Kinetic Antiferromagnetism

Magnetism from hole motion:
CounterNagaoka-Thouless theorem on frustrated lattices

Sriram Shastry

UCSC, Santa Cruz, CA

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Plan of the talk

- Setting for the talk, introduction to electronic frustration
- For matters of nature of order, variational ideas should be abandoned! Two states with very different order can be incredibly close in energy.
- Method used for getting definitive results, towers of states (Paris group: Bernu, Misguich, Lhuillier..)
- Calculation for single hole in J=0 models in 2d and 1d.
- Calculation for many holes in t-J model
- Prospects and general applicability.

Jan Haerter UCSC coauthor of main paper

Thanks to Claire Lhuillier and Olivier Cepas for useful discussions about clusters

Single slide summary:

In certain metallic cases, with strong correlation, we find

Athough:

$$J=0$$

Yet:

$$\Theta_{C-W} \sim cx|t|$$

Real kinetic processes lead to AFM

Real in contrast to virtual kinetic processes a la Superexchange

Kinetic Antiferromagnetism

Where does it belong?

	Ferro	Antiferro
Metals	•Stoner (ZrZn2) •Kanamori (Ni) •Double exchange (CMR) •Nagaoka (High Tc)	•SDW AFM (Chromium)(Weak coupling FS instability) •Kinetic AFM (strong coupling)
Insulators	•Direct exchange •Superexchange with small angles Goodenough Anderson rules	•Anderson's superexchange

NEW

Electronic Frustration

The Model, The states

$$H = - \sum_{i,j,\sigma} t_{i,j} c^{\dagger}_{\vec{R}_j,\sigma} c_{\vec{R}_i,\sigma}$$

$$c^{\dagger}_{\vec{R}_i,\uparrow} c^{\dagger}_{\vec{R}_i,\downarrow} = 0$$

t's are hopping elements on the lattice, C's electron destruction operators.

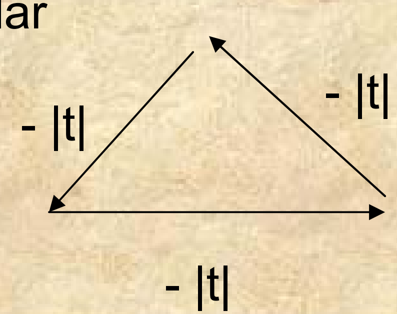
Heart of the matter.

Infinite U constraint implies vanishing of pairs of occupied sites.

Single hole:

Frustration is defined for triangular type lattices by condition **t>0**

Product of **electron hops** over basic closed loop is negative for frustrated case! Flux π per trgl



$$
\begin{array}{cc} \hline a & d \\ \hline 0 & m \\ \hline \end{array}
\quad
\begin{array}{cc} \hline a & d \\ \hline m & 0 \\ \hline \end{array}
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\begin{array}{cc} \hline a & 0 \\ \hline m & d \\ \hline \end{array}
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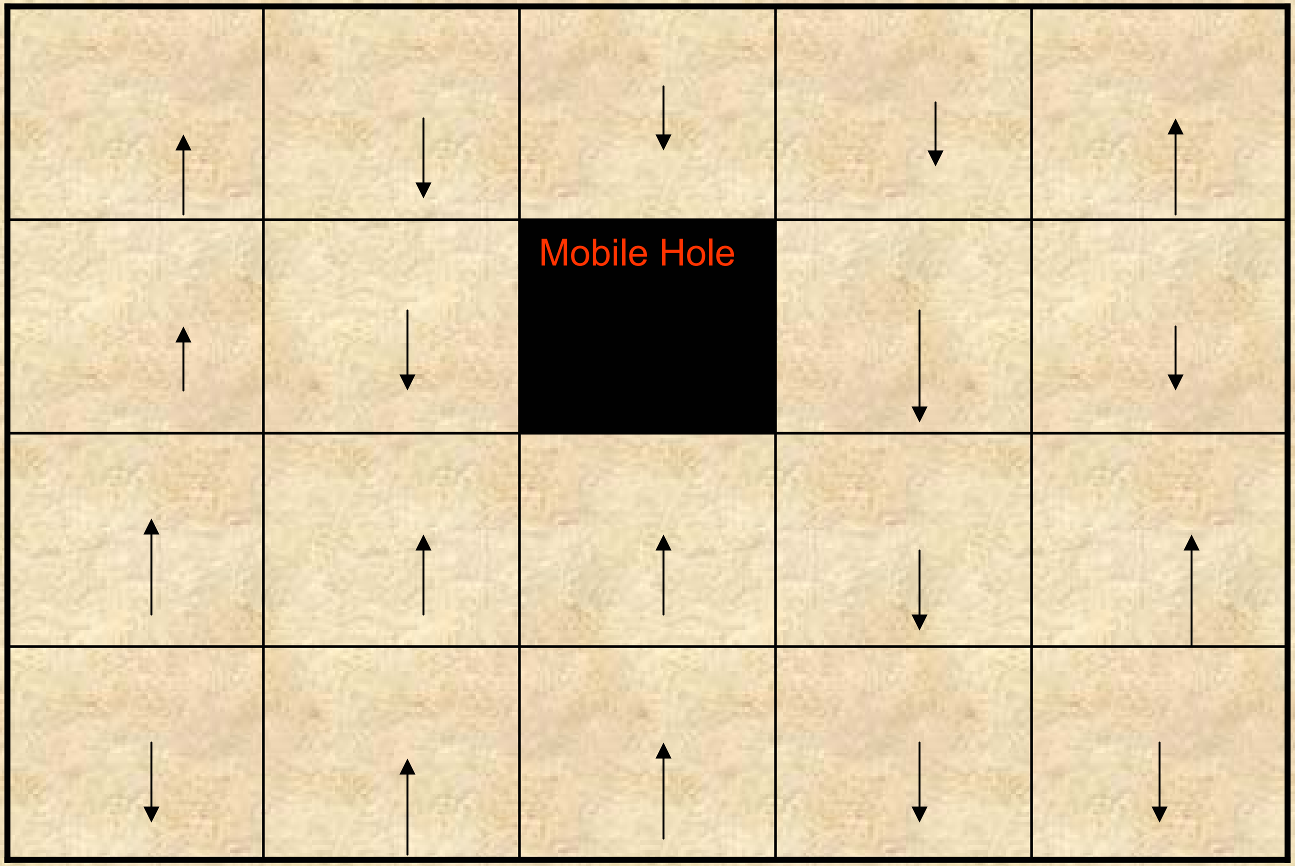
\begin{array}{cc} \hline 0 & a \\ \hline m & d \\ \hline \end{array}
\quad
\begin{array}{cc} \hline m & a \\ \hline 0 & d \\ \hline \end{array}
$$

