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SPRING COLLEGE IN CONDENSED MATTER
ON QUANTUM PHASES
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SERIES EXPANSIONS FOR QUANTUM SPIN SYSTEMS

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

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SERIES EXPANSIONS FOR QUANTUM SPIN SYSTEMS

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We will cover

- The general idea behind series expansion/extrapolation method
- What kinds of problems/questions are they suited to
- What are some general limitations
- What has been done for Quantum Spin Systems
- What are some of the problems of current and future interest
- Relationship with other numerical/analytic approaches

We will focus on

- Details of series generation methods for Heisenberg/t-J models
- Details of series analysis and extrapolation (how can one take advantage of existing additional knowledge/assumptions)

References

1. Phase Transitions & Critical Phenomena Vol 3: Domb/Green Ed
2. Perturbation Theory for Quantum Many Body Systems
   Gelfand, Singh and Huse J Stat Phys, 59, 1093 (1990) (and references therein)
3. Finite temperature properties of the spin-1/2 Heisenberg Antiferromagnet on the triangular lattice
   Elstner, Singh and Young, PRL 71, 1629 (1993)
4. Quantum Critical Scaling in a moderately doped antiferromagnet Sokol, Glenister and Singh PRL, 72, 1549 (1994)

General Idea Behind Series Expansions

Consider a model Hamiltonian $\mathcal{H}\{J_i, S_j\}$ — J_i: coupling constants; S_j: spin variable

In statistical mechanics we are interested in (an ensemble)

$$Z = \mathrm{Tr}\, e^{-\beta \mathcal{H}} \qquad P(\{S_j\}) = \frac{1}{Z} e^{-\beta \mathcal{H}}$$: Gibbs distribution

from which one can calculate Physical properties

F, E, C_v, χ, κ, ...

Let us assume that such a physical property can be expanded in terms of a suitable parameter

$$F = \sum_n a_n x^n$$

x (expansion parameter)

e.g. $\beta J (= \frac{J}{T})$, $e^{-\beta J} (= e^{-J/T})$, $\frac{J}{T}$, $1/d$,

(βJ, $\frac{J}{T}$: high T; $e^{-\beta J}$, $e^{-J/T}$: low T; $\frac{J}{T}$: coupling constant)

Series method:

Calculate as many a_n's as possible

Use these coefficients to obtain F for as large an x as possible

Typically: small x is of limited interest

[No true small parameter in our difficult problem]

Still by carrying out the expansion to high orders we hope to learn the properties of the model when x gets 'large'

Problems addressed by Series Expansion Methods

- Different phases of a model Hamiltonian
  Equilibrium, thermodynamic phases
- Quantitative Estimates of phase-boundaries
  (specially 2nd order phase boundaries)
- Studies of critical point phenomena
  (Calculations of critical exponents, amplitudes, scaling functions, crossovers etc. and their dependence on symmetry / dimensionality etc.)
- Dynamics of quantum spins
  Matsubara Susceptibilities, Green's functions
  Relaxation rates
- Role of quenched impurities
  Dilution, Spin-glass, Bose-glass etc.

Relation to other numerical approaches

Closely related to finite size diagonalization studies.

Advantage: Effective size explored is much larger than what can be diagonalized. Essentially the large problem is broken up into a counting problem and many smaller problems.

Disadvantage: Series extrapolation is based on many assumptions, which are not always ~~exhibited~~ proven. Must be compared with other numerical schemes wherever possible.

Another advantage: Going from one-dimension to 2, 3 or higher dimension requires only marginal increase in computer power.

Disadvantage: Generating high order expansions can be a full time business

SERIES EXPANSIONS

A general method for Statistical models

Some thermodynamic property $f(x)$ is expanded

$$f(x) = \sum_n a_n x^n$$

A finite number of a_n, $n \le N$ are calculated exactly

[Finite number of coefficients → complete answer at small x]

Use series extrapolations (resummation) to get to large x.

[High temperature / low temperature expansions]

1st Lecture

Calculating series coefficients by cluster expansions

Closely related to exact diagonalization methods

End Lecture

$T=0$ expansions for Heisenberg models,

Ising & Dimer expansions for $d=1, 2$

Third Lecture

High temperature expansions for

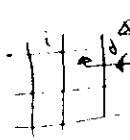
Heisenberg / t-J models

Series analysis will come in 2nd and 3rd lectures

Wednesday

Cluster Expansions

[Keep in mind high-T expansion for Heisenberg / Ising models]



sites S_j (spins / spin operators)

bonds J_{ij} (interactions)

Assume: high-T expansion exists

$$f\left(\frac{J}{T}\right) = \sum_n f_n \left(\frac{J}{T}\right)^n$$

, wish to calculate $f_0, f_1, \ldots f_N$

[Most models, such an expansion can be rigorously shown to exist]

Cluster Expansions: Conceptually simple and convenient for a computer algorithm

[Not a unique method]

Consider a multi-variable expansion

$$K_{ij} = J_{ij}/T$$

$$f(\{K_{ij}\}) = \text{const} + \sum_{\langle i,j\rangle} \sum_{n=1}^{\infty} a_n^{(i,j)} K_{ij}^n + \sum_{\langle i,j\rangle,\langle k,l\rangle} \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} a_{n,m}^{(i,j),(k,l)} K_{ij}^n K_{kl}^m + \sum_{\langle i,j\rangle,\langle k,l\rangle,\langle m,n\rangle} \cdots + \cdots$$

terms which depend on only one interaction coeff. K_{ij}

terms which " on exactly two " " $K_{ij} K_{kl}$

" " " n " "

" "

Define a graph by a set of bonds on the lattice. An N-bond graph is a graph with N bonds

