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Workshop on Synergies between Field Theory and Exact Computational Methods in Strongly Correlated Quantum Matter

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Linked Cluster Series - Expansion Methods

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LINKED CLUSTER SERIES-EXPANSION METHODS

R. R. P. Singh (UC Davis)

OUTLINE

- Introduction and Examples
- Basic Formalism (Linked-Cluster Methods)
- Selected Results (Heisenberg and other models)

  Thermodynamics

  Ground State Properties

  Excitation Spectra

  Square/ Triangular/ Honeycomb/ **Kagome Lattices**
- Entanglement Entropies
- Summary and Conclusions

LINKED CLUSTER SERIES EXPANSION METHODS

A class of methods where you compute properties of a Lattice Statistical Model in the thermodynamic limit by summing over contributions from all (real space) Linked clusters of varying sizes.

Domb and Green Vol 3

Gelfand, Singh, Huse J. Stat. Phys 1990

Gelfand, Singh Adv. Physics 2000

Oitmaa, Hamer and Zheng –Recent Book

High Temperature Expansions:

$$\exp -\beta H = 1 - \beta H + \frac{(-\beta)^2}{2!} H^2 + \ldots$$

An extensive (intensive) property P:

F, C_v, $\chi(q)$, $\ldots$

$C(R) = \Sigma_r < S(r)S(r+R) >$

Can be expanded as a power series in β

$$P/N = \ a_0 + \ a_1\beta + \ a_2\beta^2 + \ \ldots$$

Lattice Statistical Model (with Short Range Couplings):

Coefficients can be calculated by:

Linked-Cluster Methods

How far down in temperature will the expansion work?

In principle: Until there is a Phase Transition

Heisenberg-Ising Models:

$$H = J_z \Sigma S_i^z S_j^z + J_\perp \Sigma (S_i^x S_j^x + S_i^y S_j^y)$$

$$H = J_z (H_0 + \lambda H_1)$$

$\lambda = 0$ is (Classical) Ising Model

$\lambda = 1$ is (Quantum) Heisenberg Model

Ground state properties can be expanded in powers of λ

$$E_0/N = \ a_0 + \ a_1 \lambda + \ a_2 \lambda^2 + \ \ldots$$

Coefficients can be calculated by:

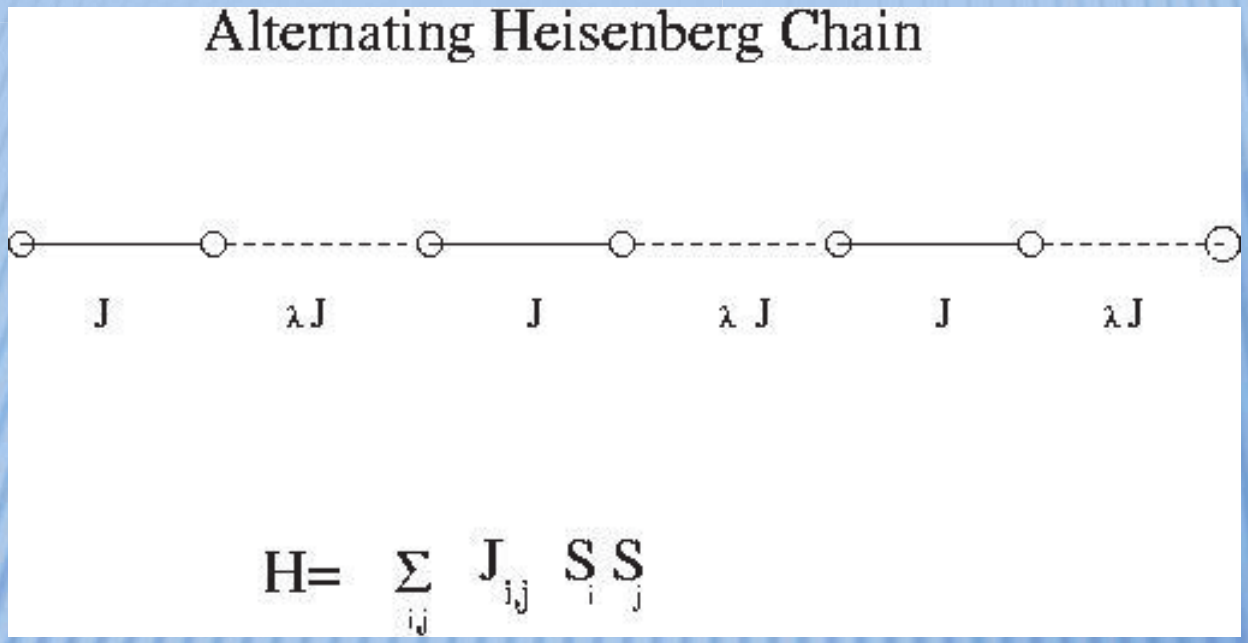
Linked-Cluster Methods

Will this expansion converge in the Heisenberg Limit?

It does so for $d = 1$ (Exact solution)

In principle: As long as ordered moment is non-zero

DIMER EXPANSIONS



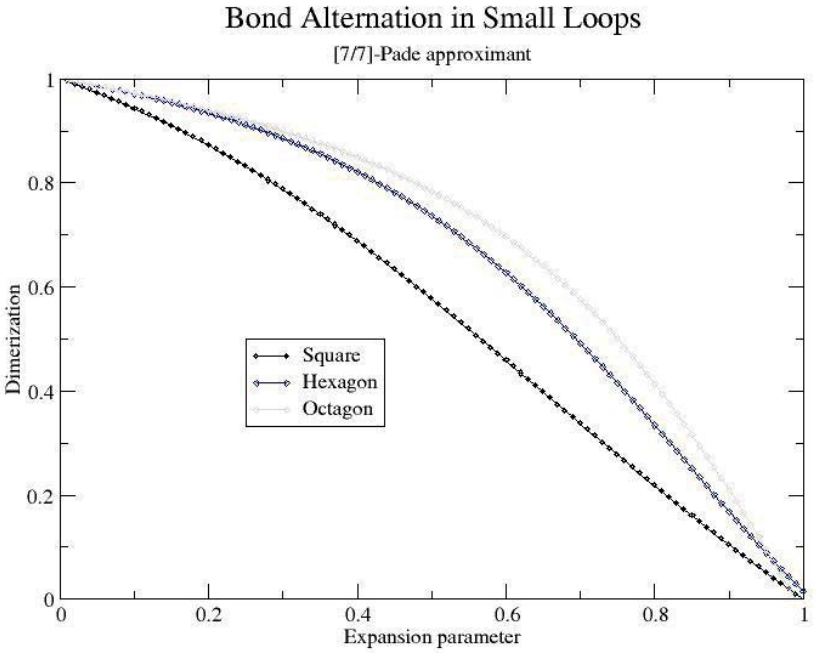
Lambda=0: Disconnected Dimers (Singlets)

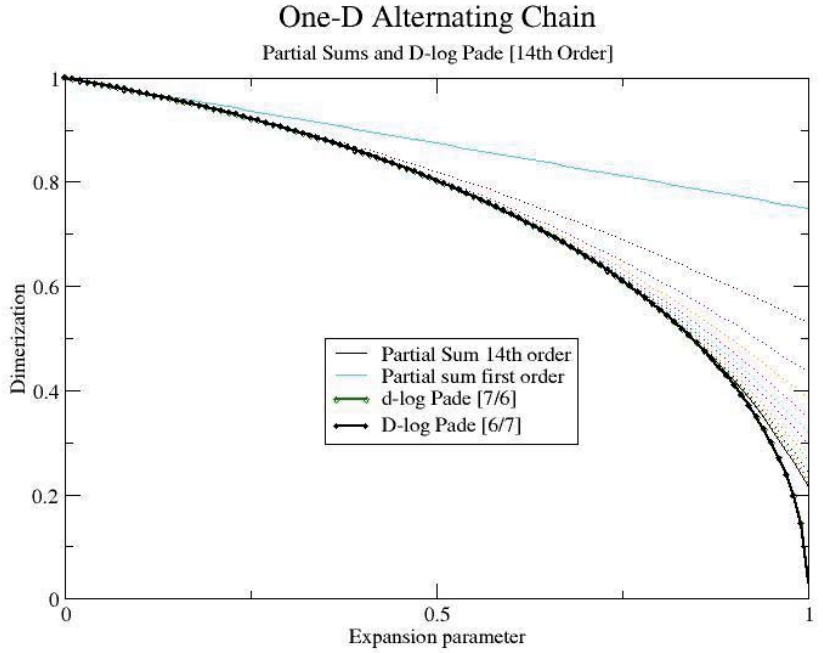
Lambda=1: Uniform Heisenberg Model

Expansion Converges until gap vanishes

Up to Lambda=1

DIMER SERIES EXPANSIONS





For small clusters series results indistinguishable from exact results:

Linear Chain is critical – requires d-log Pade extrapolation

Other models: may need to create expansion parameter:

Hubbard Model at half-filling

$$H = H_U + J_z(1-\lambda)\Sigma S_i^z S_j^z + \lambda H_t$$

$$H = (H_0 + \lambda H_1)$$

: $\lambda = 0$ is On-site term plus Ising anisotropy

: $\lambda = 1$ is Hubbard Model with rotational symmetry

Triangular Lattice Heisenberg Model

: Rotate Basis so Classical Ordered State is Ferromagnetic

: Introduce Ising anisotropy λ

λ interpolates between gapped Ising-like models and gapless models with Heisenberg symmetry

Need Series Extrapolation for gapless excitations

Basic Formalism of Linked Cluster Expansions

Consider a multi-variable expansion:

$$\begin{aligned} P &= A_0 + (a_1 J_1 + a_2 J_1^2 + \ldots) \\ &+ (a_{11} J_1 J_2 + a_{21} J_1^2 J_2 + a_{12} J_1 J_2^2 + \ldots) \\ &+ (a_{111} J_1 J_2 J_3 + \ldots) \end{aligned} \tag{1}$$

And, view it as

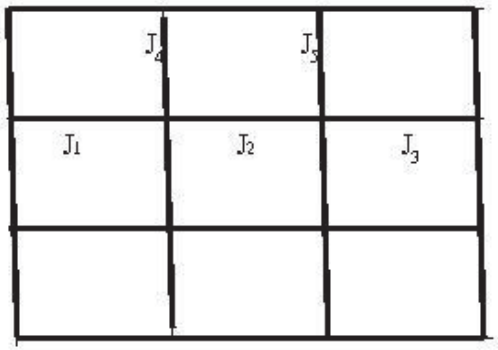
$$W(.) + W(J_1) + W(J_1, J_2) + W(J_1, J_2, J_3)$$

A natural graphical correspondence

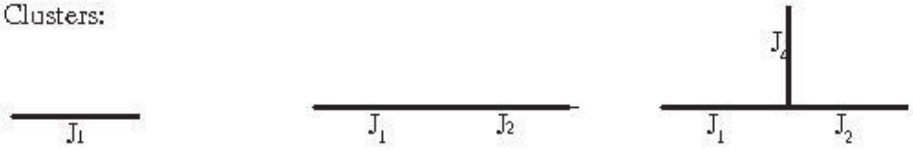
When do only 'Linked Clusters' contribute?

If a cluster C is made up of $A \cup B$
where, $[H_A, H_B] = 0$
Then $P_C = P_A + P_B$,
And the cluster does not contribute: $W(C) = 0$

Lattice



Clusters:



To obtain Weight for a cluster, set all Js not in the cluster to zero. Define the property for this case as $P(c)$. Then,

$$P(c) = \sum_{s \subseteq c} W(s)$$

Hence,

$$W(c) = P(c) - \sum_{s \subset c} W(s)$$

Obtain W(c) recursively

Thus, for a Lattice L (using symmetries)

$$P(L) = N \sum_{g} L(g) \times W(g)$$

L(g): Lattice Constant of graph g: Count per site

W(g): Weight of graph g (Finite cluster property)

Finite Cluster: Like any ED study
H: finite dimensional matrix
Recursion Relations in finite-dimensional Hilbert space

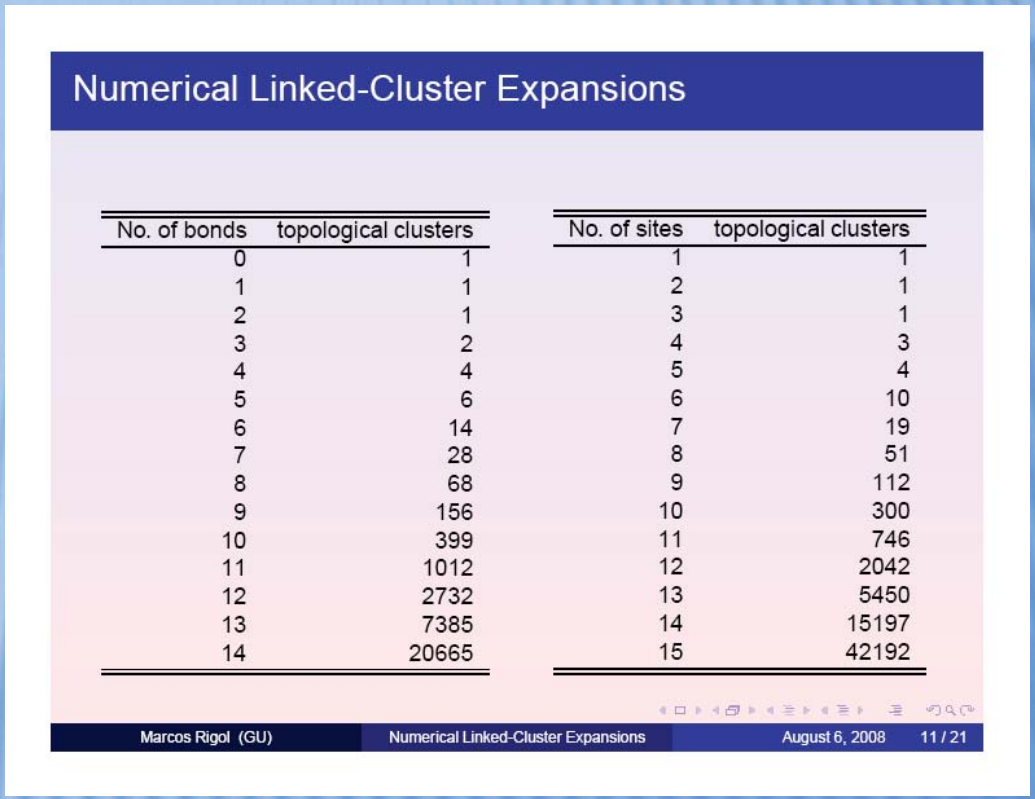
CLUSTERS AND LATTICE CONSTANTS

- Same as Ising Models

Domb and Green Vol 3

Group together all graphs with same connectivity (Hamiltonian)