Hole motion can rearrange patterns:

•Basis of childrens game (mobile squares). Todays science is tomorrows toy, and sometimes vice versa!!

•Also Nagaoka type theorems. In fact metallic magnetism is partly based on this idea.

a	b	c
d		f
g	h	i



PHYSICAL REVIEW VOLUME 147, NUMBER 1 8 JULY 1966

Ferromagnetism in a Narrow, Almost Half-Filled *s* Band*

YOSUKE NAGAOKA†
Department of Physics, University of California, San Diego, La Jolla, California
(Received 17 January 1966)

What do Nagaoka and Thouless prove?

•For frustrated case nothing. (our work)

•Single hole, unfrustrated case ($t<0$) infinite U

•$E_0(S_{max}) \leq E_0(S_{any})$ Thus the maximal spin state cannot be beaten (Remember for each S there are 2S+1 states with different projection)

•In 2d and 3d the inequality can be strengthened to give

$E_0(S_{max}) < E_0(S_{any})$ (tricky part of theorem) hence true ground state. However in 1-d it is a superparamagnet, in the sense that all S states are degenerate.

•Many questions (finite T, many holes etc) remained, and infact regarded as pathological for many years.

More recently Shastry Krishnamurthy Anderson (1989) suggested robustness of this state against hole filling using variational w fns. Triangular lattice for unfrustrated case a strong case for FM order at any filling.

Anderson, Rice, Lee, Randeria, Trivedi and Zhang suggest Nagaoka Ferromagnetism is responsible for weakening J as

$J_{eff}= J- 4 x |t|$

for finite hole density (i.e. a thermodynamic state) in High Tc.

Main new work

PRL **95,** 087202 (2005) PHYSICAL REVIEW LETTERS week ending 19 AUGUST 2005

Kinetic Antiferromagnetism in the Triangular Lattice

Jan O. Haerter and B. Sriram Shastry
Physics Department, University of California, Santa Cruz, California 95064, USA
(Received 25 May 2005; published 19 August 2005)

We show that the motion of a single hole in the infinite U Hubbard model with frustrated hopping leads to weak metallic antiferromagnetism of kinetic origin. An intimate relationship is demonstrated between the simplest versions of this problem in 1 and 2 dimensions, and two of the most subtle many body problems, namely the Heisenberg Bethe ring in 1-d and the 2-dimensional triangular lattice Heisenberg antiferromagnet.

Technique used:

Construct momentum and spin eigenstates of H on clusters that are well chosen, i.e. do not prevent any kind of expected order, e.g. three sublattice order. We take clusters of upto 27 sites with one hole, so the ground state spin is integer, 0, 1, 2, etc, and in each sector compute excitation energies for different momentum.

For the Heisenberg model, we know that if the ground state is ordered in the thermodynamic limit, then the finite sized spectrum will reflect rotator kind of spectrum:

$$\mathrm{J}\ \vec{S}_i.\vec{S}_j \sim J/N^2 \vec{M}_a.\vec{M}_b$$

$$\mathrm{E}_0(S) = E_0(0) + J\frac{S(S+1)}{I}$$

Where J is the O(1) exchange energy and I is a moment of inertia type number, which is O(N) if the thermodynamic limit possesses LRO.

Further for say S=1 sector, we expect AFM magnons so the excitation spectrum above the GS will look like a tower of states with a typical energies:

$$\epsilon = Jc\frac{2\pi \mathrm{i}nteger}{L}$$

Symmetries:

$$S^+ = \sum c^\dagger_{i,\uparrow} c_{i,\downarrow}$$
$$S_z = \frac{1}{2} \sum_i (n_{I,\uparrow} - n_{I,\downarrow})$$
$$\vec{S}^2_{tot} = S^2_x + S^2_y + S^2_z$$

[H,Q]=0

Hence in each subspace of S_z we set up the Hamiltonian matrix.