* The sites which are connected by these bonds will be called sites of the graph

N bond graph has M sites with $M \leq 2N$

Definition : Weight of an N-bond graph are all terms in the multivariable expansion which depend on exactly N-bonds, i.e they have one or more powers of each interaction in the graph and no dependence on any other interaction

K_{12} (1 — 2)

$$W(\cdot\!-\!\cdot) = a_1 K_{12} + a_2 K_{12}^2 + \cdots$$

$$W(\cdot\!-\!\cdot\!-\!\cdot) = b_{11} K_{12} K_{23} + b_{21} K_{12}^2 K_{23} + b_{12} K_{12} K_{23}^2 + \cdots$$

(1 — 2 — 3)

It follows from this definition that

(a) $f(\{K_{ij}\}) = \sum_{\text{all graphs}} \text{constant} + \sum_{\text{graphs}} W(\text{graphs})$

each term is contained in the weight of one and only one graph.

(b) Weight of an N-bond graph is Nth order has at least N powers of K_{ij}

(c) For a uniform system $K_{ij} = K$, weight of all graphs related by a symmetry [translation or reflection, rotation] is the same.

More generally for uniform quantities only the topology (or connectedness) of graphs matter

Same connectedness but different embedding

We will restrict ourselves to uniform quantities

Generalization for $\vec{r}_i, \vec{r}_j$ dependence will be easy.

d) For calculating weight of a graph g we can set all interactions not in the graph to zero. Then carry out the multivariable interactions. Weight is unaffected.

The sites not in the graph are free. Do not contribute to the weight.

This Weight can be gotten by calculating th. expansion for a finite graph.

Multivariable expansions are cumbersome. We need only carry single variable expansion and use the fact that

$$F(g) = W(g) + \sum_{\substack{\text{proper} \\ \text{subgraphs } s}} W(s) + \text{constant}$$

$$W(g) = F(g) - \sum_{\text{subgraphs } s} W(s) - \text{constant}$$

If we calculate weights of successively larger graphs, then from the expansion for $F(g)$ we can get expansion for $W(g)$

$$F(g) = \sum_n \alpha_n K^n$$

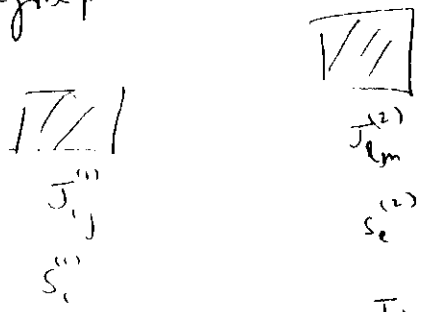
$$W(s) = \sum_n C_n(s) K^n$$

$$\boxed{C_n(g) = \alpha_n - \sum_s C_n(s)}$$

Entirely a matter of finite size calculations.

In statistical mechanics we are interested in Extensive / Intensive quantities in the thermodynamic limit.

For these weights of disconnected graphs vanish



Disconnected graph : Two sets of bonds commuting diff erent sets of spins

$$\mathcal{H} = \mathcal{H}^{(1)} + \mathcal{H}^{(2)} \quad \text{commuting parts}$$

$$\text{Tr}\, e^{-\beta \mathcal{H}} = \text{Tr}\, e^{-\beta \mathcal{H}_1} e^{-\beta \mathcal{H}_2}$$

$$Z = Z_1 Z_2 \qquad \ln Z = \ln Z_1 + \ln Z_2$$

$\Rightarrow$ Weight of graph is zero

$$\sum \langle S_i^z S_j^z \rangle = \frac{\text{Tr} \sum S_i^z S_j^z e^{-\beta \mathcal{H}}}{\text{Tr}\, e^{-\beta \mathcal{H}}} = \sum \langle S_i^z S_j^z \rangle_1 + \sum \langle S_i^z S_j^z \rangle_2$$

No term which is a product of all interactions.

Lattice Constant of a graph g

$L(g) \equiv$ # of embeddings per lattice site (in the thermodynamic limit)

For an extensive quantity

$$\frac{F}{N} = \sum_g L(g) \cdot W(g)$$

Advantage of this method

- Graph counting and Lattice dependence is completely separated from the nature of spins or field, in the problem.

High T expansion for very different models (Ising, Potts, Heisenberg, Hubbard, t-J, spin-glass) the country is the same.

It will be different for the types of interaction, second neighbor interactions, lattice anisotropy etc.

The price one pays is that the weight calculation is non-trivial. Almost requires a diagonalization of a finite system.

Steps in Graph Counting

- Finding all distinct graphs to a given order
- Finding their Lattice Constant on the given lattice
- Finding their subgraphs

Trivial for $d = 1$

only N bond connected graph is the chain of length N. It has N 1-bond subgraphs, N-1, 2-bond subgraph, etc.

Higher d

How do we represent a graph { the topology of / by numbers or symbols }

[Low connectivity of a graph] # of sites

Adjacency Matrix $(M \times M)$

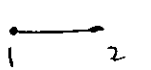
$A_{ij} =$ # of connections between (i,j)

$= 1$ if connected

$= 0$ otherwise

Symmetric matrix.

One-bond graph



$$A_{ij} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Recursion:

We can generate all (N+1)-bond connected graphs from all the set of N-bond connected graphs by one of two methods.

a) Add a site to the graph and connecting it to one of the existing sites

b) Add a bond between two existing sites

Proof: If the (N+1) bond graph has a free end it can be obtained by method (a)

If it has no free end then it must have a closed loop. Removing one bond from the closed loop will leave it connected

Thus it can be obtained by (b).

In terms of A_{ij}

(a) ⇒ Add a column with a one and rest zeros

$M \times M \Rightarrow (M+1) \times (M+1)$ matrix

(b) ⇒ Change a zero into a one in upper and lower triangles of the matrix.