Weak and Strong Embeddings



Numerical Linked-Cluster Expansions

No. of bonds	topological clusters
0	1
1	1
2	1
3	2
4	4
5	6
6	14
7	28
8	68
9	156
10	399
11	1012
12	2732
13	7385
14	20665

No. of sites	topological clusters
1	1
2	1
3	1
4	3
5	4
6	10
7	19
8	51
9	112
10	300
11	746
12	2042
13	5450
14	15197
15	42192

NUMERICAL LINKED CLUSTER METHOD RIGOL, BRYANT, SINGH

- No small parameter
- Weights can be defined numerically at any set of parameters (T etc.)
- Which embeddings should one use?
- Considerable flexibility

To obtain Weight for a cluster, set all Js not in the cluster to zero. Define the property for this case as $P(c)$. Then,

$$P(c) = \sum_{s \subseteq c} W(s)$$

Hence,

$$W(c) = P(c) - \sum_{s \subset c} W(s)$$

Obtain W(c) recursively

Thus, for a Lattice L (using symmetries)

$$P(L) = N \sum_{g} L(g) \times W(g)$$

L(g): Lattice Constant of graph g: Count per site

W(g): Weight of graph g (Finite cluster property)

1

WEAK/STRONG EMBEDDINGS

Numerical Linked Cluster Expansions

i) Find all clusters that can be embedded on the lattice

Bond clusters

	c	$L(c)$
	1	1
	2	2
	3	2
	4	4
	5	4
	6	2
	7	4
	8	4
	9	8

Numerical Linked-Cluster Expansions

Site clusters

	c	$L(c)$
	1	1
	2	2
	3	2
	4	4
	5	4
	6	2
	7	1
	8	4
	9	8

No. of sites	topological clusters
1	1
2	1
3	1
4	3
5	4
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14	15197
15	42192

Numerical Linked-Cluster Expansions

Square clusters

	c	$L(c)$
	1	1
	2	1/2
	3	1
	4	1
	5	2

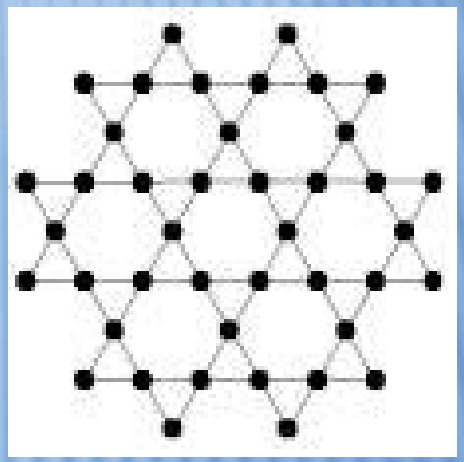
No. of squares	topological clusters
0	1
1	1
2	1
3	2
4	5
5	11

NUMERICAL LINKED CLUSTER

- What controls the convergence?
- Can it be accurate down to T=0?

Kagome Lattice Ising Model

- Exactly Soluble
- Finite entropy at T=0
- Small correlation length



A lattice of corner-sharing triangles: Triangle NLC

KAGOME-LATTICE ISING MODEL

Triangle-based expansion

Entropy at T=0 (k=1)

For one site: $S(0)= \ln(2) = W(0)$

For one triangle: $S(1)= \ln(6)$

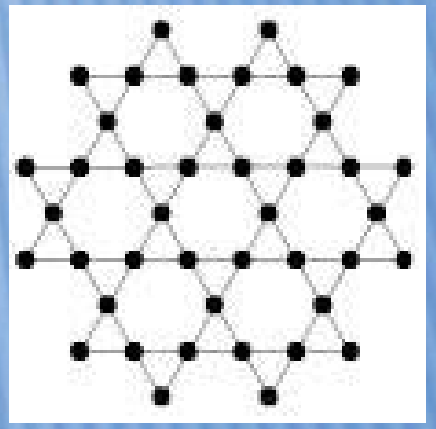
$W(1)= \ln(6)- 3\ln(2)$

Entropy per site in the thermodynamic Limit

$S/N= W(0)+(2/3)\, W(1) =0.50136$ (Pauling)

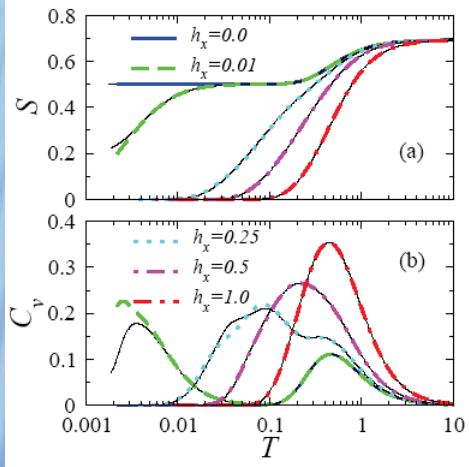
Next correction: 6-triangles 0.50182

Exact result: 0.50183…



KAGOME-LATTICE TRANSVERSE ISING

7-8
triangles



HOW TO CALCULATE SPECTRA

- Real Space Clusters
- Spectra of translationally invariant system are eigenstates of q

Gelfand:

Spectra are Fourier Transforms of effective one-particle Hamiltonian-- for Dressed one-particle states-- And can be obtained by Linked Cluster Methods

SPECTRA OF ALTERNATING CHAIN

Ground State

s s s s

One Particle States (Energy J) (Triplons)

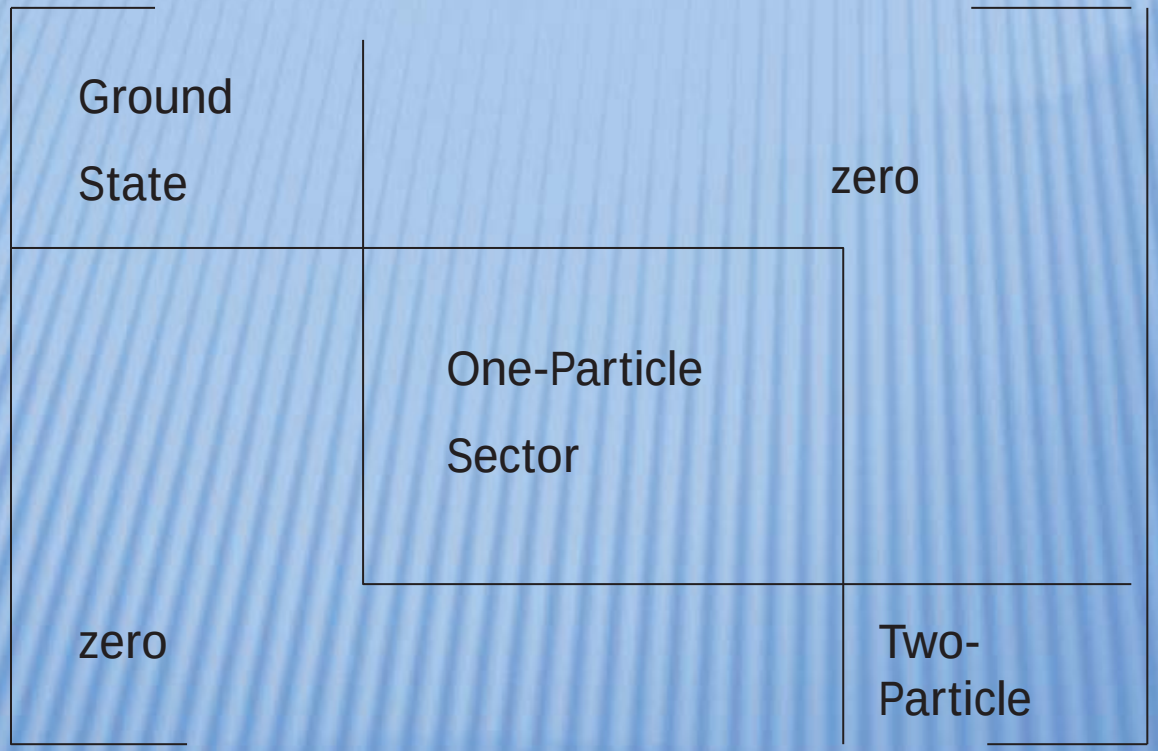
s s t s

Two Particle States (Energy 2J) (2-Triplons)

s t t s

Two triplons can combine into spin 0,1,2

SIMILARITY/ORTHOGONALITY TRANSFORMATION
FIRST BLOCK DIAGONALIZE THE HAMILTONIAN



Dressed one-particle states: The right mix of one-particle states orthogonal to other n

DIAGONALIZING THE BLOCK HAMILTONIAN

- For the infinite system with translational symmetry H_eff (i,j)=H_eff(i-j)
- One-Particle spectra obtained by Fourier Transformation

- Two particle states H_eff(i,j:k,l)
- Two-Particle States: Need to solve the Schrodinger equation in relative coordinates--numerically

SERIES EXTRAPOLATION

Let, $f(x) = a0 + a1\,x + a2\,x^2 + a3\,x^3 + \ldots$

Going beyond partial sums (analytic continuation):

- Pade Approximants $f(x) = \frac{P(x)}{Q(x)}$,

$P(x)$and $Q(x)$polynomials in x.

- D-log Pade Approximants $\frac{df(x)/dx}{f(x)} = \frac{P(x)}{Q(x)}$

Polynomials can be determined to give same expansion to desired order. Extrapolations allow one to build various singularities.

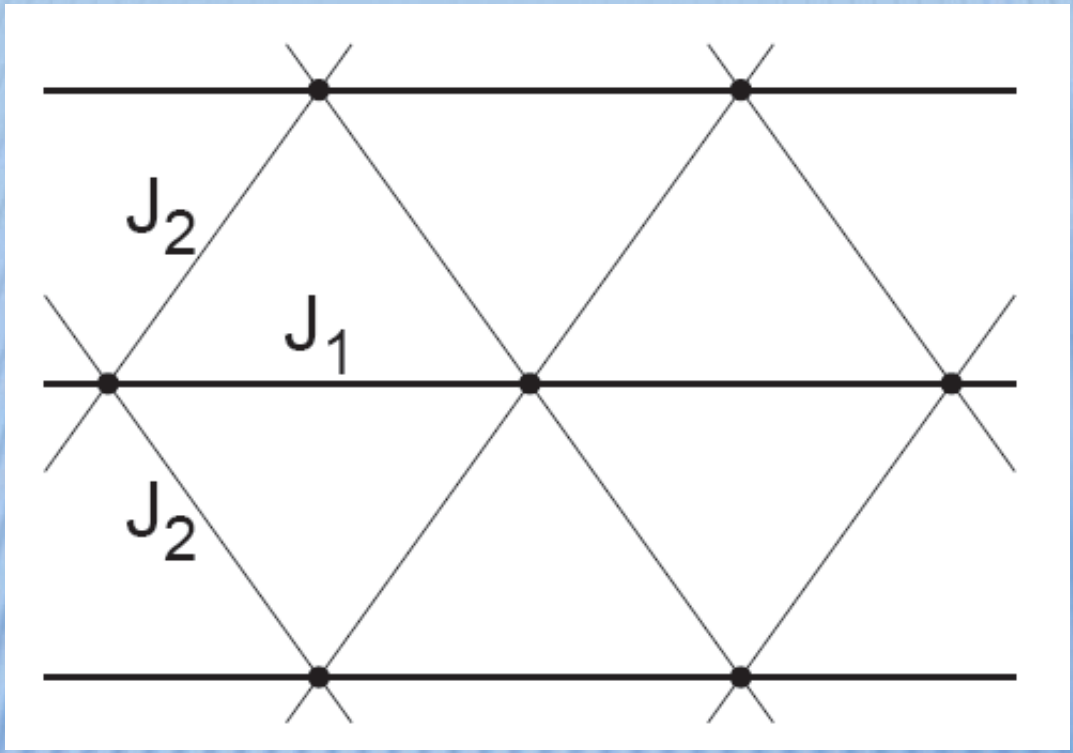
- Change of Variables (Euler, tanh, Huse, ...)

SELECTED RESULTS

- Susceptibility of Anisotropic Triangular Lattice
- Finite-T comparison of Square and Triangular Lattices
- Spectra of Square Lattice HM
- Spectra of Triangular Lattice HM
- Search for VBC Order for KLHM

ENTANGLEMENT ENTROPIES

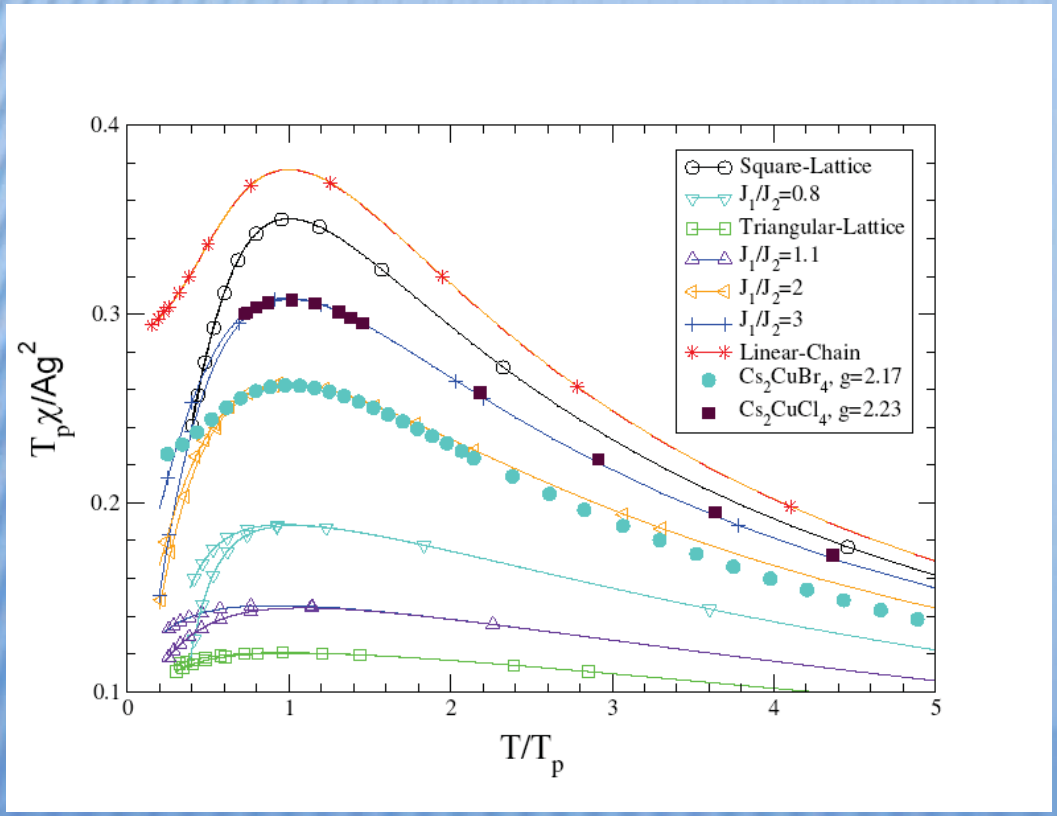
S = ½ Heisenberg antiferromagnet on an anisotropic triangular lattice