We also use time reversal invariance so that under a global transformation $\sigma_j \to -\sigma_j$, its eigenvalues are $\kappa = \pm 1$. If $(L-1)/2$ is odd (even) the even spin states have $\kappa = -1(1)$, the odd spin states the opposite value.

To understand this, note that each pairwise singlet changes sign under time reversal, whereas a triplet does not. Decomposing a global state to count the number of pairwise singlets and pairwise triplets gives this very useful rule. (Surprisingly not been used before)

Lexical Ordering: Phase factor crucial

Let us locate the hole at site $\vec{R}_{i_0}$,

Let us write a basis state $|\alpha, i_o\rangle = (-1)^{i_0} c^{\dagger}_{\vec{R}_1,\sigma_{\vec{R}_1}} c^{\dagger}_{\vec{R}_2,\sigma_{\vec{R}_2}} \ldots . c^{\dagger}_{\vec{R}_N,\sigma_{\vec{R}_N}} |0\rangle$

Thus the hole state is characterized by the spin configuration as well as hole location: There are N 2^{N-1} states in this manifold.

Collapse to one label |a>=| i , R1,R2,...>

Matrix in this space <a| H | b>

Hamiltonian hops the holes and shuffles the spin background. It is a matrix in the above dimensions.

0	t	t	t	t
t	0	t	t	t
t	t	0	t	t
t	t	t	0	t

Matrix elements are mostly 0, there are "z" non zero entries t where z is the coordination number. Notice that the matrix is not "systematic" cannot e.g. fourier transform.

Nagaoka Thouless say that if $t<0$, we can easily find ground state bypassing the labeling issues and also determine the GS spin.

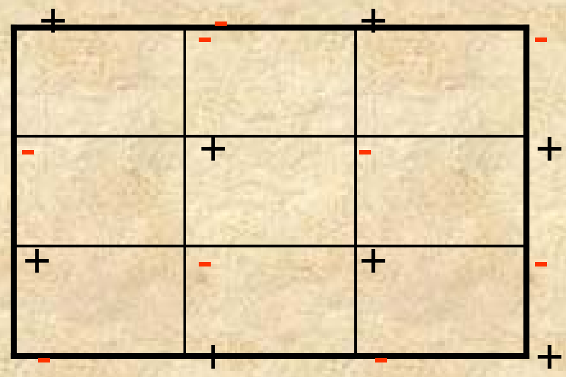
Take a sum state over all configurations with equal weight $|\Phi\rangle = \Sigma\ |a\rangle$. Clearly eigenstate with ev $\lambda = z\ t = -z\ |t|$

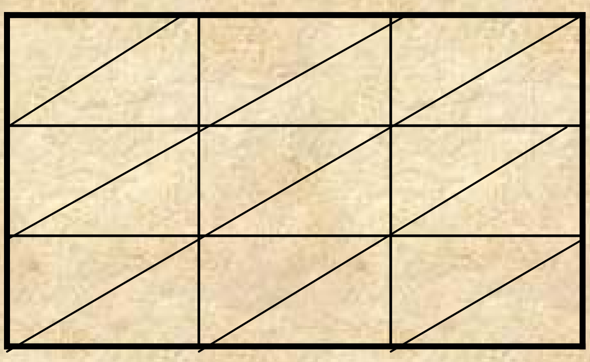
Such a state is in fact a ferromagnetic state since it occurs in each Sz subspace and moreover by action of S^+ and S^- , we can ladder up and down various subspaces.

It is infact the ground state since the lower bound on energy is the same number $-z\ |t|$.

• Sign of hopping crucial t<0 always ferromagnetic

If lattice is bipartite, we can always change sign of t, and hence for sc, bcc, we can always arrange to have Nagaoka theorem fulfilled. Not so for triangular lattice or fcc.





Triangular lattice: Counter Nagaoka Thouless case

We first use a different representation that maps the fermionic hole problem into a pure spin problem. Essential idea is to locate the hole at one site and make use of translation operators.

Localize the hole at site $\vec{R}_{i_0}$, and write $|\alpha\rangle = c^\dagger_{\vec{R}_1,\sigma_{\vec{R}_1}} c^\dagger_{\vec{R}_2,\sigma_{\vec{R}_2}} ... c^\dagger_{\vec{R}_N,\sigma_{\vec{R}_N}} |0\rangle$.

This is now a momentum eigenstate with spin pattern α

$$\psi(\vec{k},\alpha) = \frac{1}{\sqrt{L}} \sum_{\vec{r}} e^{(-i\vec{k}.\vec{r})} T_{\vec{r}} |\alpha\rangle$$

$$T_{\vec{r}} c^\dagger_{\vec{R}_i,\sigma} T^\dagger_{\vec{r}} = c^\dagger_{\vec{R}_i+\vec{r},\sigma}$$

T is a translation operator

$$\langle\beta|H^{\vec{k}}_{eff}|\alpha\rangle = \sum_{\vec{\delta}} t_{\vec{\delta}}\, e^{-i\vec{\delta}.\vec{k}} \langle\beta|T_{\vec{\delta}}\, c_{\vec{R}_{i_0}-\vec{\delta},\sigma} c^\dagger_{\vec{R}_{i0},\sigma} |\alpha\rangle.$$

