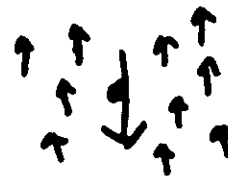
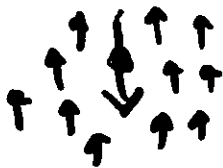


$$\vec{S}_1 + \vec{S}_2 = 1, \quad \vec{S}_1 + \vec{S}_2 + \sum_k \vec{S}_k = S' - 1$$

$$E = -K(S+1) + \frac{J}{4} = K'(S'+1)$$

Latter wins when  $K'(S'+1) > J$

Configuration:



$$S_{\text{tot}} = 2S + S' - 1$$

cf.  $S_{\text{ferro}} = 2S + S' + 1$

Treating  $S, S'$  as classical, can solve with prior assumptions the 2 polaron problem:

$$Z = Z_1 Z_2 \int_0^{\sqrt{2}} e^{-\frac{\beta J}{4}(x^2-1)} \left( \mathcal{F}\left(\frac{\beta K' x}{\sqrt{2}}\right) \right)^{N_3} x dx$$

$$\Rightarrow \langle \cos \theta_{12} \rangle = \frac{\int_0^{\sqrt{2}} e^{-\beta J(x^2-1)/4} \left\{ \mathcal{F}\left(\frac{\beta K' x}{\sqrt{2}}\right) \right\}^{N_3} (x^2-1) x dx}{\int_0^{\sqrt{2}} e^{-\beta J(x^2-1)/4} \left\{ \right\}^{N_3} x dx}$$

etc.

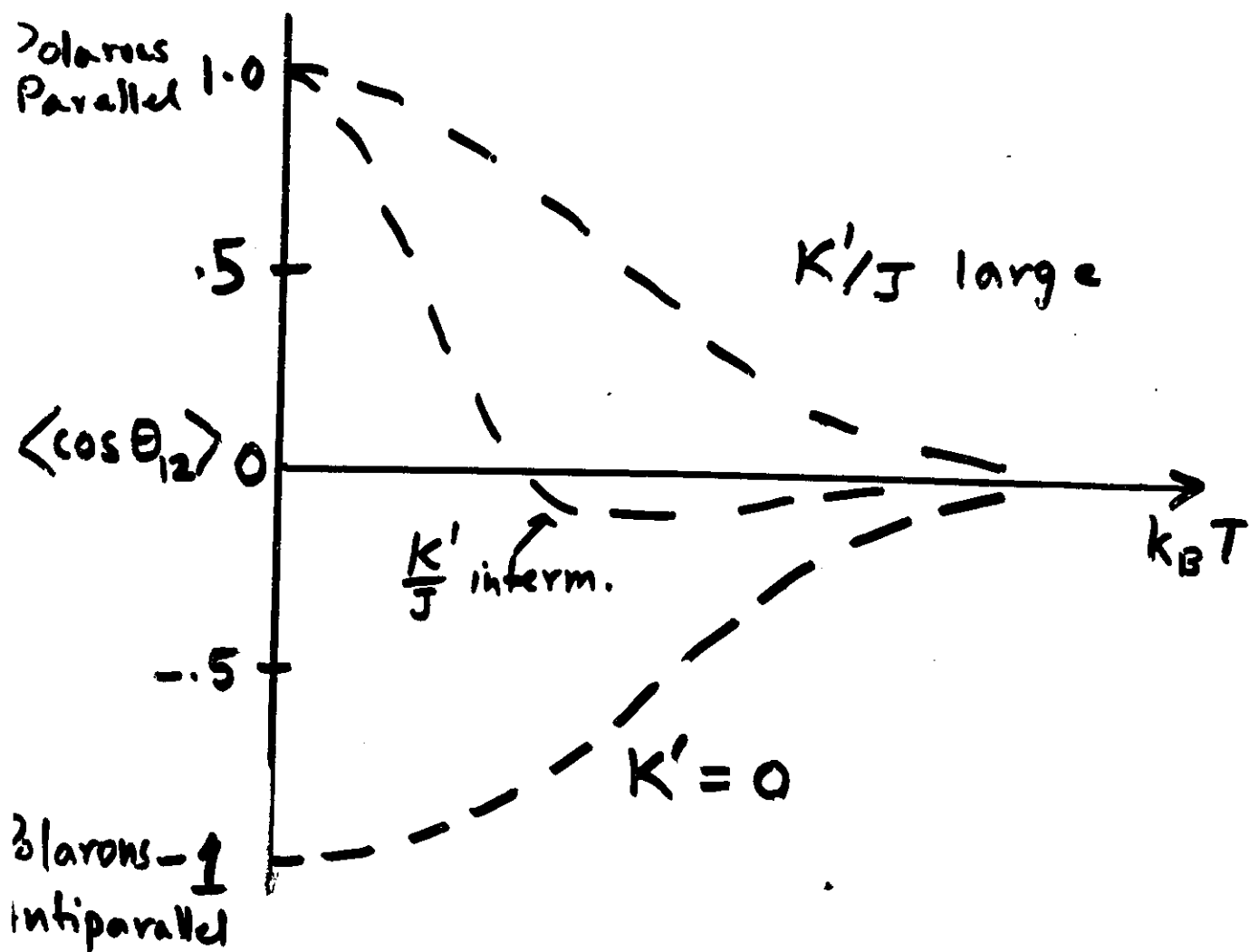
## MANY POLARONS

If "superexchange" wins, ferromagnetism likely outcome, even if some cases af.

Decimate like Bhatt-Lee, to long distances

$K' > J$ , then ferromag. takes over.

Avg. angle between polaron moments



## SUMMARY

**SPIN CHAINS** : Not all Gaps are the same.

Dimerized spin- $\frac{1}{2}$  and spin-1 chain in Haldane phase retain non-trivial topological structure even when gap  $\rightarrow 0$  (finite randomness)

Non-universal thermodynamics, but similar to RS phase

Short range spin-spin corr., but persisting Topological order

Eventual transition to RS in spin-1 case, but weak signature in thermodynamics.

spontaneously dimerized (MG or biquadratic spin-1)

unstable to arbitrarily weak disorder, divergent  $\chi$  immediately.

## DILUTED MAGNETIC SEMICONDUCTORS (3D) :

Intervening free Mn give rise to effective Ferromagnetic coupling between polarons.

At  $T=0$  (Ground state) ALMOST Ferromagnetic with only AF interactions in  $\text{Mn}^{2+}$ . ( $\frac{J_{FM}}{J} \sim 10^{-4}$ )

Ferromagnetic Insulator-Metal Transition.

QUANTUM (ANTIFERRO) MAGNETS WITH QUENCHED DISORDER HAVE MANY INTERESTING PHASES, WITH MORE SURPRISES TO COME.