$M \times M$ matrix with N+1 bonds

But This procedure applied to all N-bond graphs will generate all (N+1)-bond graphs. But it will generate any graph many-many times.

We don't wish to overcount. Need to remove duplicates

(Time consuming / Bottleneck for bcc Ising 21st order sum)

When are two graphs the same?

[When adjacency matrices agree on a permutation of nodes

$M!$ possible comparisons are needed in comparing two ~~node~~ graphs.

Define a Canonical Labelling scheme. Label each graph canonically. Then graphs are identical if A_{ij} agree.

Lexicographic Ordering of matrices

$M_1 > M_2$ if $(M_1)_{ij} = (M_2)_{ij}$ upto some (a,b)

$(M_1)_{ab} > (M_2)_{ab}$

in row order

$\begin{pmatrix} & & \\ & \vdots & \\ & & \end{pmatrix}$

Adjacency matrix of a graph must be labelled canonically (N! choices) (not for every pair of graphs)

Skeleton graph: Suppress all sites of valency two [Valency of a site] left with nodes, bridges and free ends

Need only consider permutation of nodes. And then check for A_{ij}

Avoid repetitive operations

Use Self Avoiding Walks for bridges

Read J L Martin in Domb/Green critical phenomena

Not the bottleneck for Quantum spins. Do not need the best algorithm.

Finding Subgraphs

Try all possible $2^N - 2$ possibilities.

List all connected ones.

Listing of graphs

to the order Baker et al Brookhaven NL Report 1967

Difficult to publish. Large data set. Could possibly have a data bank set up.

Standardize notation

Lattice Constants [Count of Embeddings]

Exhaustive search

Dumb algorithm

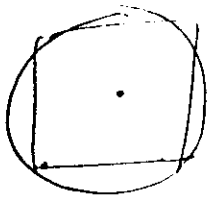
Place 1st site at origin

Determine a size such that all embeddings are contained in it

Place all other sites one by one at all possible sites in that finite region

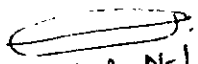
Once every site is placed, check to see if there is no double occupancy and all neighbors are unit distance apart.

Exhaustively count all allowed embeddings.



Efficient algorithm

Backtracking: An algorithm which leads from one allowed algorithm to the next in a regular way. ~~Needs~~ From one embedding to a nearby algorithm



Stack of N-1 sites in acceptable

Put nth in all acceptable positions

∴ (N-1)th in next position

Weight Calculation

Calculating $F(g)$ for a finite graph

$$T\chi = \left\langle \sum_i \sum_j S_i^z S_j^z \right\rangle$$

$$= \frac{\mathrm{Tr}\, e^{-\beta \mathcal{H}} \sum_i \sum_j S_i^z S_j^z}{\mathrm{Tr}\, e^{-\beta \mathcal{H}}}$$

$$= \frac{\sum_n \frac{(-\beta)^n}{n!} \sum_\alpha \langle \alpha | \mathcal{H}^n \sum S_i^z S_j^z | \alpha \rangle}{\sum_n \frac{(-\beta)^n}{n!} \sum_\alpha \langle \alpha | \mathcal{H}^n | \alpha \rangle} = \frac{\sum_n a_n \beta^n}{\sum_n b_n \beta^n}$$

$$\left.\begin{aligned} \frac{\sum_n a_n \beta^n}{\sum_n b_n \beta^n} &= \sum_n c_n \beta^n \\ a_0 &= c_0 b_0 \qquad c_0 = a_0/b_0 \\ a_1 &= c_0 b_1 + c_1 b_0 \qquad c_1 = \frac{a_1 - c_0 b_1}{b_0} \end{aligned}\right\}$$ in any

need to sum over all $|\alpha\rangle$ and operate by $\mathcal{H}^n$

[Can use block-diagonal structure]

S^z_{tot} is conserved

given S^z_{tot} for state $|\alpha\rangle$ $\mathcal{H}^n$ will not change it.

Reduces size of Hilbert space. No more difficult than Lanczos

High-Temperature Expansion with Fermions

t-J model

$$\mathcal{H} = \sum_{\langle ij\rangle \sigma} P (c^{+}_{i\sigma} c_{j\sigma} + h.c.) P + J \sum_{\langle ij\rangle} \vec{S}_i \cdot \vec{S}_j$$

$$\vec{S}_i = \sum_{\sigma,\sigma'} \frac{1}{2} c^{+}_{i\sigma} \vec{\sigma}_{\sigma\sigma'} c_{i\sigma'}$$

Grand Ensemble

$$\Xi = \mathrm{Tr}\, z^N e^{-\beta \mathcal{H}}$$

$$= \sum_{\substack{\text{complete set} \\ \text{of states with} \\ \text{all particle number}}} \langle \psi | z^N e^{-\beta \mathcal{H}} | \psi \rangle$$

Choose $|\psi\rangle = |\varphi_1, \varphi_2, \ldots\rangle$

Constraint dealt with exactly

$$\varphi_i = \begin{cases} n_{i\uparrow} = 1, & n_{i\downarrow} = 0 \\ n_{i\downarrow} = 1, & n_{i\uparrow} = 0 \\ n_{i\uparrow} = 0, & n_{i\downarrow} = 0 \end{cases}$$

$$\sum \Rightarrow \sum_{\varphi_1} \cdot \sum_{\varphi_2} \cdots$$

Trace factorizes

allowed all states at a site independent of others

Collect all $z^N = \prod z^{n_i}$

to show

collect all operators at a given site

$$\prod \langle \varphi_i | S_i^{\beta} | \varphi_i \rangle \quad c_{i\sigma} c_{i\sigma'} \cdots$$