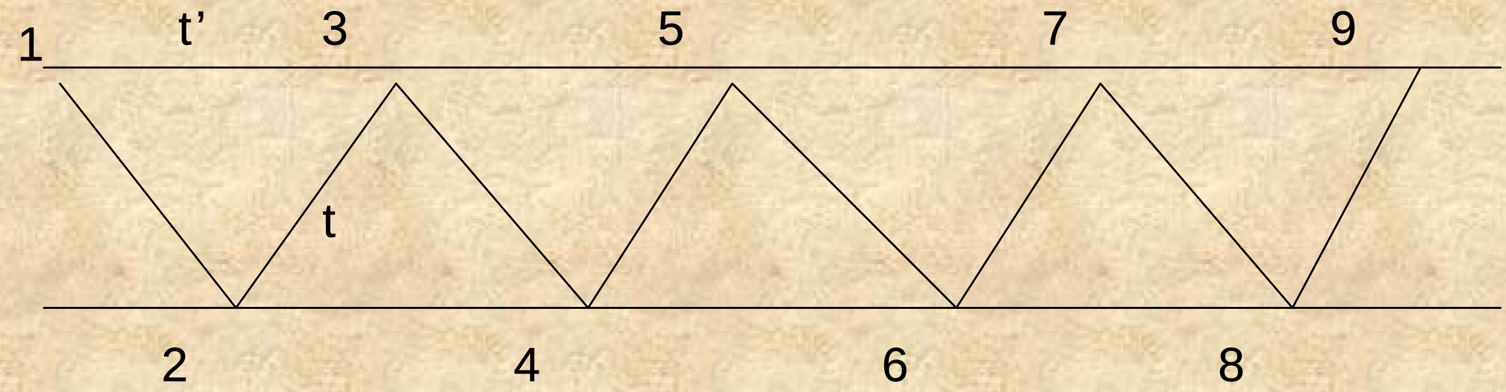
C creates a hole which is brought back to “origin” by T

Making use of [H,T]=0   Hence only PBC’s OK

Not yet spin problem since fermionic signs remain.

However, for **any** cluster, we prove that it can be “decoloured”, and a translation operator that moves spins only, rather than spin and charge as in **T**

Example 1-d Frustrated system



t is nearest neighbor hop and t’ second nbr hopping amplitude

Frustration= sign of products of hopping around shortest closed loop. (Just as in spin glasses, but with t’s)

$$|\sigma_1, ..\sigma_N\rangle = c^\dagger_{1,\sigma_1} c^\dagger_{2,\sigma_2} .. c^\dagger_{N,\sigma_N} |0\rangle$$

$$P_{i,j} = \tfrac{1}{2} + 2\vec{S}_i.\vec{S}_j$$

$$\mathcal{T} = P_{1,2} P_{2,3} ... P_{N-1,N}$$ ⟵ Right shift

$$H_k^{t,t'} = te^{-ik}\mathcal{T} + t'e^{-2ik}P_{1,2}(\mathcal{T})^2 + hc,$$

- The full spectrum is obtained by varying k.
- The hole has been eliminated, and we arrive at an impurity bond model residing on the deleted L-1 site lattice.
- The first term bodily translates all spin configurations, hence all spin states remain degenerate.
- The second term discriminates between the configurations through the single exchange term P.

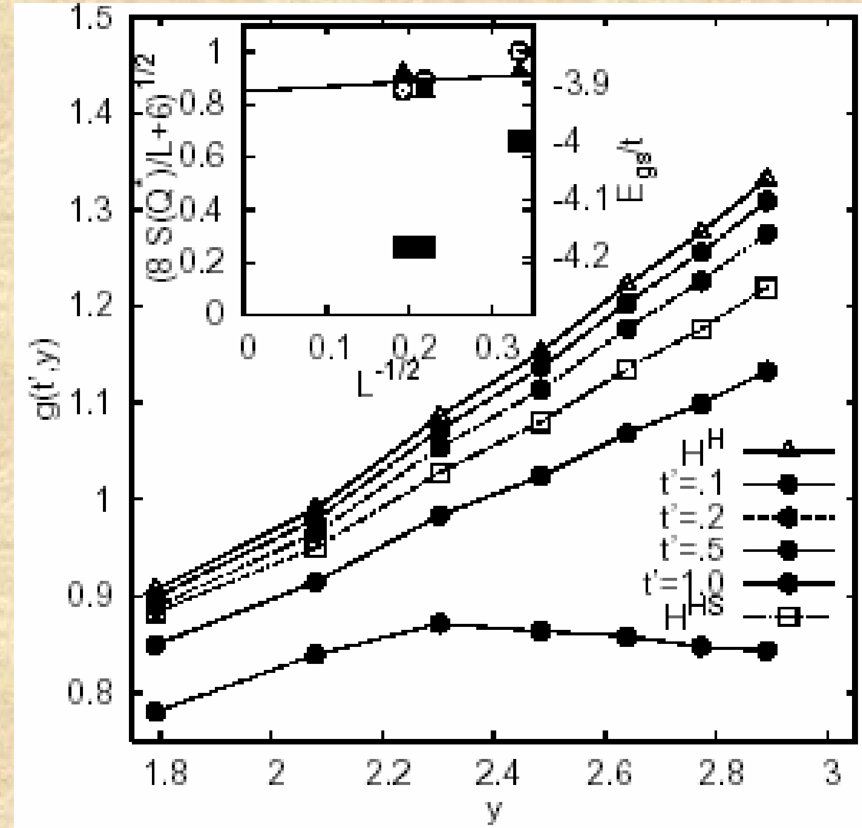
GS found for L up to 27. Spin spin correlations are antiferromagnetic, and seem to be powerlaw: This is familiar from antiferromagnetic Heisenberg model- Bethe solution. Power law usually of the form