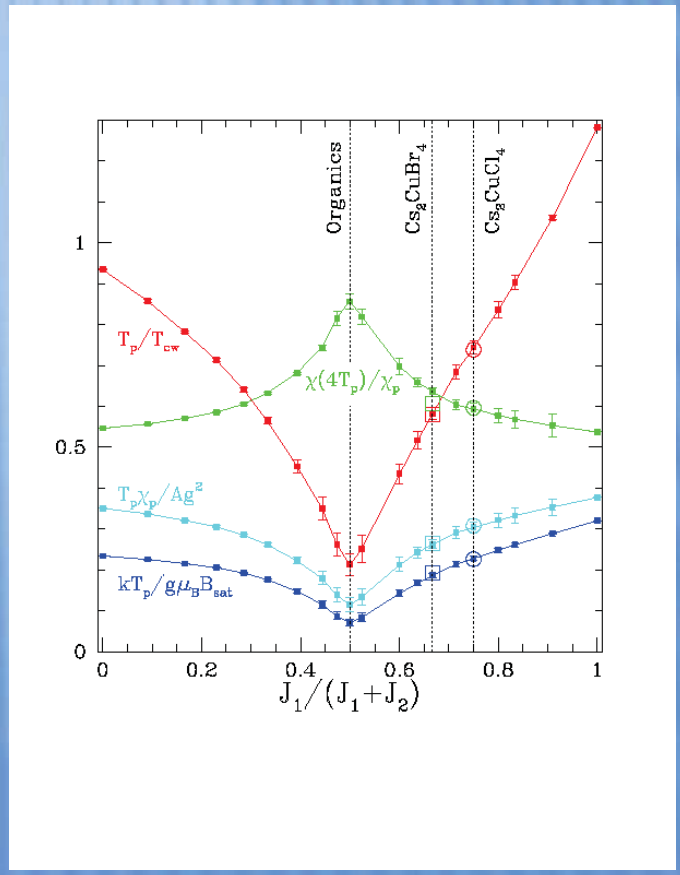


Special cases:
- $J_1/J_2 = 0$: Square lattice model
- $J_1/J_2 = 1$: Triangular lattice model
- $J_1/J_2 = 2$: Cs_2CuBr_4
- $J_1/J_2 = 3$: Cs_2CuCl_4
- $J_1/J_2 = \infty$: Decoupled chains

THERMODYNAMICS

Susceptibility of Anisotropic Triangular Lattice

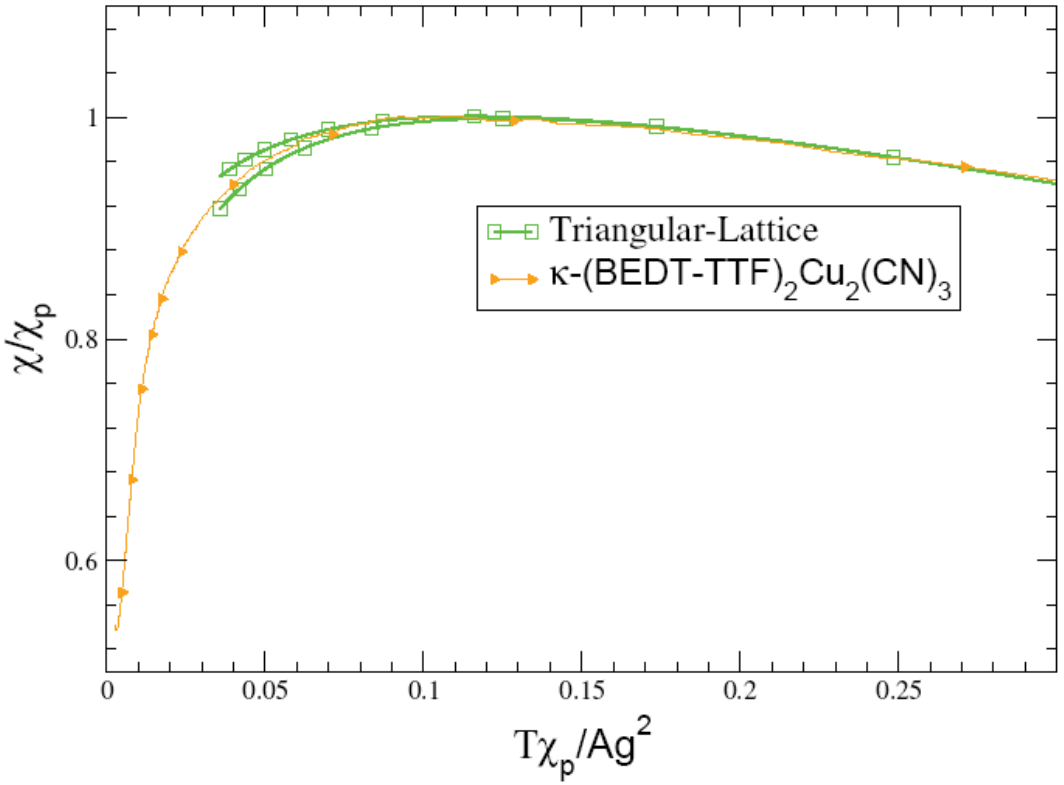




Weihong, RRPS, McKenzie, Coldea

ISOTROPIC MATERIAL

Spin-Liquid Candidate



SQUARE VS TRIANGULAR LATTICE HM

Elstner, RRPS, Young PRL, JAP

Entropy
AFM Structure Factor
AFM Correlation Length

Renormalized Classical Behavior
Chakravarty, Halperin, Nelson
Azaria et al

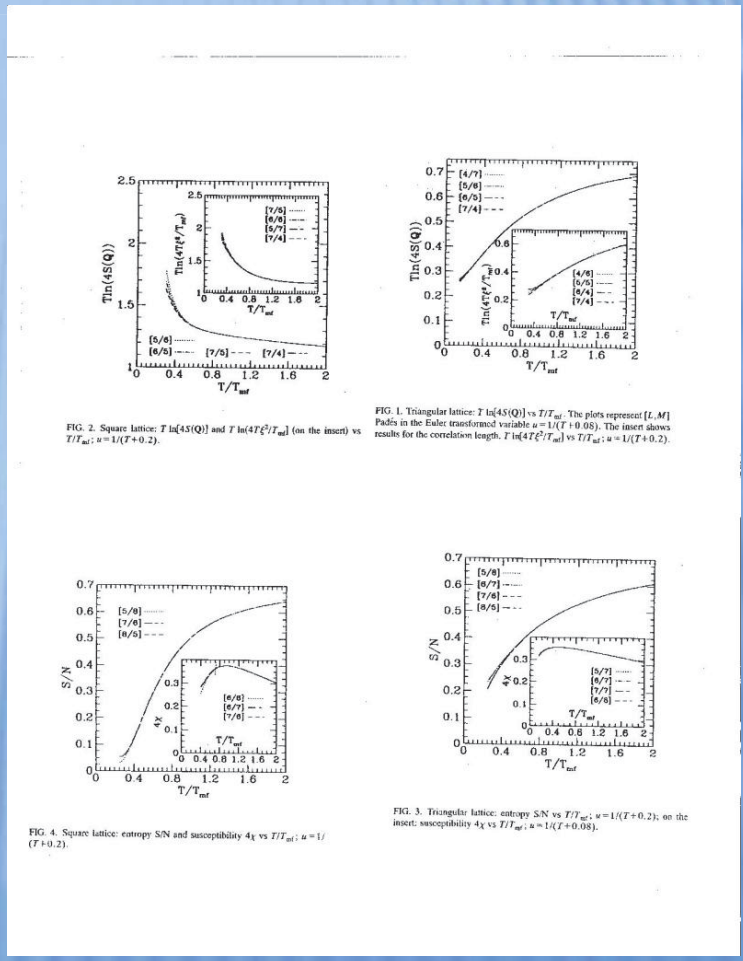


FIG. 2. Square lattice: $T \ln[4S(Q)]$ and $T \ln(4T\xi^2/T_{mf})$ (on the insert) vs T/T_{mf}; $u = 1/(T+0.2)$.

FIG. 1. Triangular lattice: $T \ln[4S(Q)]$ vs T/T_{mf}. The plots represent $[L,M]$ Padés in the Euler transformed variable $u = 1/(T+0.08)$. The insert shows results for the correlation length. $T \ln(4T\xi^2/T_{mf})$ vs T/T_{mf}; $u = 1/(T+0.2)$.

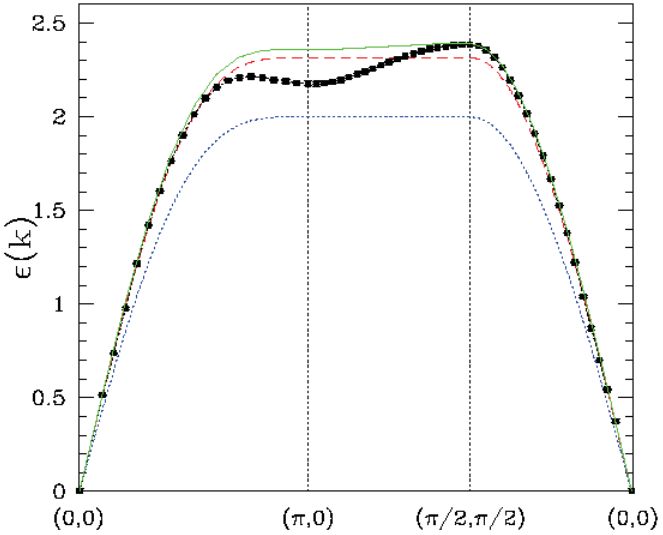
FIG. 4. Square lattice: entropy S/N and susceptibility 4χ vs T/T_{mf}; $u = 1/(T+0.2)$.

FIG. 3. Triangular lattice: entropy S/N vs T/T_{mf}; $u = 1/(T+0.2)$; on the insert: susceptibility 4χ vs T/T_{mf}; $u = 1/(T+0.08)$.

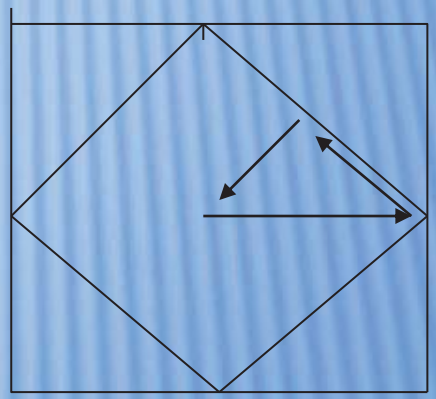
SELECTED SPECTRAL RESULTS

- Spectra for Square-Lattice AFM
- Spectra for Triangular Antiferromagnet

MAGNON SPECTRA IN 2D (DIP AT (PI,0)) RENORMALIZED UPWARDS



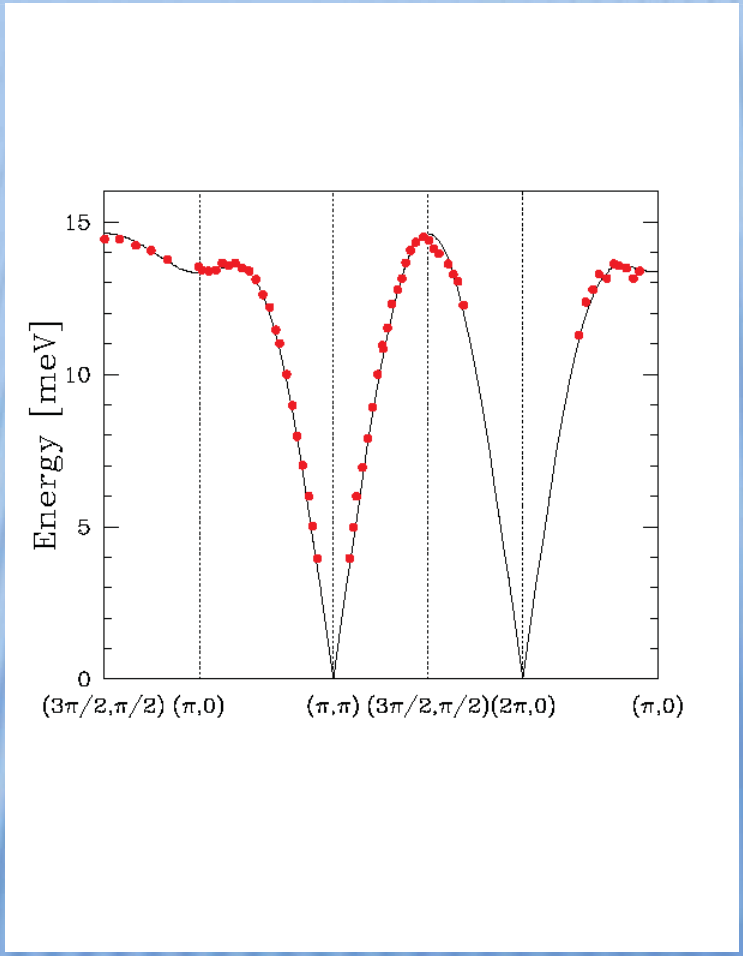
Antiferromagnetic
Brillouin Zone



Sandvik+RRPS (QMC)

Zheng, Oitmaa and Hamer PRB 71, 184440 (2005)

COMPARES WELL WITH SPECTRA IN CFTD

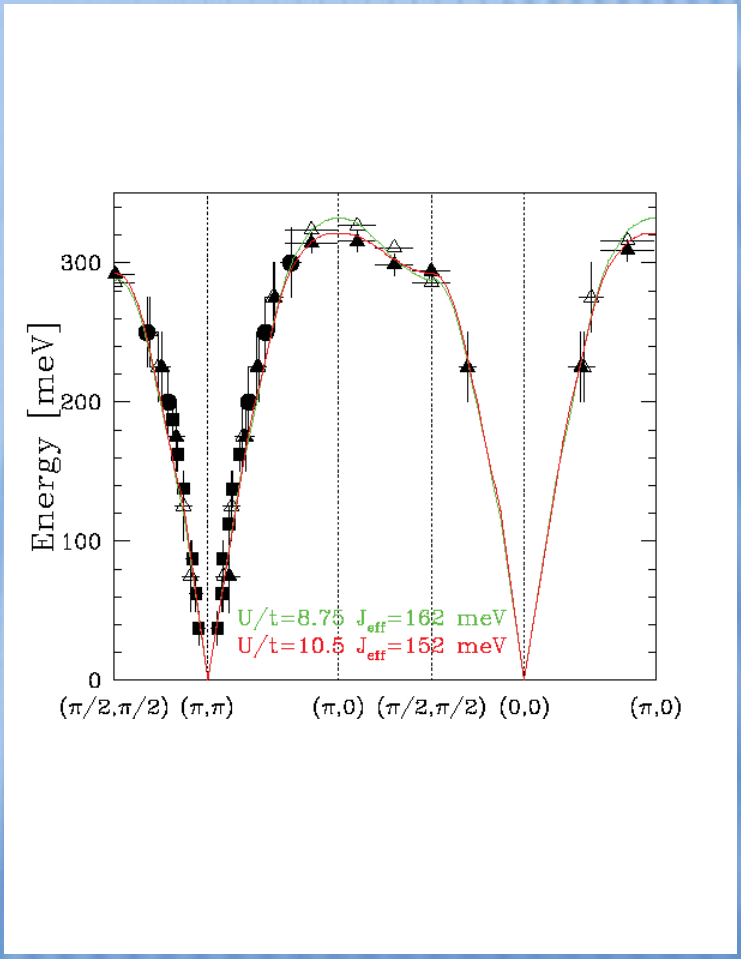


Ronnow et al PRL 87, 037202 (2001)