In bringing operators of a given site together need to worry about signs

We get

$$F = \sum_n \beta^n \sum_{m=0}^{n} a_{n,m}(z)\, J^m\, t^{n-m}$$

For J, t

$$F = \sum_n \beta^n \bar{a}_n(z)$$

$$+ \sum_n \beta^n \bar{r}_n(z)$$

obtain

$$f = \frac{1}{N} \sum_i \langle n_i \rangle = \frac{2z}{1+2z}$$

ρ_0

can invert

$$\rho_0 = \rho + \sum_m \beta^m r_m''(\rho)$$

Kubo

Substitute in F to get

$$F = \sum_n \beta^n a_n'(\rho)$$

Expansion in β for fixed t, J, ρ

Series Expansion at T=0

Ising expansion

$$\mathcal{H} = J \sum_{\langle ij \rangle} \left[S_i^z S_j^z + \alpha \left(S_i^x S_j^x + S_i^y S_j^y \right) \right]$$

$J > 0$

Expand in powers of α

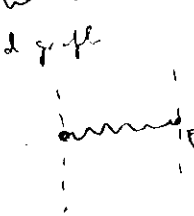
(gap in the spectrum at $\alpha = 0$)

$$\frac{E}{N} = e_0 + \alpha^2 e_2 + \alpha^4 e_4 + \cdots$$

$$\frac{M^+}{N} = m_0 + \alpha^2 m_2 + \alpha^4 m_4 + \cdots$$

The multivariable scheme will work. A different α_{ij} for every bond. But the J_z part of the Hamiltonian present everywhere for any graph

On bond ij

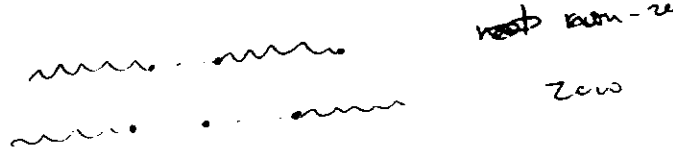


J_z interaction apply staggered field on active spins. Choose one ground state

$\Rightarrow$ Energy gap at $\alpha = 0$. Perturbation theory is simple (non-degenerate)

However, graph counting more difficult.

When is a graph connected (disconnected)?



$$\mathcal{H} = \mathcal{H}_0 + \alpha \mathcal{H}_1 + \mathcal{H}_2$$

$[\mathcal{H}_1, \mathcal{H}_2] = 0 \Rightarrow$

$E = \text{const} + E_1(\alpha) + E_2(\alpha)$

$\psi = \psi_1(\alpha) \cdot \psi_2(\alpha)$

If they apply staggered field on each other they do not commute.

There is a better way to do this

Low temperature (Strong Embedding scheme)

Specify a graph by a set of sites and which are nearest neighbor in the graph. Every such bond will be considered part of the graph.

Weight of the graph: all terms where the state of each site in the graph was changed (non-changed back)

$\langle \Psi_0 | \cdots \frac{1}{E - H_0} H' \frac{1}{E - H_0} H' | \Psi_0 \rangle$

An M site graph will contribute in order d^M

⟹ can not have the embedding ⊔

Counts are different.

From the coordination number and the coordination in the graph know the staggered field on the site. Do not need to consider outside J_z bonds.

Special for magnetically ordered system

Heisenberg

Half-filled Hubbard

Dimer (Cluster) Expansion

1 λ 1 λ 1 λ

$H = H_0 + \lambda H_1$

$\frac{1}{N} \quad e_0 + \lambda e_1 + \lambda^2 e_2 + \cdots$

$\chi \langle ss \rangle = a_0 + \lambda a_1 + \cdots$

Two-dimension

Many possible cluster shapes

Need a gap

Magnetic susceptibility

Dimer

A natural scheme ... clusters

$\frac{1}{4}$ filled t-J / Hubbard model

For a finite system how do we calculate the perturbation expansion.

Exists a basis in which

$(H_0)_{ii}$ is diagonal / known

$(H_1)_{ij}$ is easily calculable

Choose 1 → ground state of H_0. M is dimension of Hilbert space

$$H_0|\psi_\lambda\rangle + \lambda H_1|\psi_\lambda\rangle - E_\lambda|\psi_\lambda\rangle \quad -(1)$$

Raleigh Schrodinger Perturbation Theory

Let

$$|\psi_\lambda\rangle = \begin{pmatrix} 1 \\ a_2^1\lambda + a_2^2\lambda^2 + \cdots \\ \\ \\ a_M^1\lambda + a_M^2\lambda^2 \cdots \end{pmatrix}$$

M is relevant dimension of Hilbert space.

~~Fock space~~

$$E_\lambda = E_0 + E_1\lambda + E_2\lambda^2 + \cdots$$

Eq. (1) is M equations. Lets work in ... components

$\langle i|$ (1) $\rangle \Rightarrow$

$$(H_0)_{ii}|\psi_\lambda\rangle_i + \lambda\sum_j (H_1)_{ij}|\psi_\lambda\rangle_j = E_\lambda|\psi_\lambda\rangle_i$$

For $i = 1$

$$(H_0)_{ii}\cdot 1 \; 1 + \lambda\sum_j (H_1)_{ij}\sum_n a_j^n\lambda^n = (E_0 + E_1\lambda + E_2\lambda^2 \cdots)\cdot 1$$

comparing coefficients of λ^{n+1}

$$\sum_j (H_1)_{1j} a_j^n = E_{n+1}$$

knowing 1 terms to order n gives E in order $n+1$

$i \neq 1$

$$(H_0)_{ii}\sum_n a_i^n\lambda^n + \lambda\sum_j (H_1)_{ij}\sum_n a_j^n\lambda^n = (E_0 + E_1\lambda + \cdots)\sum_n a_i^n\lambda^n$$

comparing coefficients of λ^{n+1}, we get

$$(H_0)_{ii}\, a_i^{n+1} + \sum_j (H_1)_{ij} a_j^n = E_0 a_i^{n+1} + E_1 a_i^n + E_2 a_i^{n-1} + \cdots$$

$$\sum_j (H_1)_{ij} a_j^n - \sum_{m=1} E_m a_i^{n+1-m} = (E_0 - (H_0)_{ii}) a_i \quad (27)$$

$$a_i^{n+1} = \frac{1}{E_0 - (H_0)_{ii}} \left[\sum_j (H_1)_{ij} a_j^n - \sum_{m=1} E_m a_i^{n+1-m} \right]$$

Important to have a non-degenerate ground state. Or one that does not couple in any finite order of perturbation theory.