$$\mathrm{C(r)} = (-1)^r\left\{\frac{A}{|r|} + \frac{B(\log|r|)^{\frac{1}{2}}}{|r|}\right\} + O(1/r^2)$$

Familiar model for spin systems has two terms:

J2/J1 controls B/A

$$H_h = J_1 \sum_n \vec{S}_n.\vec{S}_{n+1} + J_2 \sum_n \vec{S}_n.\vec{S}_{n+2}$$



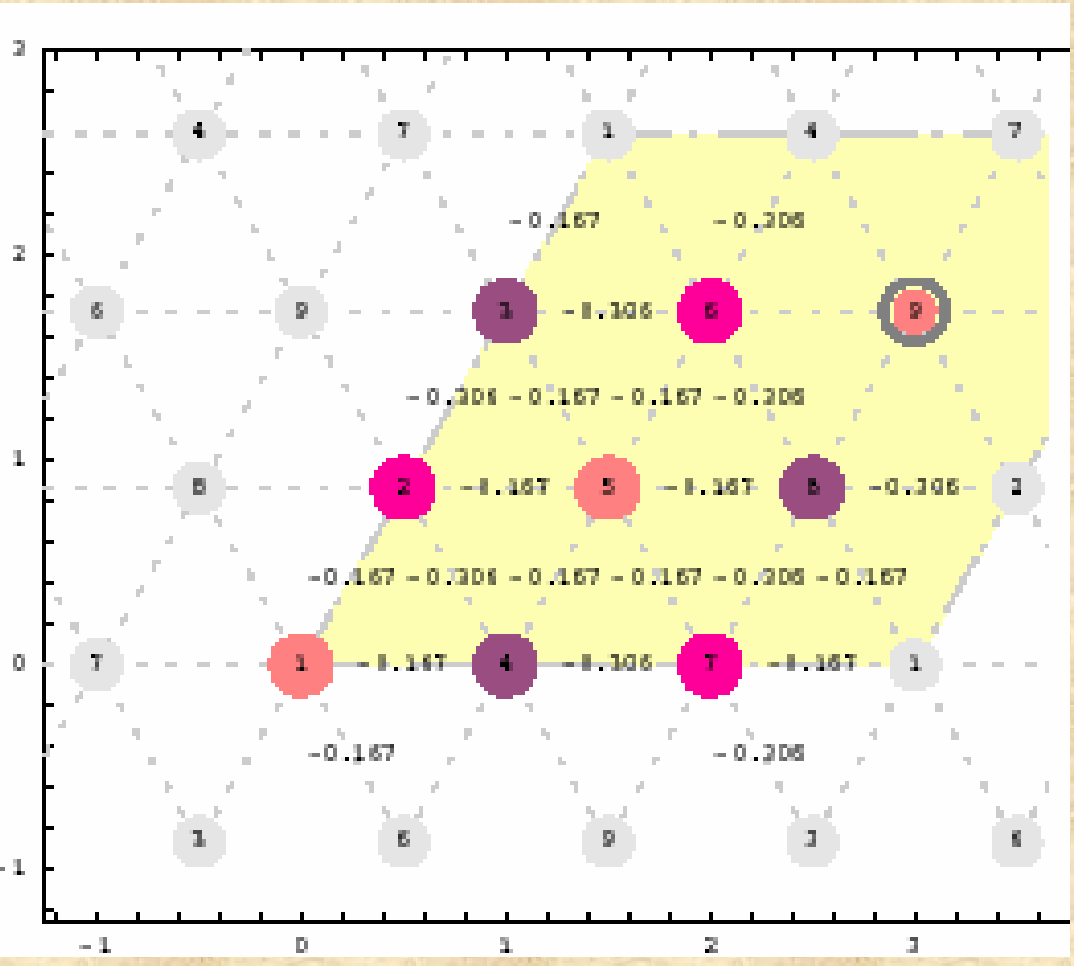
$$g(y,t') = \sum_{r=1}^{N}(-1)^r C(r)$$

Y= Log(r)