NOT WITH SPECTRA FOR LA2CUO4

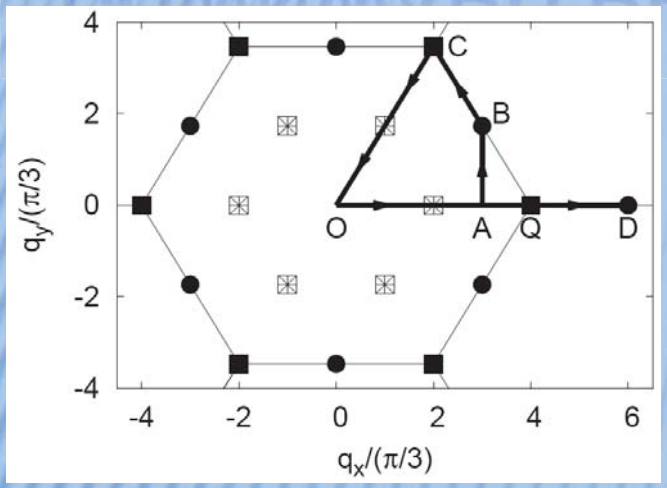
Zone boundary dispersion is opposite: Second neighbor J will make it worse

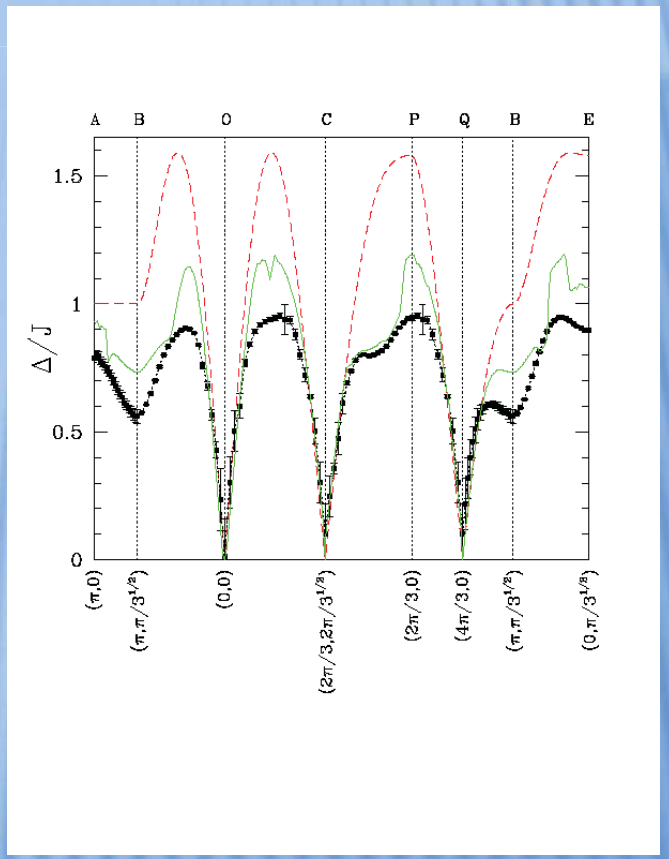
Finite-U changes zone boundary dispersion

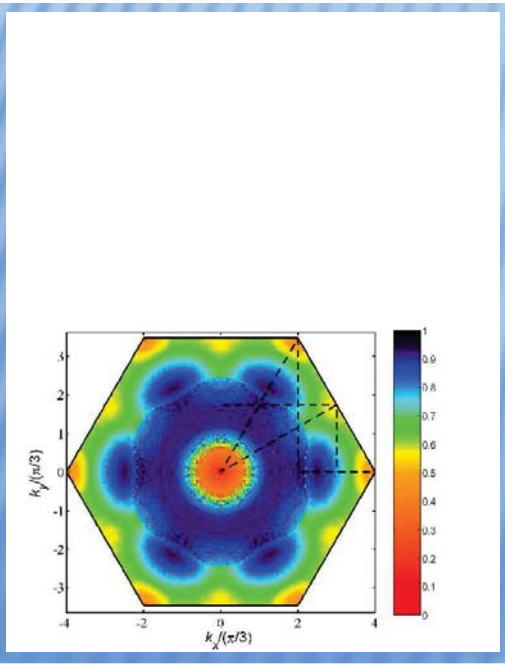


Coldea et al PRL 86, 5377 (2001)

TRIANGULAR-LATTICE SPECTRA DOWNWARD RENORMALIZATION







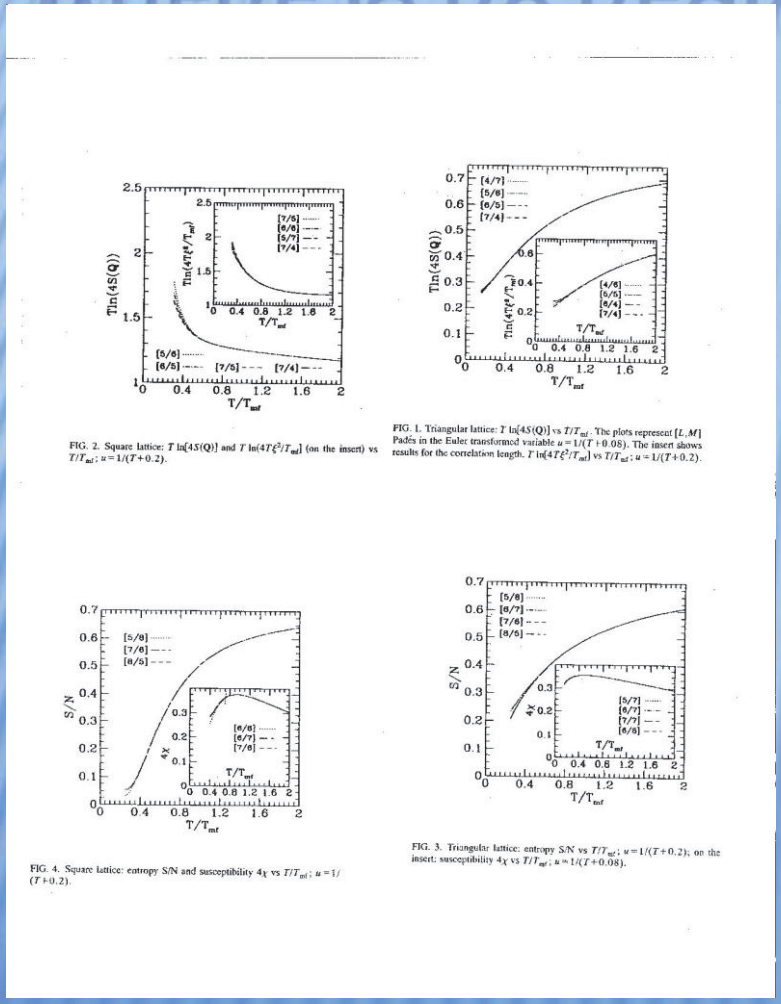
SWT, (1/S), Series

Zheng et al

Starykh,Chubukov

Chernyshev, Zhitomirsky (magnon-decay)

THERMODYNAMICS OF SQUARE AND TRIANGULAR LATTICES: WHERE IS RC REGION?



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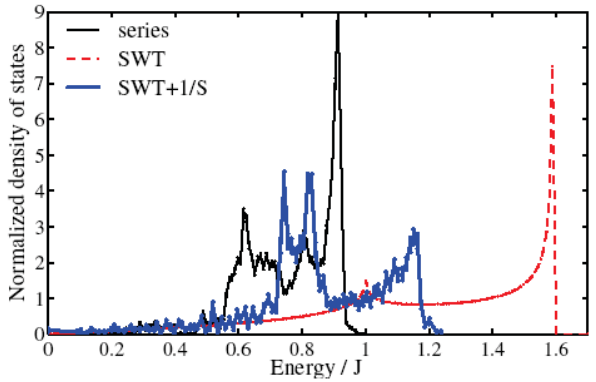


Elstner, RRPS, Young

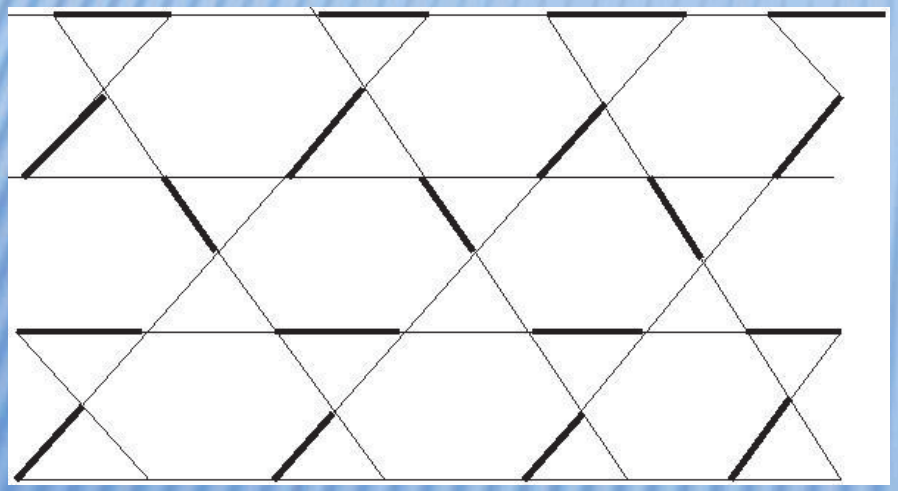
Density of States

KAGOME LATTICE HEISENBERG MODEL

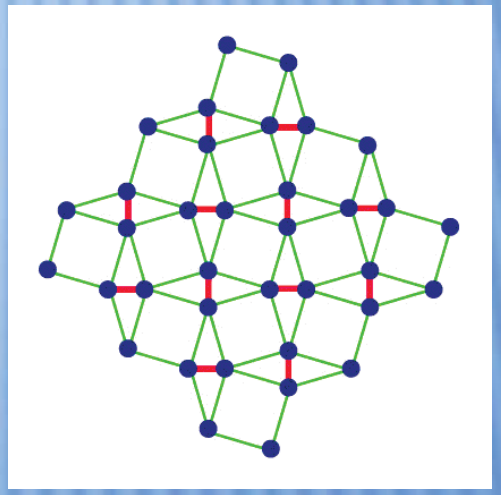
WHAT IS THE DOMINANT VBC PATTERN?

EMPTY TRIANGLES ARE KEY

THE REST ARE IN LOCAL GROUND STATE



Kagome Lattice

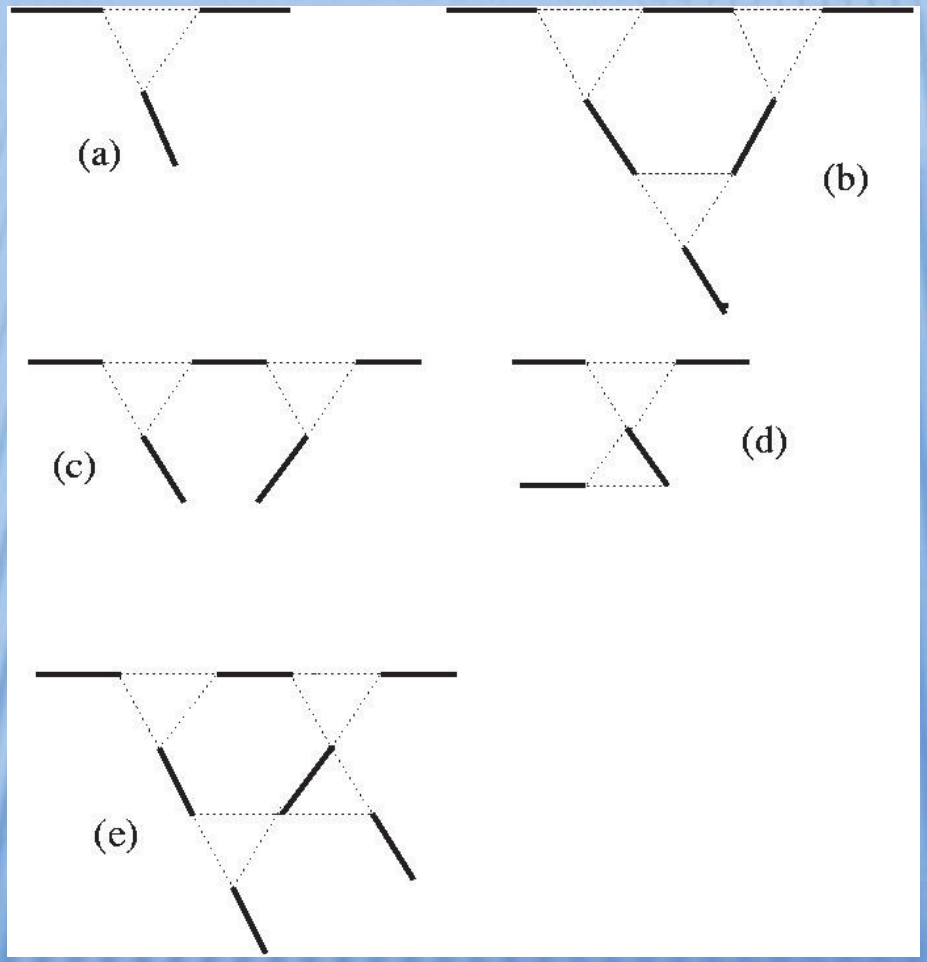


Shastry-Sutherland Lattice

SERIES EXPANSION AROUND ARBITRARY DIMER CONFIGURATION (RRPS+HUSE)