Once we know $|\Psi_g\rangle$ we can get $\frac{\langle \Psi_g | O | \Psi_g \rangle}{\langle \Psi_g | \Psi_g \rangle} = \sum_n O_n \lambda^n$

Excited states? Can not use this

|1⟩ ↑ ↓ ↑ GS

|2⟩ ↓ ↓ ↑ } excited states of H_0 are degenerate!

|3⟩ ↑ ↓ ↓

Can not do this, to calculate E_2 or E_3 need degenerate perturbation theory. & more and more higher order degeneracies, more longer graphs!

Do we know expansions are correct? (28)

Independently on 2 continents

Ising expansion for M^+, $\chi_\perp$, E_g

Myrheim, Weihong, Oitmaa & Hamer

High T expansion for ~~t-J~~ Heisenberg

Baker et al, Elstner, Elstner (10th order)

t-J model

Gros, Rice, Putikka, Luchini,

Internal checks

Weights subgraph subtraction

Low order is crucial

Graphs calculate known series and check

Series Analysis (Extrapolation / Summation)

With T=0 expansions for Heisenberg model

First discuss d=2 (come back to d=1)

Ising Expansions

$$\mathcal{H} = \sum_{ij}\left[S_i^z S_j^z + \alpha\left(S_i^x S_j^x + S_i^y S_j^y\right)\right]$$

Dawis 1950's
Parinello etal 1970's

expand in powers of α

$M^+ = S - \cdots$ (transparency)

Can we estimate M^+ for $\alpha = 1$?
Terms are decreasing slowly. Not enough to add

1988 Huse: Need extrapolation
Extrapolate partial sum with inverse power of N.
Huse: Critical phenomena problem with known exponent

If ordered ~~convergent~~ for x = 1, then we must have gapless excitations (Goldstone, spin-waves). Series must become singular at x = 1.

TABLE 1. Series coefficients for the ground-state energy per site E_0/N, the staggered magnetization M^+, staggered parallel susceptibility χ^s_{zz}, and the mass gap m. Coefficients of x^n are listed for both the spin-½ and spin-1 models.

n	E_0/N	M^+	χ^s_{zz}	m
Spin ½ model				
0	-1/2	1/2	0	2
2	-1/6	-1/9	0.148148148148E+00	-5/3
4	0.925925925926E-03	-0.177777777778E-01	0.108691358025E+00	0.317129629630E+00
6	-0.158156966490E-02	-0.947129349682E-02	0.798717918565E-01	-0.419233764146E+00
8	-0.825212846235E-03	-0.744291529381E-02	0.774790791855E-01	0.270996990417E+00
0	-0.311850649269E-03	-0.437691024484E-02	0.636977861687E-01	-0.389433514875E+00
2	-0.241942079720E-03	-0.360570635434E-02	0.602759642393E-01	
4	-0.151122678477E-03	-0.260100515146E-02	0.558300121347E-01	
pin 1 mode'				
0	-2	1	0	4
2	-0.285714285714E+00	-0.816326530612E-01	0.466472303207E-01	-0.238095238095E+01
4	-0.252298721686E-01	-0.269590990605E-01	0.373146890919E-01	-0.401853664099E+00
6	-0.723812205411E-02	-0.136997515033E-01	0.305409765642E-01	-0.199264281768E+00
8	-0.328119045071E-02	-0.880047084950E-02	0.267818056353E-01	-0.129254232622E+00
0	-0.179344795467E-02	-0.625519624340E-02	0.241638397155E-01	-0.892317430503E-01
2	-0.110240947222E-02	-0.473624235610E-02	0.222072275325E-01	

Weihong, Oitmaa, Hamer

TABLE 2. Series coefficients for the perpendicular susceptibility $\chi_\perp$. Coefficients of x^n are listed for both the spin-½ and spin-1 models.

n	Spin ½	Spin 1
0	1	1
1	-1/3	-0.285714285714E+00
2	0.354166666667E+00	0.289285714286E+00
3	-0.379629629630E+00	-0.299831800852E+00
4	0.383522247942E+00	0.301344414137E+00
5	-0.393158923672E+00	-0.306189718951E+00
6	0.395868009007E+00	0.306873914417E+00
7	-0.402954211929E+00	-0.309864843278E+00
8	0.405315646692E+00	0.310323237180E+00
9	-0.409211981572E+00	-0.312399393569E+00
10	0.411027697321E+00	0.3[illegible]10344E+00
11	-0.414448978063E+00	
12	0.415617280171E+00	
13	-0.418179085518E+00	

Nature of singularity determined by SWT

$$M^+ = S - \int \frac{d^d k}{\omega_k}$$

for small k

$\omega_k \approx ck$ Heisenberg $\alpha = 1$

$= c\sqrt{k^2 + 1 - \alpha^2}$ $\alpha \neq 1$

$\Rightarrow \tilde{S} - \text{const}\sqrt{1-\alpha^2}$

Quite generally expect the power to remain unchanged

Given: $M^+ = A_1 - A_2\sqrt{1-x}$

$= \sum_n c_n x^n$

How do we estimate A_1, A_2

$\Rightarrow$ What is the error if we add N terms?