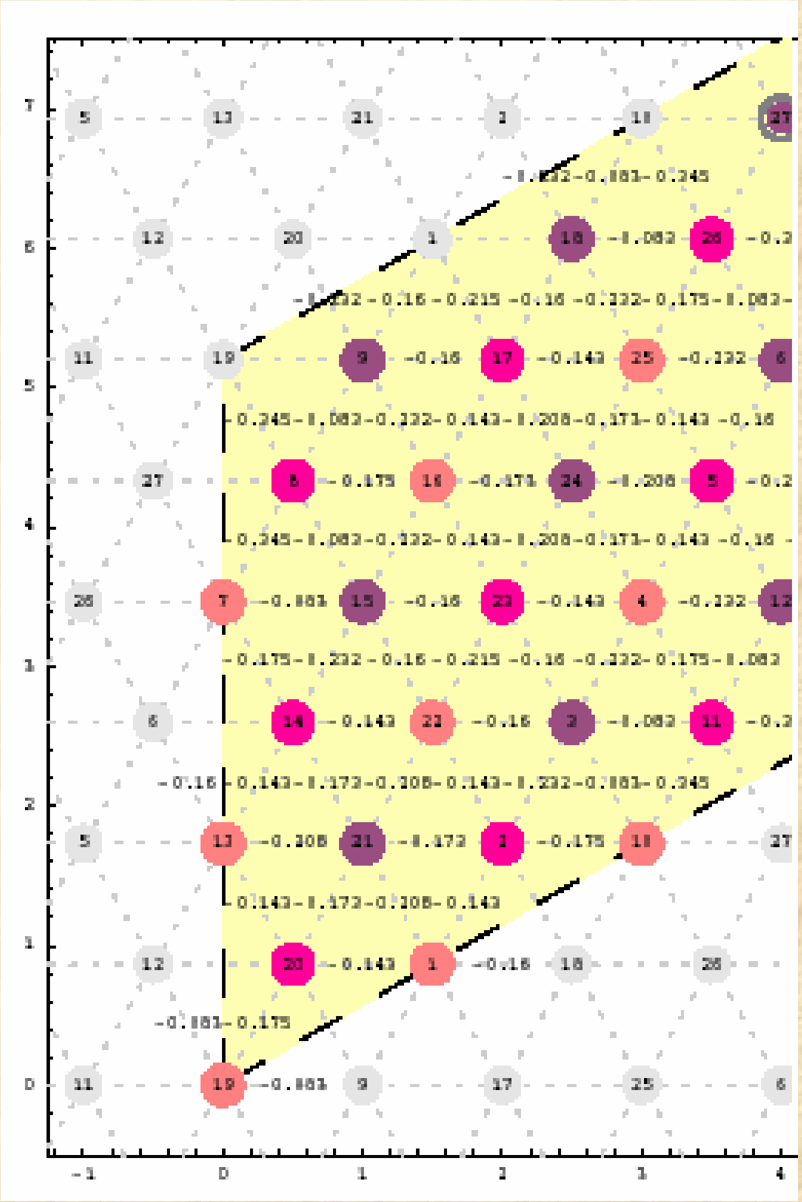
Linear plot implies B =0
and B>0 gives y^1.5

t'->0 tends exactly to Heisenberg
Bethe chain: J2=0!!

Triangular lattice:



- 9 site cluster PBC’s
- Supports 3 sl structure
- Same gs as for Heisenberg model!
- Hole at site 9