Graphs defined by triangles

All graphs to 5^{th} order



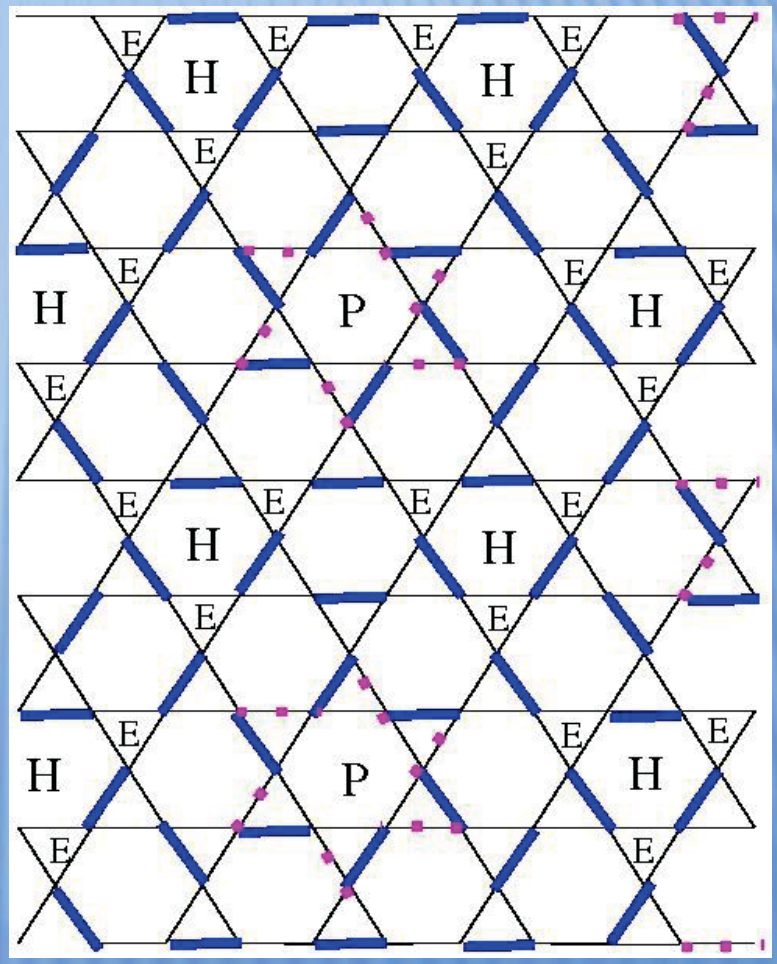
DEGENERACY LIFTS IN 3RD/4TH ORDER BUT NOT COMPLETELY

3rd Order: Bind 3Es into H—maximize H

4th Order: Honeycomb Lattice

Leftover: Pinwheels

24*2^(N/36) Low energy states



SERIES SHOW EXCELLENT CONVERGENCE

Order	Honeycomb	Stripe VBC	36-site PBC
0	-0.375	-0.375	-0.375
1	-0.375	-0.375	-0.375
2	-0.421875	-0.421875	-0.421875
3	-0.42578125	-0.42578125	-0.42578125
4	-0.431559245	-0.43101671	-0.43400065
5	-0.432088216	-0.43153212	-0.43624539

Ground State Energy per site

Estimated H-VBC energy: -0.433(1) (ED, DMRG)

36-site PBC: Energy=-0.43837653

Recent DMRG by Yan et al: RVB: E =-0.437

SPIN GAP

- Lowest triplet at q=0 (reduced zone)

  Gap Series:

  1 –0.5 –0.875 +0.440625+0.07447-0.04347-0.02336

  Estimated Gap =0.08 (.02) (agrees with ED/DMRG)

- Lowest triplet for 36-site PBC

  Gap Series:

  1 –0.5 –0.875 +0.440625+0.486458-0.16984-…

  Estimated Gap =0.2 (cf 0.164 exact answer ED)

Entanglement Entropies:

Divide a Lattice into two mutually exclusive set of sites $AB = A \cup B$, with Hamiltonian

$$\hat{H} = \hat{H}_A + \hat{H}_B + \hat{H}_{AB}$$

The Density Matrix is Defined as

$$\hat{\rho} = \exp(-\beta \hat{H})/Z(\beta),$$

with

$$Z(\beta) = Tr_{A,B} \ \exp(-\beta \hat{H}).$$

The reduced density matrices are partial traces

$$\hat{\rho}_A = Tr_B \ \hat{\rho}, \qquad \hat{\rho}_B = Tr_A \ \hat{\rho}.$$

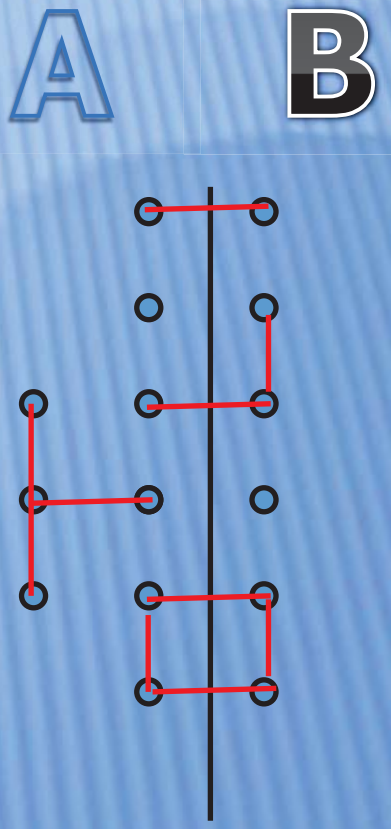
Von Neumann entropies are ($\alpha = A,\ B$, or AB):

$$S_\alpha = -Tr\alpha \ \hat{\rho}_\alpha \ \ln \hat{\rho}_\alpha$$

Renyi entropies of index n are

$$S_\alpha^n = \frac{1}{1-n} \ln Tr \hat{\rho}_\alpha^n$$

Von Neumann entropy follows from $n \to 1$ limit.



Work done with A. Kalin, M. Hastings and R. Melko

These entropies have Linked Cluster Expansions, will be extensive (depend on Volume).

Define Mutual Information as

$$M_{AB} = S_A + S_B - S_{AB}$$

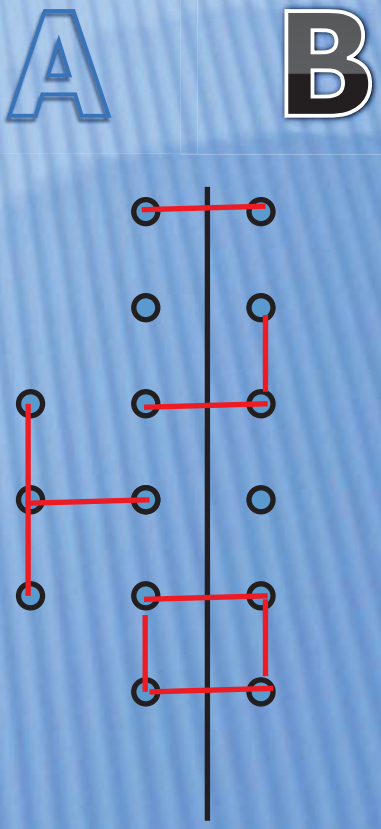
Clusters entirely in A (or B) will not contribute.

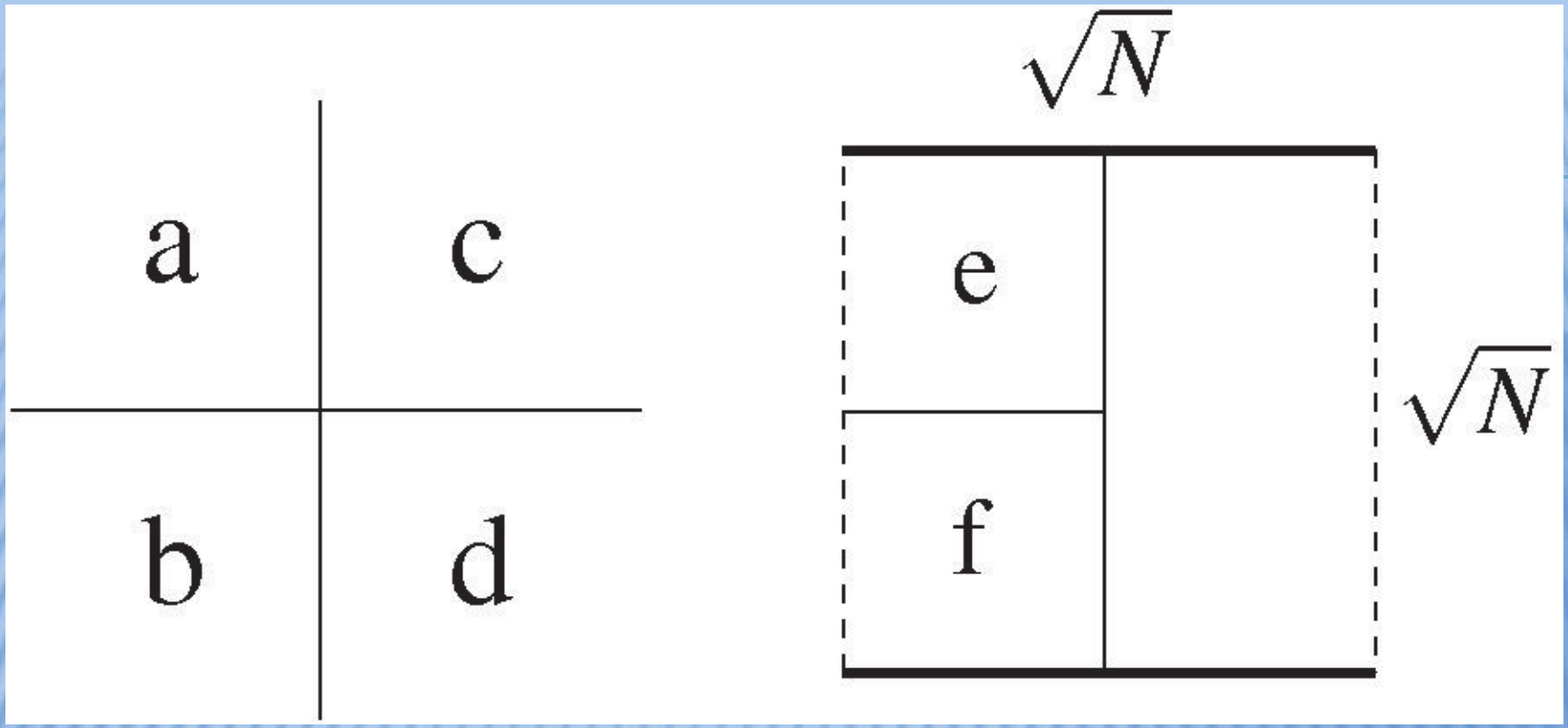
Proof:
For such a cluster, $\hat{H} = \hat{H}_A$, $\hat{\rho}_{AB} = \hat{\rho}_A \times \hat{I}$.
Hence, $S_{AB} = S_A + S_B$, $M_{AB} = 0$.

M_{AB} has an area law. To contribute a cluster must cut across the boundary. If we divide a lattice along a line, clusters related by translation along the line will have same contribution. Count will be per unit length not per site.

One can obtain series for M_{AB}/ℓ.

Corners can be separately calculated by suitable choice of regions A and B. Only clusters, whose rectangular envelop includes the corner can contribute.





(i) A=a, B=bdc
(ii) A=d, B=bac
(iii) A=ab, B=dc
(iv) A=ac, B=bd

CORNER = (M(i)+M(ii)-M(iii)-M(iv))/2

Can use real REPLICAS but is not necessary

$$M_{AB} = \frac{1}{1-n} \ln \frac{Z[A,n,\beta]Z[B,n,\beta]}{Z[n\beta]Z[\beta]^n}$$

where

$$Z[A,n,\beta] = Tr_A[Tr_B \exp(-\beta \hat{H})]^n$$

This can be evaluated by introducing replicas. Let there be n copies of B variables B_i. Then

$$Z[A,n,\beta] = Tr_A \prod_i Tr_{B_i} \exp(-\beta \hat{H}_i),$$

where

$$\hat{H}_i = \hat{H}_A + \hat{H}_{B_i} + \hat{H}_{AB_i}$$

Note that different B_i have completely independent existence, but they all couple to same A variables. It is as if the lattice consists of different sheets of B_i all joined to a single sheet of A along the boundary of AB.

Calculation can also be done without replicas, by treating the n variable analytically.

- Every Power of β brings a power of n
- Coefficient of β^m : Polynomial in n Order m
- Vanishes (before division) for n=1 and n=0
- M_AB: Polynomial of order (m-1)
- Analytic continuation to Von Neumann is easy
- β_c scales as 1/n
- Renyi-n is Singular at n T_c

XXZ MODEL, BIPARTITE LATTICE

Arbitrary n

Consider the XXZ model on a bi-partite lattice

$$\mathcal{H} = \sum_{<i,j>} (S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z)$$

Five traces are needed for full calculation to 4th order.

$$A_2 = \frac{Tr(\sigma_1 \cdot \sigma_2)^2}{Tr(1)} = 2 + \Delta^2$$

$$A_3 = \frac{Tr(\sigma_1 \cdot \sigma_2)^3}{Tr(1)} = -6\Delta$$

$$A_4 = \frac{Tr(\sigma_1 \cdot \sigma_2)^4}{Tr(1)} = (2 + \Delta^2)^2 + 4(1 + 2\Delta^2)$$

$$B_4 = \frac{Tr(\sigma_1 \cdot \sigma_2 \; \sigma_2 \cdot \sigma_3 \; \sigma_1 \cdot \sigma_2 \; \sigma_2 \cdot \sigma_3))}{Tr(1)} = \Delta^4 - 4\Delta^2$$

$$C_4 = \frac{Tr(\sigma_1 \cdot \sigma_2 \; \sigma_2 \cdot \sigma_3 \; \sigma_3 \cdot \sigma_4 \; \sigma_4 \cdot \sigma_1))}{Tr(1)} = 2 + \Delta^4$$

For the Square-Lattice, Mutual Information per unit length to 4th order is:

$$(\frac{\beta}{4})^2 \frac{nA_2}{2} - (\frac{\beta}{4})^3 \frac{n(n+1)A_3}{6} + (\frac{\beta}{4})^4 [n(n^2+n+1)(\frac{A_4}{24} - \frac{A_2^2}{8}) + n(n^2+n-1)(\frac{B_4 - A_2^2}{2} + C_4)]$$