Expand $(1-x)^{1/2} = 1 - \frac{1}{2}x + \frac{\frac{1}{2}(\frac{1}{2}-1)}{2!}(-x)^2 + \frac{\frac{1}{2}(\frac{1}{2}-1)(\frac{1}{2}-2)}{3!}(-x)^3$

$$c_n = -\frac{1 \cdot 3 \cdots (2n-3)}{2^n\, n!} = \frac{(2n-3)!}{2^{2n-2}\, n!\,(n-2)!}$$

Use Stirling's approximation

$n! \simeq \sqrt{2\pi n}\; n^n e^{-n}$

$c_n \sim \frac{1}{n^{3/2}}$

Partial sum $S_N = \sum_{n=0}^{N} c_n$

Error $\sum_{n=N+1}^{\infty} c_n \sim \sum_{n=N+1}^{\infty} \frac{1}{n^{3/2}} \sim \frac{1}{N^{1/2}}$

Plot S_N vs $1/N^{1/2}$

Quite generally

$$(1-\mu x)^{-\gamma} = \sum_n a_n x^n$$

$$a_n \approx \text{const}\ \mu^n\, n^{\gamma-1}$$

Our case was $\mu = 1$, $\gamma = -1/2$

Error after N terms for $\gamma > 0$

$$\sim \frac{\text{const}}{N^{\gamma}}$$

$$\text{Energy} \sim E_0 + E_1(1-x) + E_2(1-x)^{3/2}$$

S_N ↑ —— $1/N^{3/2}$

What about $\chi_\perp$ [Perpendicular susceptibility]

[$\chi_{11} = 0$: cannot change $S^z = 0$]

$$\mathcal{H} = \mathcal{H}_0 + h\frac{G_x}{2}$$

$$E = E_0 - \tfrac{1}{2}\chi_\perp h^2$$

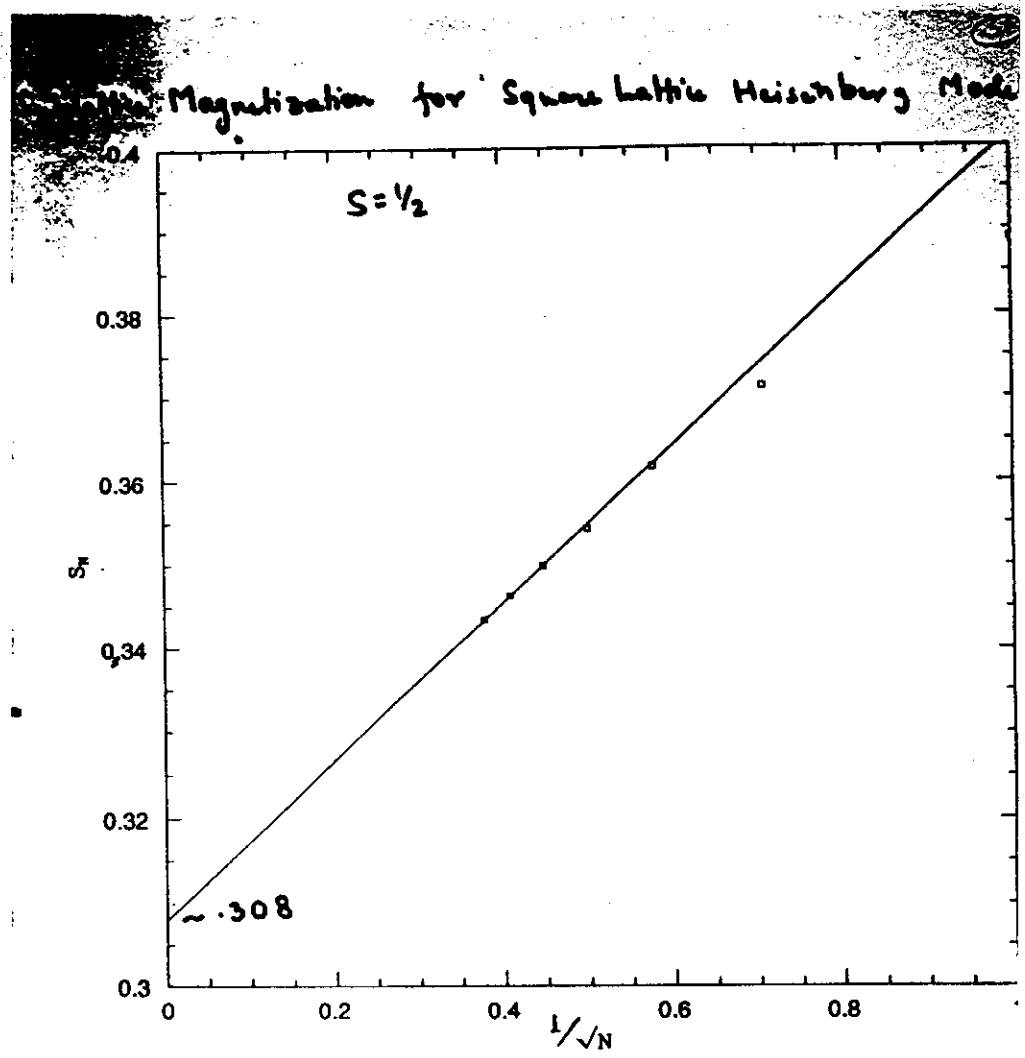
Does not decay, oscillates

$\alpha = -1$ ferromagnetic XY order (divergence $\alpha = -1$)

Singularity moving transformation

[$x = -1 \Rightarrow z = \infty$ for removed!]