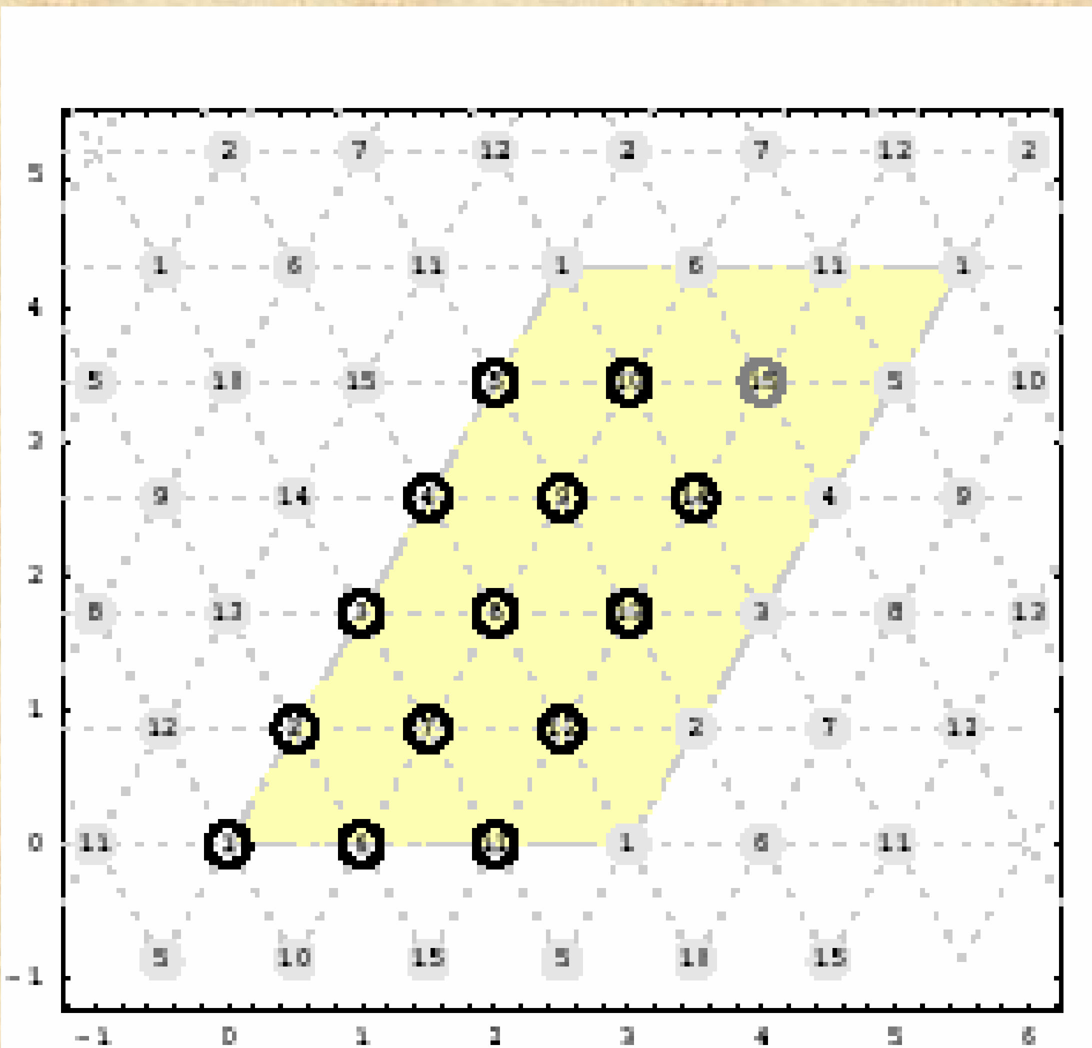


27 site cluster (26 particles)

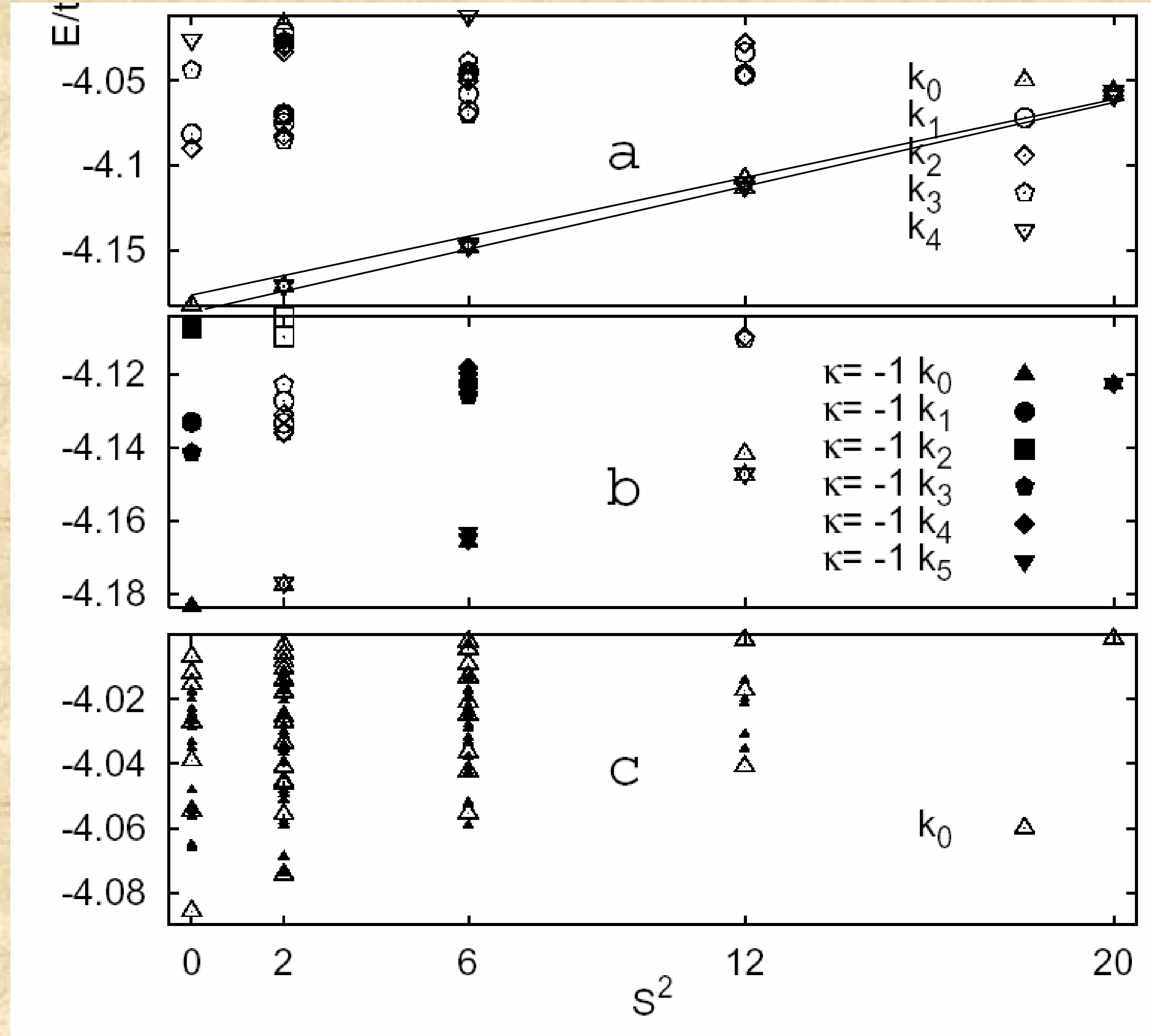
Singlet gs

Strongly 3 sublattice order

Charge soliton picture



Bad cluster: what not to do! It frustrates 3 sl structure and end up having higher gs energy than good clusters