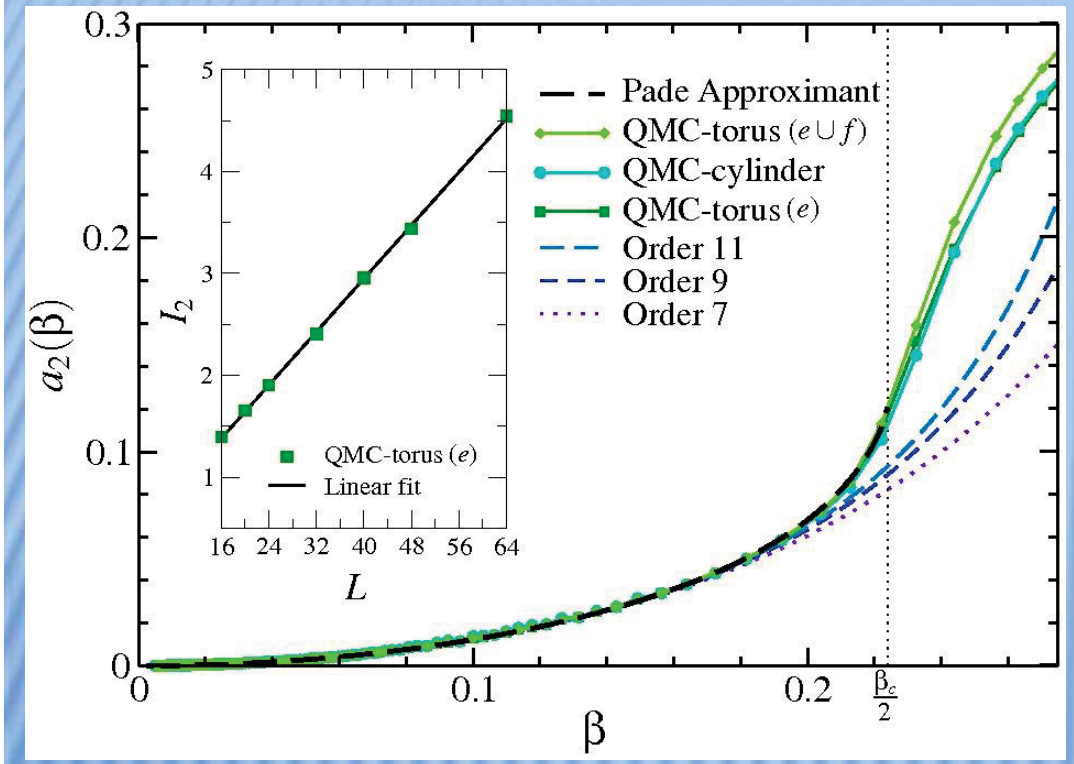
For the Simple Cubic Lattice Lattice, Mutual Information per unit area to 4th order is:

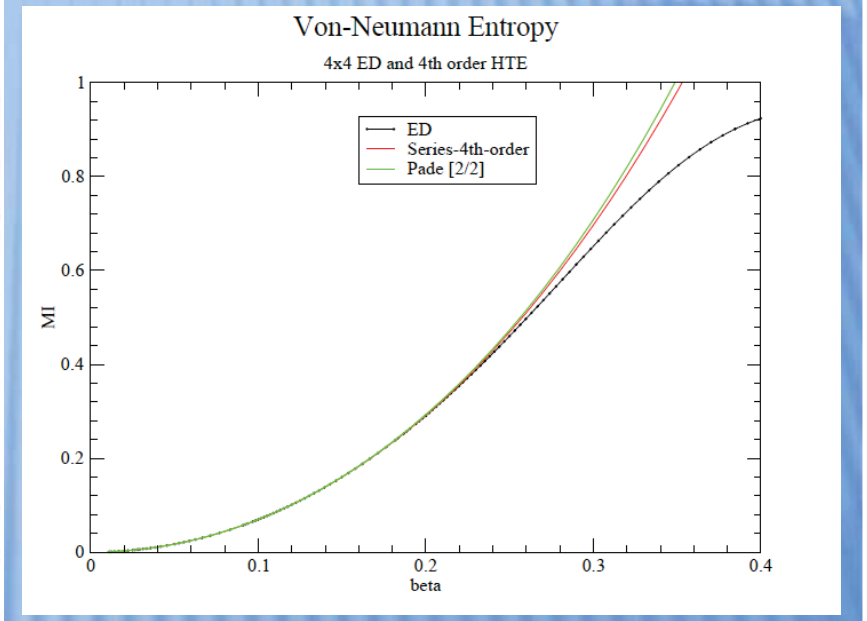
$$(\frac{\beta}{4})^2 \frac{nA_2}{2} - (\frac{\beta}{4})^3 \frac{n(n+1)A_3}{6} + (\frac{\beta}{4})^4 [n(n^2+n+1)(\frac{A_4}{24} - \frac{A_2^2}{8}) + n(n^2+n-1)(\frac{5(B_4 - A_2^2)}{6} + 2C_4)]$$

Note:

1. The only changes between 2D and 3D are that in the β^4 term coefficient of $(B_4 - A_2^2)$ 1/2 is replaced by 5/6 and for coefficient of C_4 1 is replaced by 2.

RRPS, Ann Kallin, Roger Melko, Matt Hastings PRL 2011





Renyi-2

Von Neumann Entropy

ISING EXPANSIONS AT T=0

At $T = 0$,

$$\hat{\rho} = |\psi_0 >< \psi_0|,$$

and reduced density matrices are,

$$\hat{\rho}_A = Tr_B\ \hat{\rho}, \qquad \hat{\rho}_B = Tr_A\ \hat{\rho}.$$

In this case $S_{AB} = 0$ and by Singular Value Decomposition $S_A = S_B$.

Now, all Renyi entropies are different (coefficients are not related by polynomial relations). For a given n calculations can be done straightforwardly.

In a suitable basis, let,

$$|\psi_0 >= \sum_{A_i} \sum_{B_j} c(A_i, B_j)|A_i > |B_j >$$

The matrix element of the reduced density matrix $\hat{\rho}_A$ is

$$\rho_{A_i,A_j} = \sum_{B_l} c(A_i, B_l)c(A_j, B_l)$$

Here, all wavefunctions are assumed real.

And, for $n = 2$

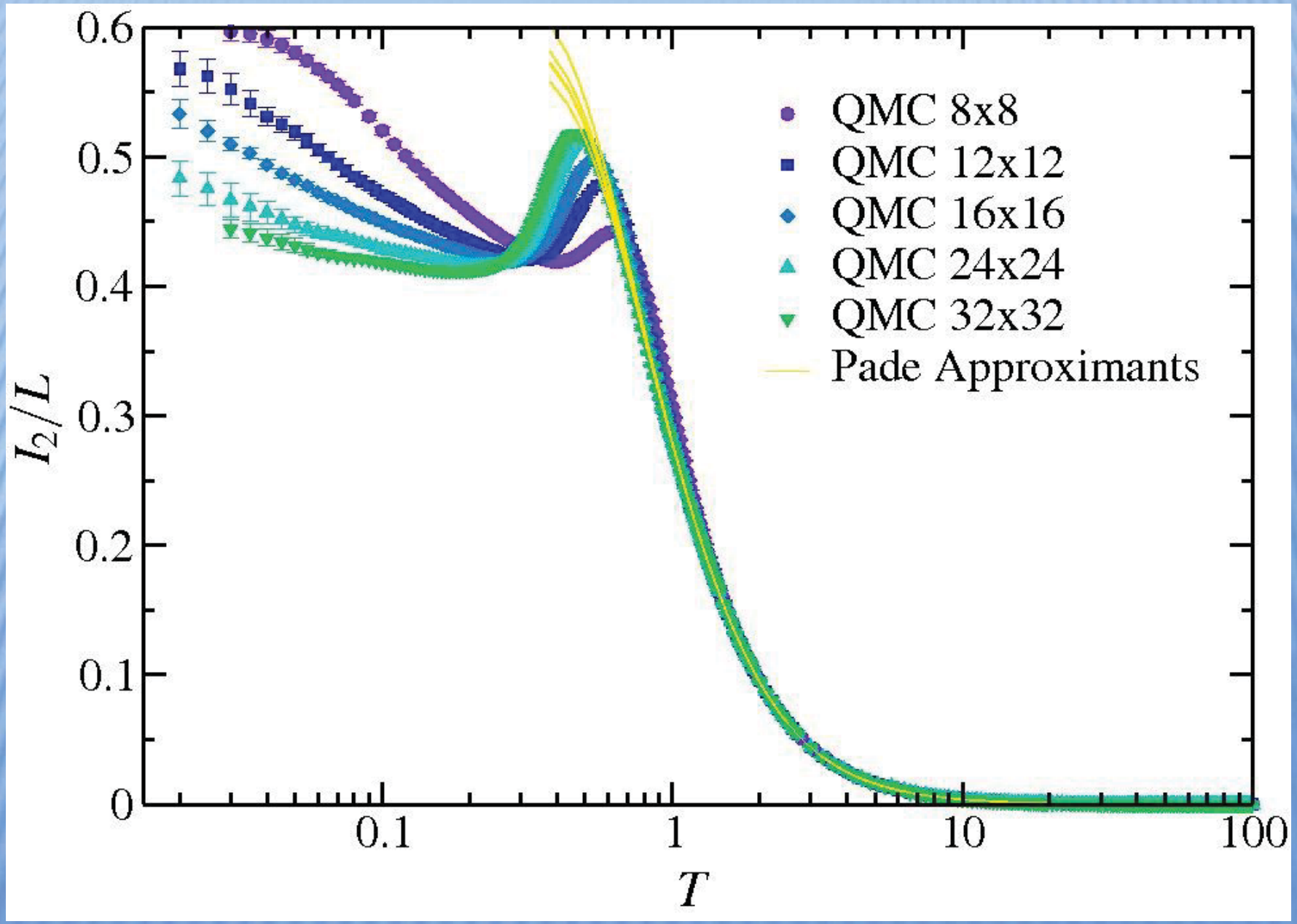
$$Tr_A(\hat{\rho}_A)^2 = \sum_{A_i,A_j}\ \rho_{A_i,A_j}\ \rho_{A_j,A_i}$$

- Von Neumann Entropy has trivial $x^2 \ln(x)$ singularity at $x=0$.
- For all n, no singularity until gap closes at $x=1$.
- Heisenberg Model is particularly interesting
- Series also developed for

  Transverse Ising Model

  Free Fermion Models

Heisenberg Model, Finite-T, Renyi-2 (A. Kallin, R. Melko, M. Hastings, RRPS)



T=0 HEISENBERG MODEL

- Area Law Terms
- Logs from Broken Symmetry (QMC, MFT)
- Logs from Corners (QMC, Series)

Numerical Results agree well.

Theoretical Understanding Remains Incomplete

CONCLUSIONS

- Series expansion methods work in thermodynamic limit----

--Advantages: No size/shape extrapolation, Spectra, Broken Symmetry, No sign problems, any-q, real omega.

--Disadvantages: Convergence problems—Finite size can be a blessing (SSE, ED), Reliance on series extrapolation- especially when gapless excitations play a role

THE END

DIMER ORDER PARAMETER WITHIN HEXAGONS

Order 0th 2nd 3rd 4th 5th 6th

Strong (within hexagon)

-.75 -.5625 -.516 -.437 -.428 -.423

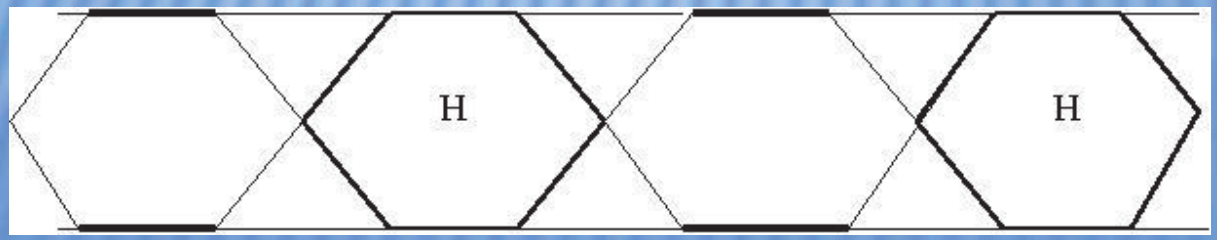
Weak (within hexagon)

0 -.1875 -.258 -.326 -.337 -.328

Resonance within hexagons restored?

Both strong and weak are stronger than mean

Mean energy per bond = -0.217



Kagome strips

White+RRPS

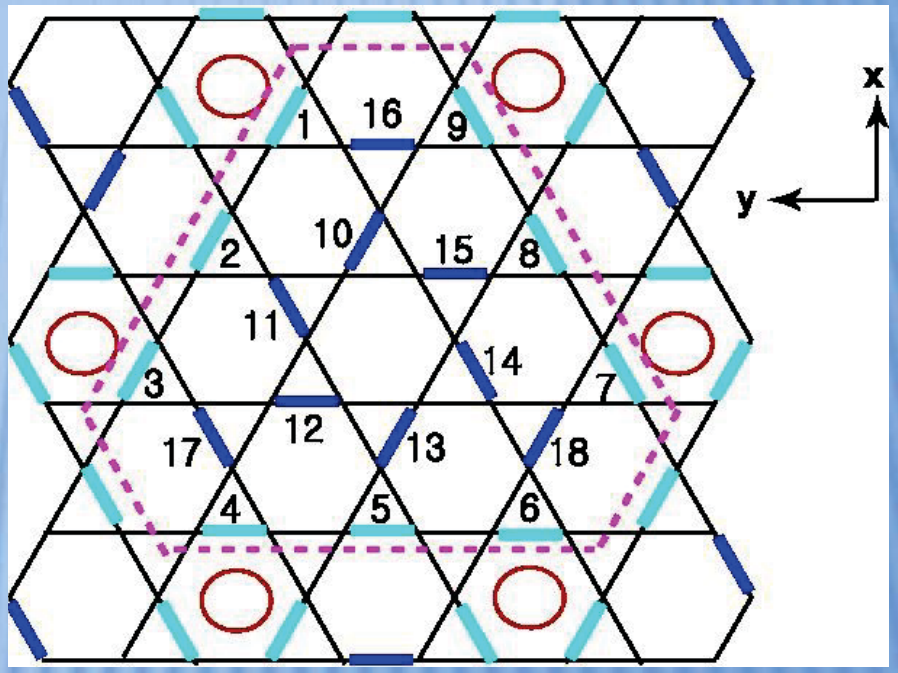
COST OF A LARGE UNIT CELL: ONE PARTICLE SPECTRA: 18X18 MATRIX (FOR EACH Q)

Heavy Triplets (Blue)

and

Light Triplets (Green)