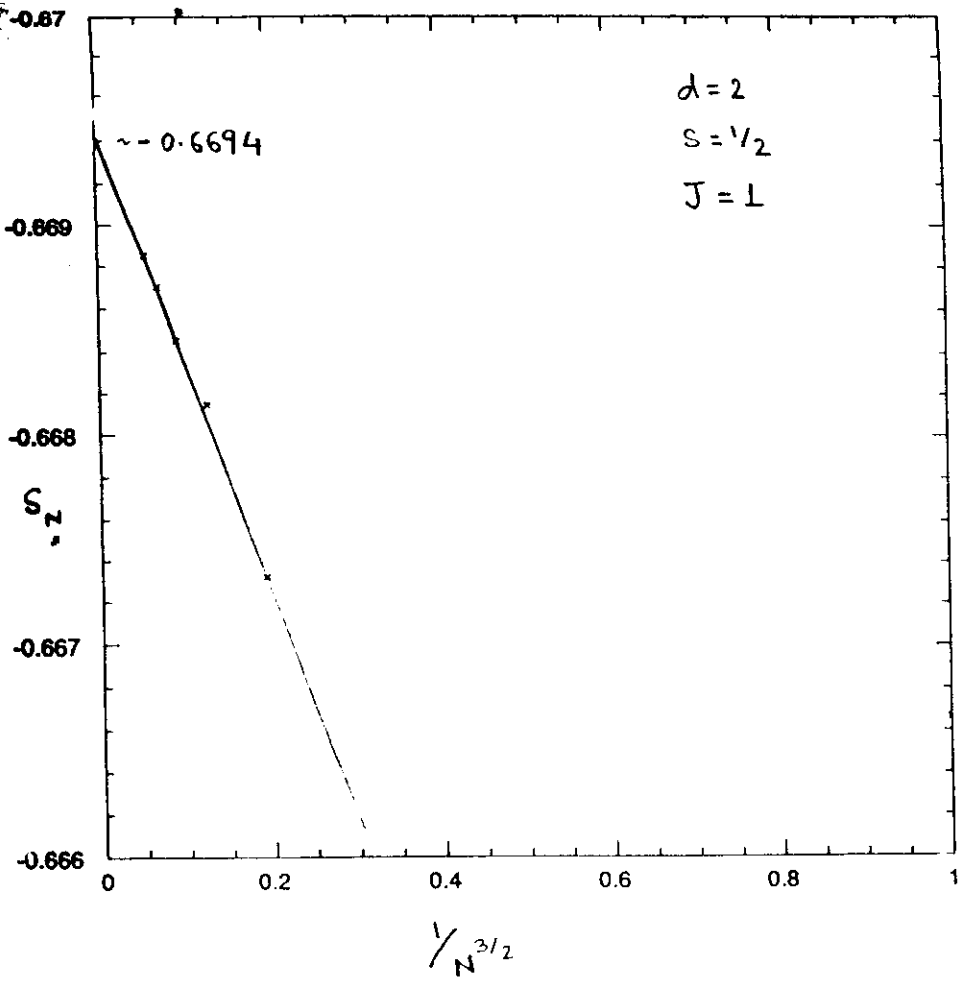
$$z = \frac{2x}{1+x}$$



SWT ($\frac{1}{2}$): $M^+ \sim .303$

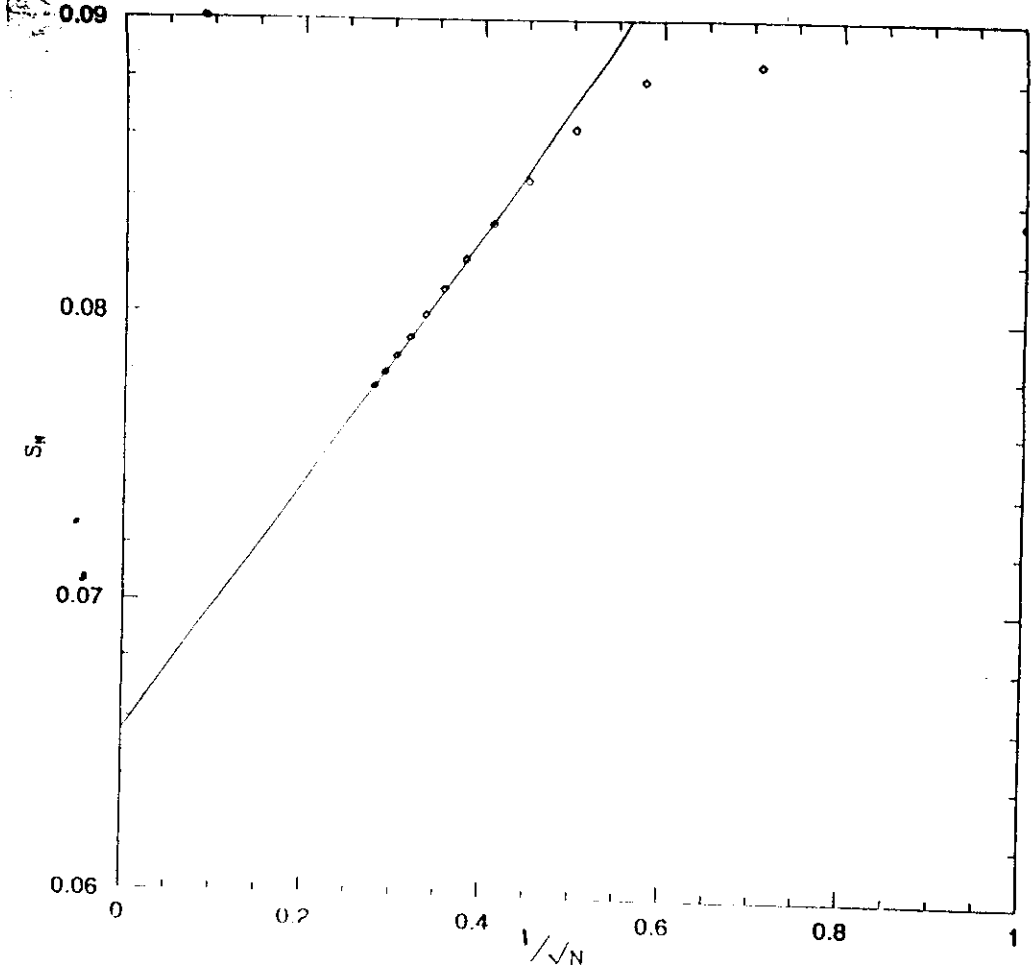
Monte Carlo : Reger and Young

Ground State Energy



$$E \sim A + B(1-x^2) + C(1-x^2)^{3/2}$$

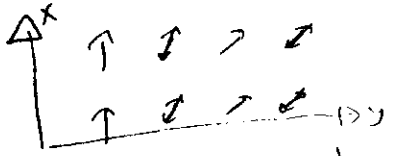
$\chi_\perp$



We have heard from Subir

$\chi_\perp$ measures stiffness in time [NLσ model]

Spatial stiffness
cost in twisting along say Y axis $(a = 1)$



Relative twist θ per in the neighbors

$$E(\theta) = E(\theta=0) + \frac{1}{2}\rho_s \theta^2 \quad \text{defines } \rho_s$$

Classically

$$E(\theta) = -JS^2(1+\cos\theta)$$

$$\rho_s = JS^2$$

Quantum fluctuations will reduce stiffness

How do we impose a twist:
Rotate axis of quantization along Y (by relative angle θ, rotation along Y axis in spin-space)

$$\mathcal{H} = J\sum \vec{S}_i\cdot\vec{S}_j = \frac{J}{4}\sum_i \vec{\sigma}_i\cdot\vec{\sigma}_{i+\hat{x}} + \sigma_i^Y\sigma_{i+\hat{y}}^Y$$