21 sites

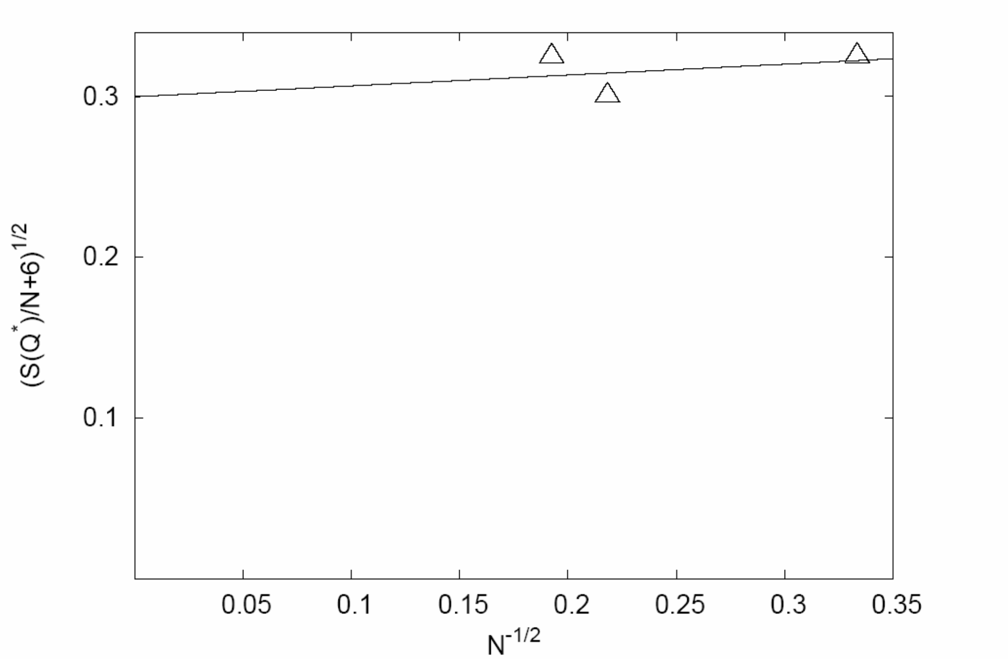
27 sites

21 site bad cluster

$E(S)-E(0) = c\ S(S+1)/L^2$

Finite moment of inertia consistent with LRO

Further, the spin structure function S(Q) shows identical behaviour to that of the Heisenberg antiferromagnet (same numbers!!).



•We find afm on a scale of J=1/N, ie. AFM per hole

Hence for thermodynamic hole density expect Jeff ~ + x |t|

•Slightly incommensurate, hence expect to be strong coupling analog of SDW order.

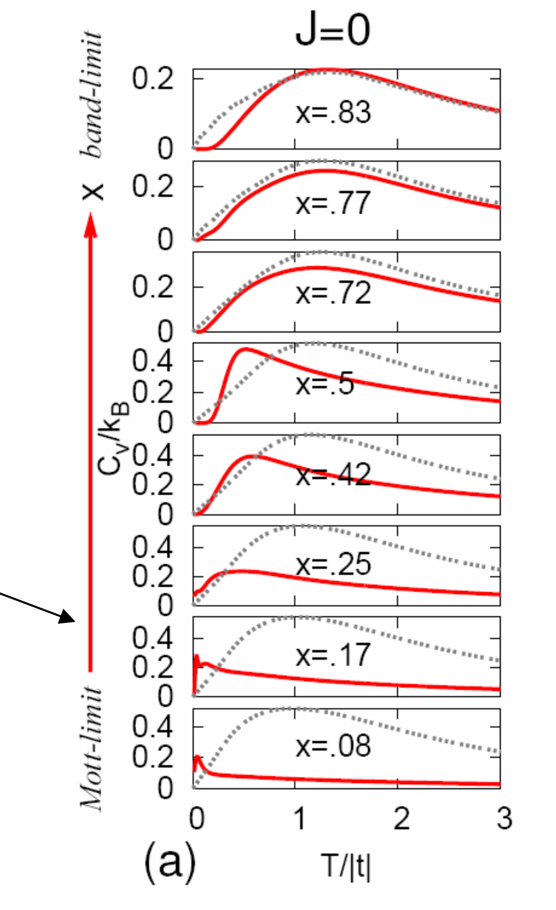
What next? Smoking gun for KAFM?

• T-J model numerics
Multi hole solutions

Strong Correlations Produce the Curie-Weiss Phase of *NaxCoO2*
Jan O. Haerter, Michael R. Peterson, and B. Sriram Shastry
Phys. Rev. Lett. **97**, 226402 (2006) and
Phys Rev B (2006)

Hint of KAFM

Bump in Cv



$$\Theta(x, J) = -cJ_{eff}(x)$$

Curie constant

$$J_{eff}(x) = J(1 + cx|t|) + cx|t| \quad \rightarrow cx|t|$$

Materials…Can we find things that are kinetic afm's?
1. NCO is possibly already a good example for x~.68
2. FCC antiferromagnetic metals in 3-d are good targets for kinetic AFM.
{ Zach Fisk suggested the name "weak antiferromagnetism"}