Shastry/Sutherland model

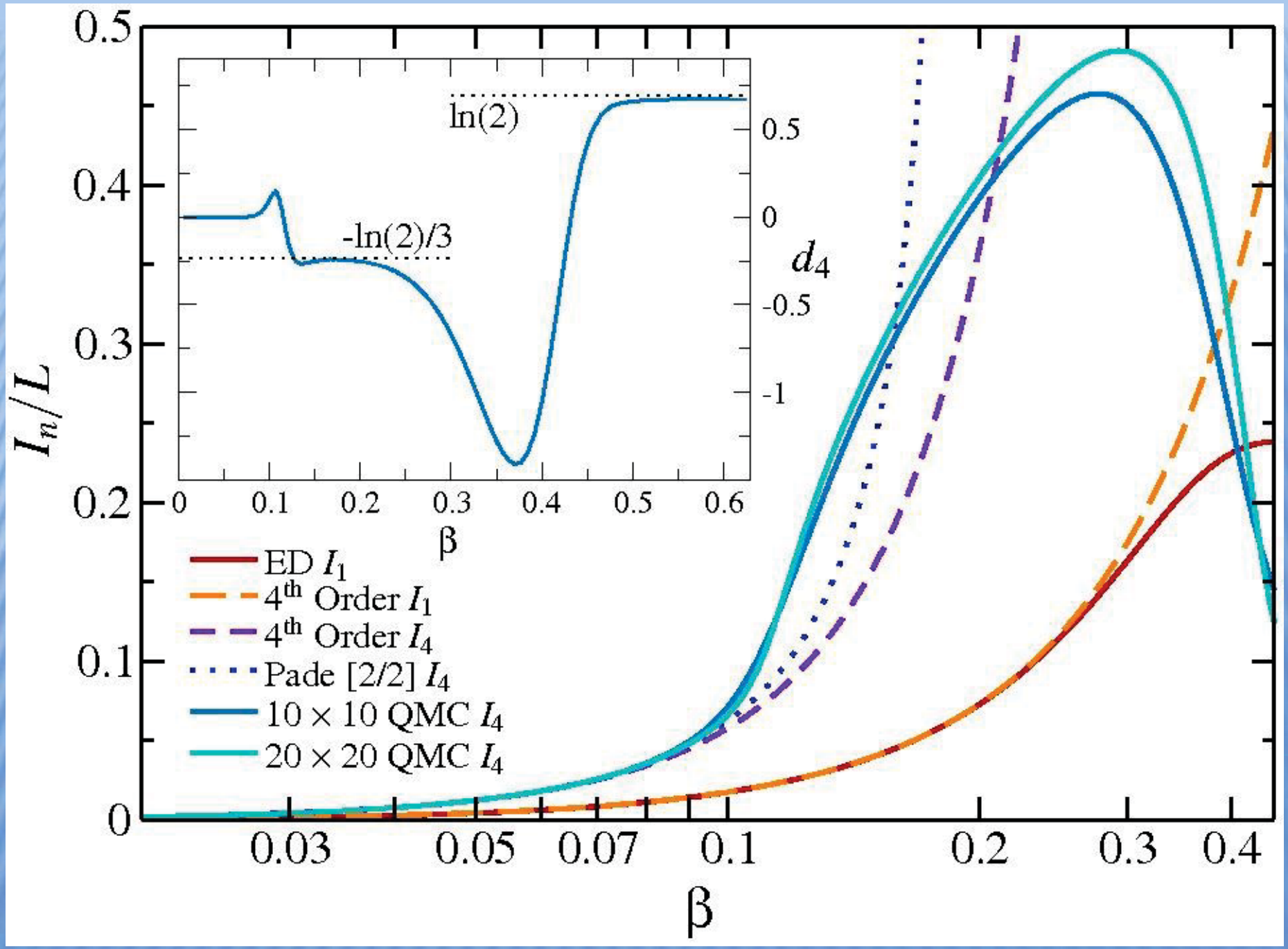


Light triplets have lower energies (9x9)

Yang, Kim, Yu and Park Center Fig. at Pinwheel

TRIPLONS

- All heavy triplets are practically fully localized.
- Light triplet wave functions emerge from degenerate perturbation theory.
- Lowest order—4 states (per q) separate to the bottom. Degeneracy lifts in 3rd order.
- Two are uniformly circulating states in perfect hexagons that hop (very weakly) from hexagon to hexagon.
- Two are pair of chiral states with non-trivial wave function mixing the 9 light triplets in a unit cell that become the lowest energy states.
- Spectral weights measure wave-functions


0.5
0.4
0.3
0.2
0.1
0
I_n/L
0.03
0.05
0.07
0.1
0.2
0.3
0.4
β
ln(2)
-ln(2)/3
0.5
0
-0.5
-1
d_4
0
0.1
0.2
0.3
0.4
0.5
0.6
β
ED I_1
4th Order I_1
4th Order I_4
Pade [2/2] I_4
10 × 10 QMC I_4
20 × 20 QMC I_4

TRIPLONS OF VBC?

- Many triplets but singlets are much lower

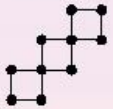
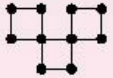
  (We have calculated several singlets states below Triplet)—Only lowest wave-functions are (stable) significant
- Most of 18 give q-independent weight
- 36-site PBC: Focus on 4 Low lying states (of which two are degenerate)—expect 3 peaks—lowest being most significant (stable and twice high)

  Leading order calculation—
- Lowest Mode dominant at g (as observed)—then f,d,h—vanishes at e---agrees Well!
- Next mode dominant at d
- Next mode dominant at e

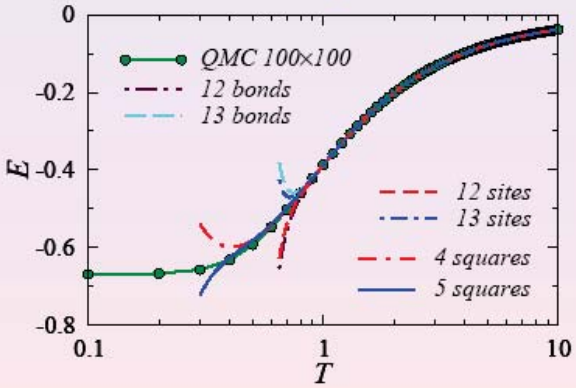
NO SERIES EXTRAPOLATION (BARE SUM)

Numerical Linked-Cluster Expansions

Square clusters

	c	$L(c)$
	1	1
	2	1/2
	3	1
	4	1
	5	2

Heisenberg Model



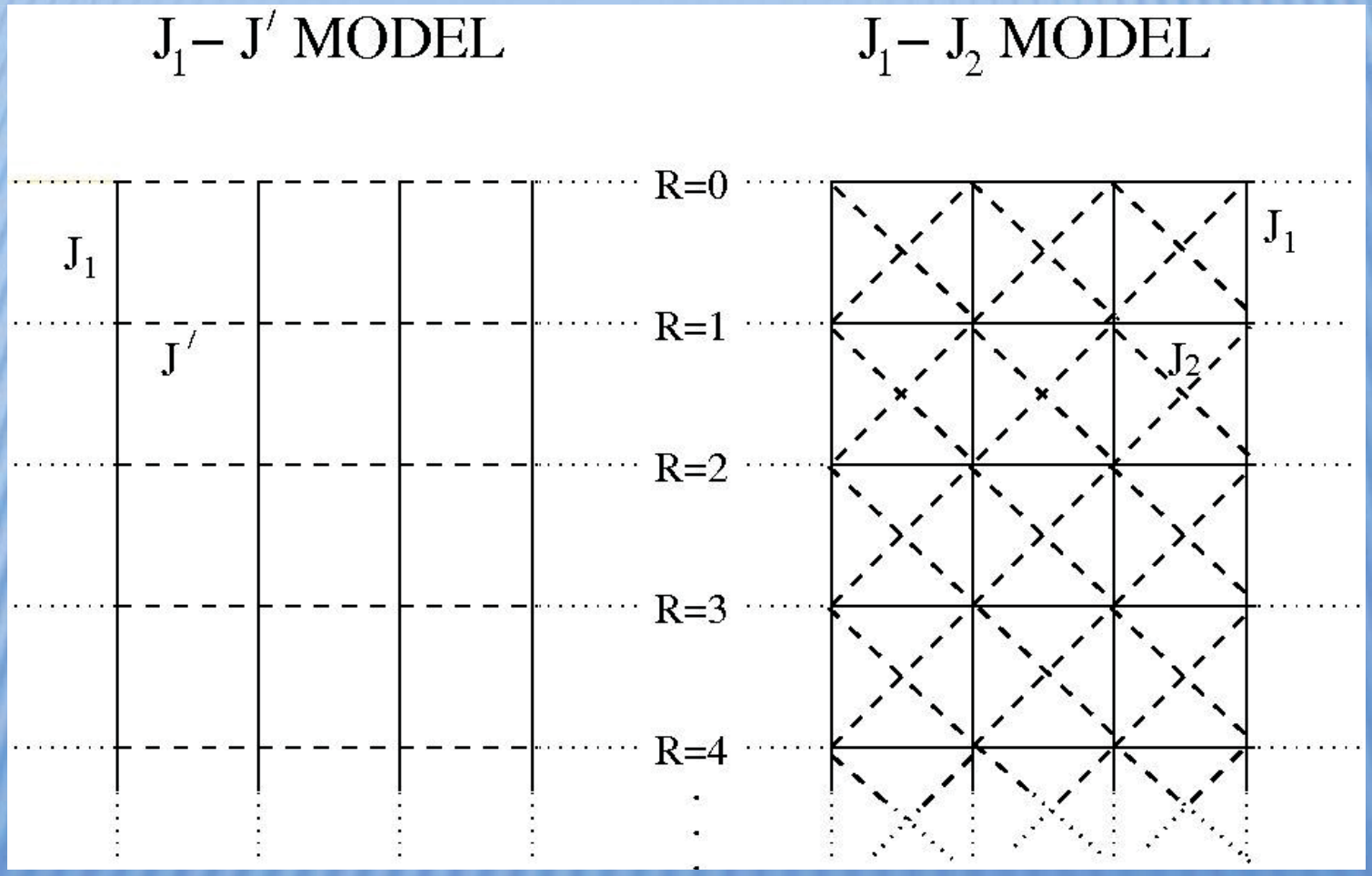
IMPURITIES AND BOUNDARIES AT T=0

- Semi-Infinite Systems
- isolated static hole
- Isolated spin-impurity (HTE by Motrunich grp)
- Cluster of impurities
- Domain Walls

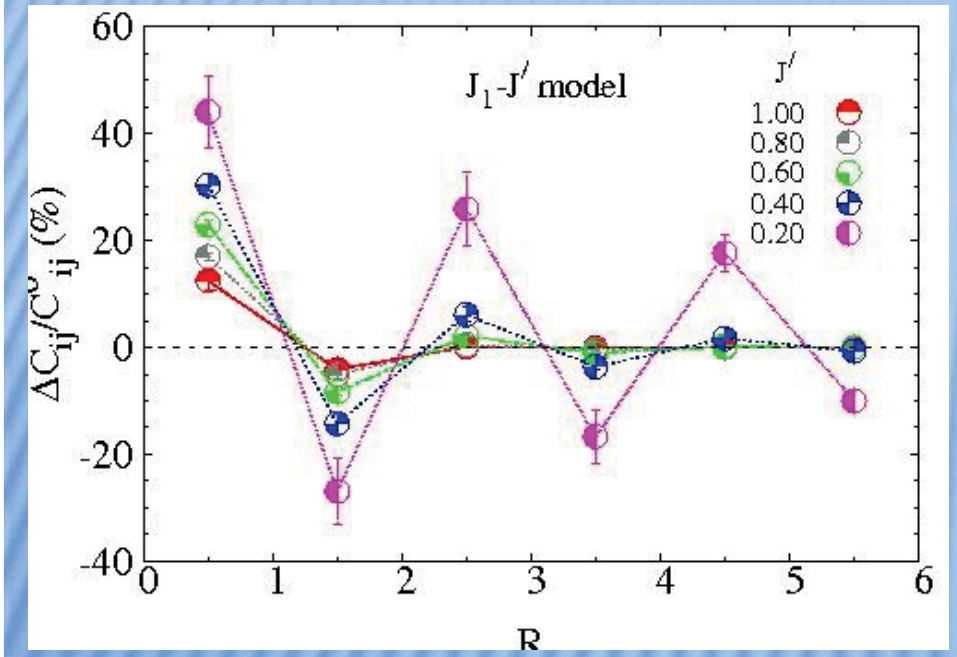
Correlations and spectra remain largely unexplored

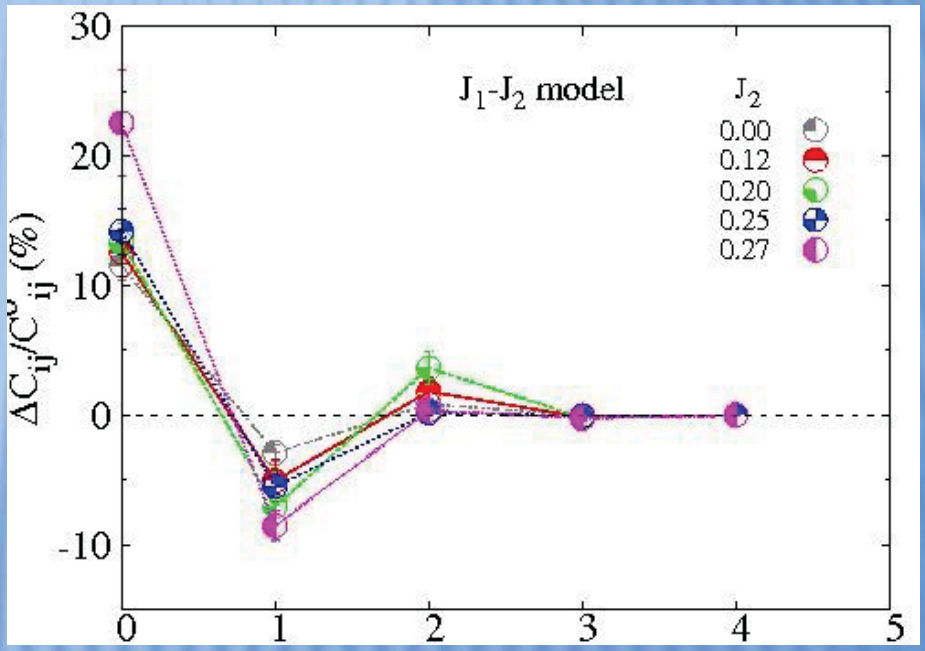
Formalism can accommodate these exactly—without further approximation

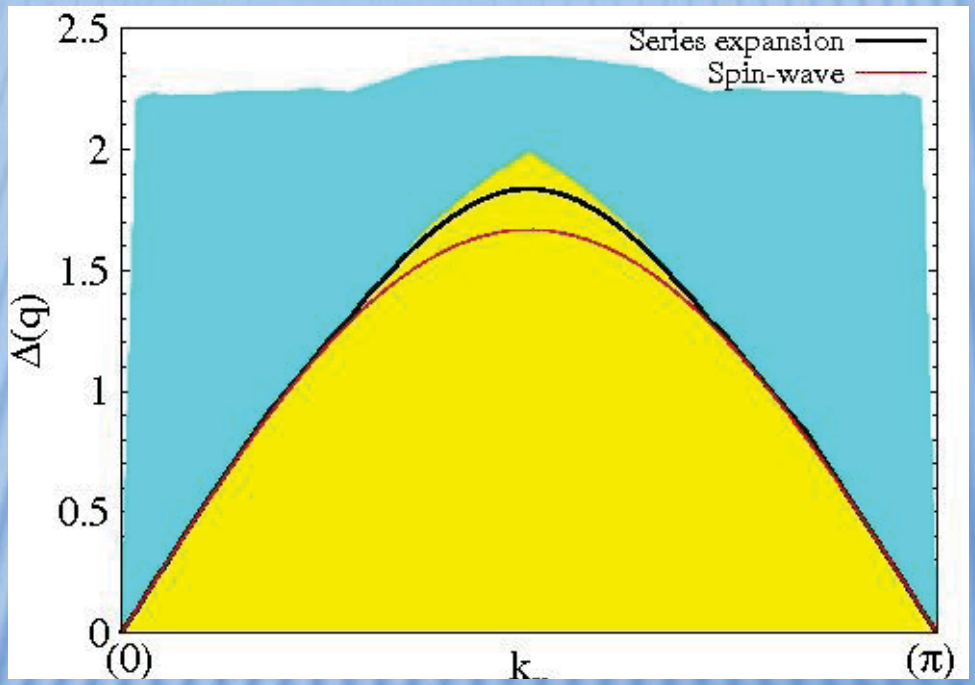
BOUNDARY CORRELATIONS (PARDINI+RRPS)



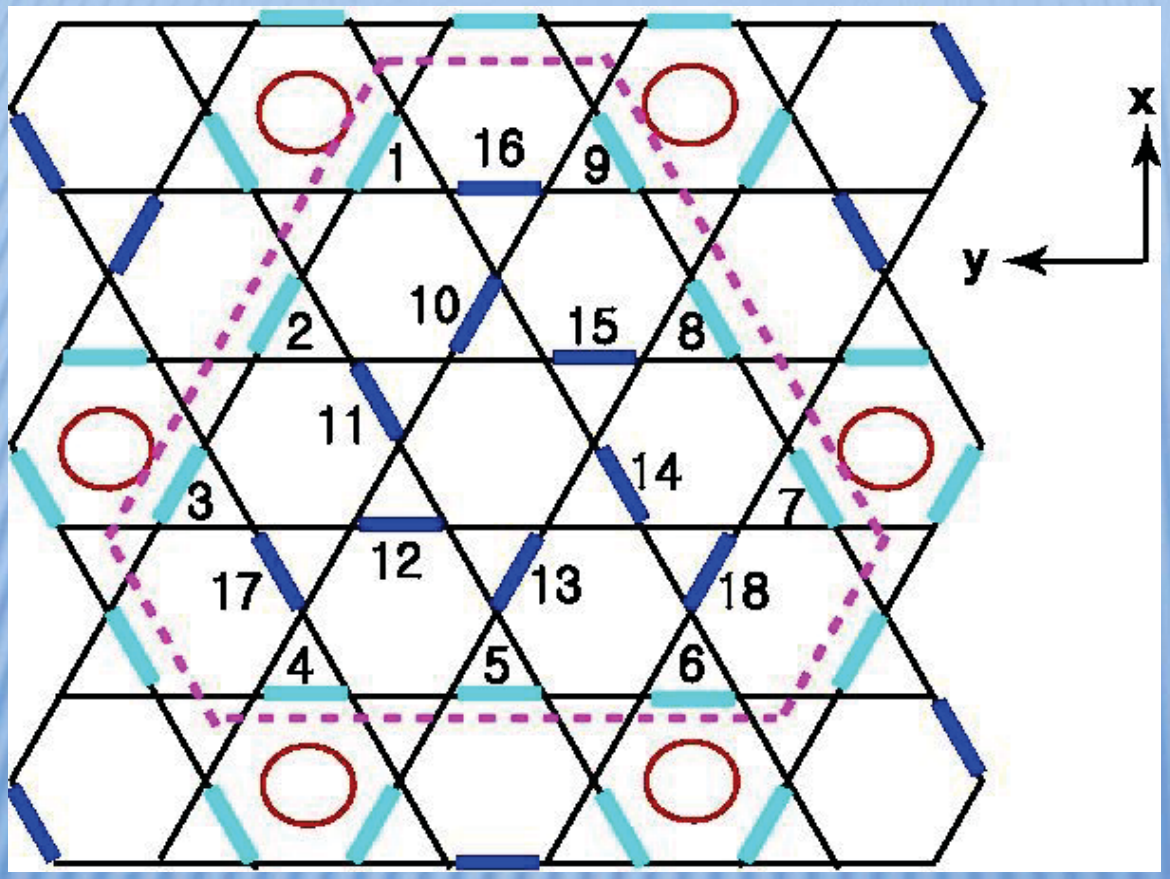
DIMER CORRELATION-LENGTH DOESN'T APPEAR TO GROW IN THE J1-J2 MODEL






Series expansion
Spin-wave
2.5
2
1.5
1
0.5
0
Δ(q)
(0)
k
(π)

TRIPLETS NEARLY LOCALIZED AT ALL SCALES



Loop: Hop along String of Green and Black

Cannot exit, has lowest energy

Spectrum of Lowest Triplets

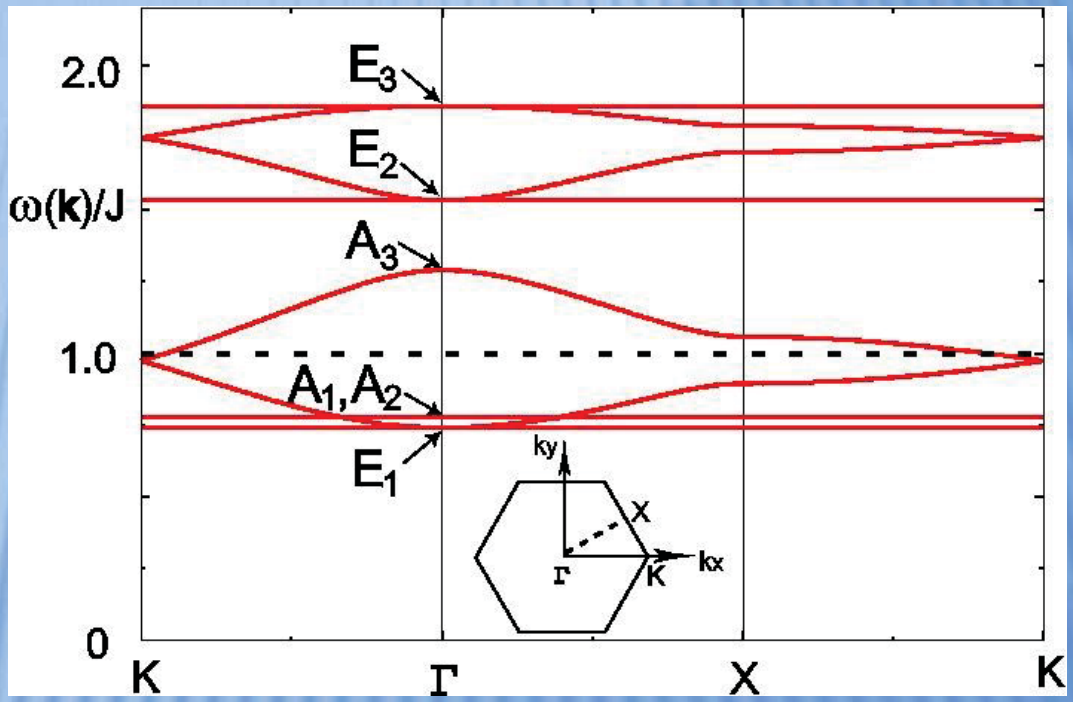
Degenerate Perturbation Theory until Degeneracy Lifts

Then Non-degenerate Perturbation Theory

Low energy structure agrees completely with Yang, Kim, Yu, Park (treat triplets as Bosons)

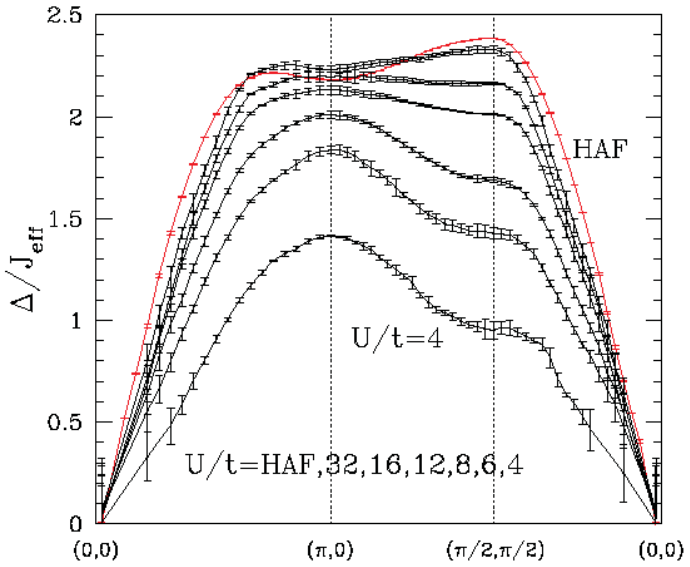
3 flat and one dispersive states that crosses them

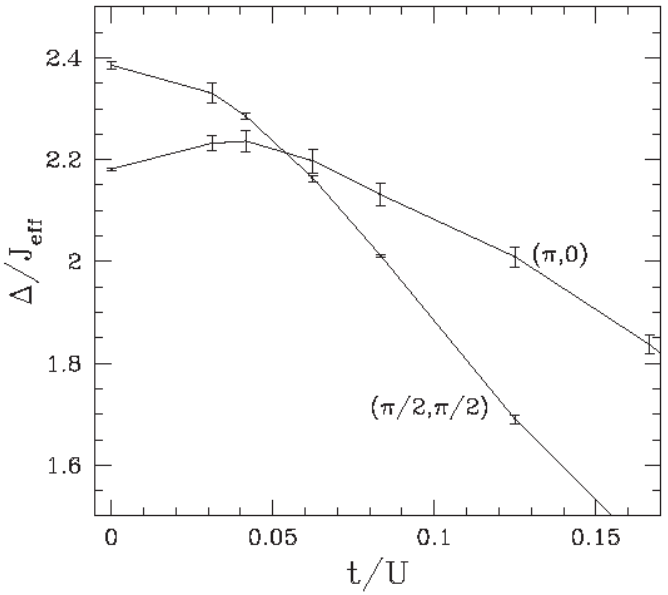
Main difference is gap + small dispersion



Any string of alternating strong and weak Empty triangle bonds: Uniform hopping same energy

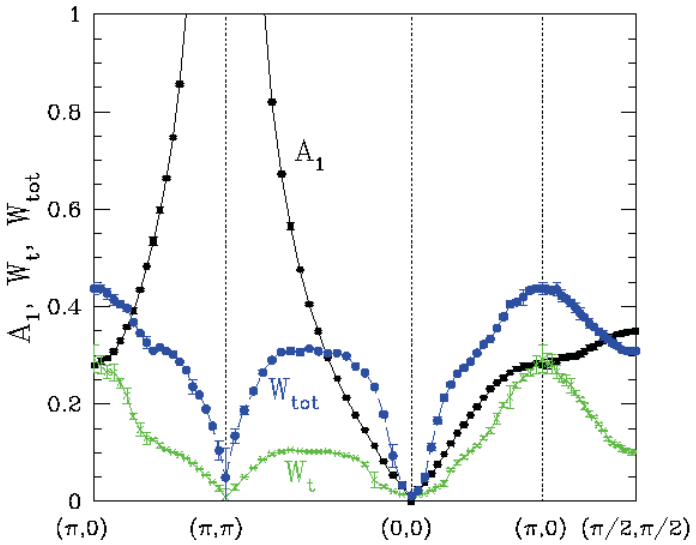
SPECTRA FOR HUBBARD MODEL (ROLE OF CHARGE FLUCTUATIONS)





Zheng et al PRB 72, 033107 (2005)

INTEGRATED WEIGHTS (PI,0) HAS MOST WEIGHT IN CONTINUUM



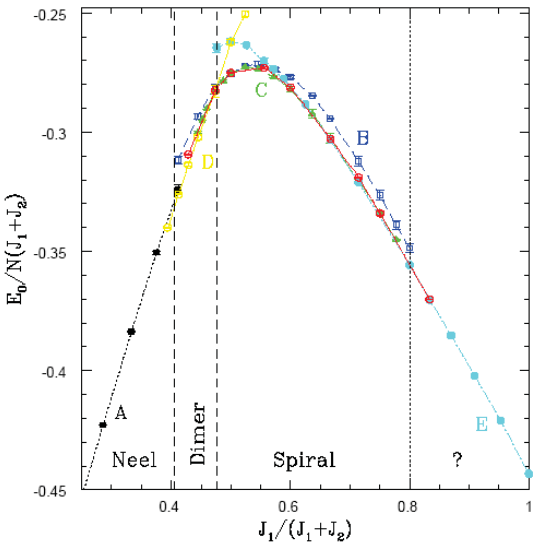
Spinons with minima at

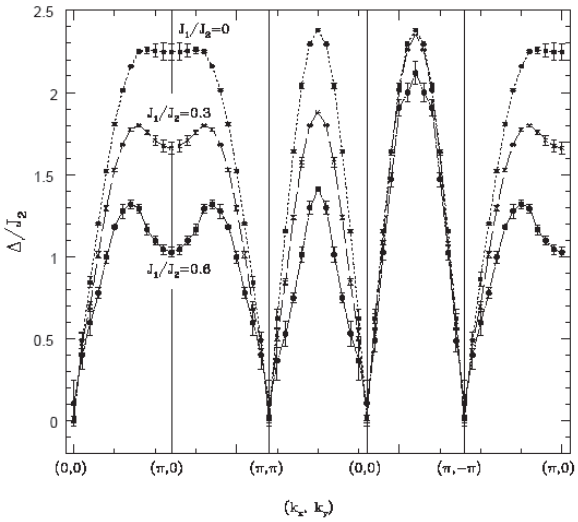
(pi/2,pi/2) ⟶

Two-spinons minima at

(pi,0)

FLUX PHASE PICTURE


-0.25
-0.3
-0.35
-0.4
-0.45
0.4
0.6
0.8
1
$E_0/N(J_1+J_2)$
$J_1/(J_1+J_2)$
A
B
C
D
E
Neel
Dimer
Spiral
?


2.5
2
1.5
1
0.5
0
Δ/J_2
J_1/J_2=0
J_1/J_2=0.3
J_1/J_2=0.6
(0,0)
(π,0)
(π,π)
(0,0)
(π,−π)
(π,0)
(k_x, k_y)