$$+ \sigma_i^x\left[\sigma_{i+\hat{y}}^x\cos\theta + \sigma_{i+\hat{y}}^z\sin\theta\right] + \sigma_i^z\left[-\sigma_{i+\hat{y}}^x\sin\theta + \sigma_{i+\hat{y}}^z\cos\theta\right]$$

Two equivalent Hamiltonian.
Twist imposed on the ground state by choosing
$H_0 + \alpha H_1$ for which σ's order antiferromagnetically,
i.e. spins S_i order with a twist.
We then calculate the energy change perturbatively
to order θ^2 as $\alpha \to 1$.

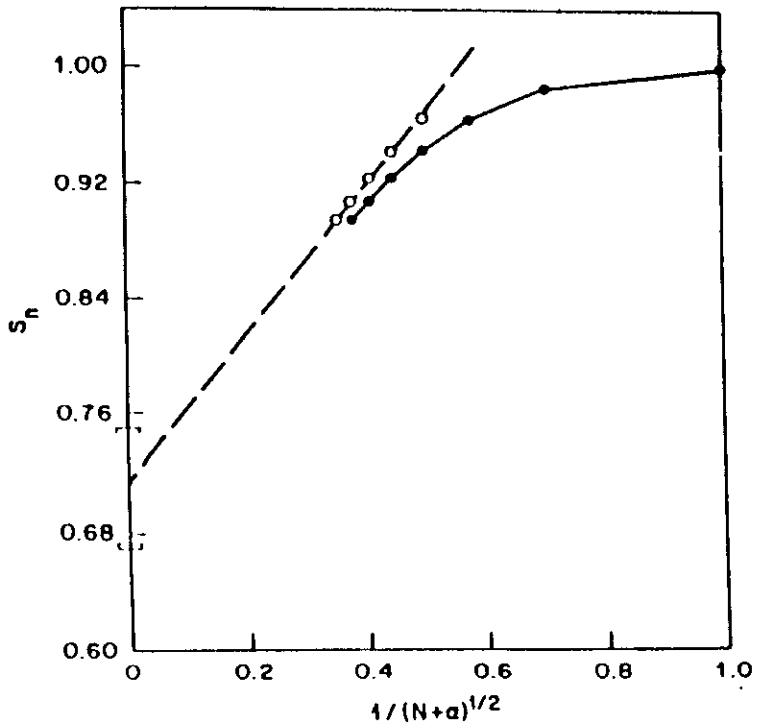
To order θ^2

$$\mathcal{H} = \frac{J}{4}\sum_i \vec{\sigma}_i\cdot\left[\vec{\sigma}_{i+\hat{x}} + \vec{\sigma}_{i+\hat{y}}\right] - \frac{1}{2}\theta^2\sum_i\left[\sigma_i^x\sigma_{i+\hat{y}}^x + \sigma_i^z\sigma_{i+\hat{y}}^z\right]$$
$$+ \theta\sum\left(\sigma_i^x\sigma_{i+\hat{y}}^z - \sigma_i^z\sigma_{i+\hat{y}}^x\right)$$

σ_i^z couplings define H_0 and as $\alpha \to 1$
we get Heisenberg model and the extra
energies can be obtained

ρ_s series can be obtained

From $\chi_\perp$, ρ_s get $c^2 = \frac{\rho_s}{\chi_\perp}$



Schwinger Bosons

$$Z_{\rho_s} = \frac{4\rho_s}{J} = 0.72 \pm 0.04$$

$$Z_\chi = 8\chi_1 J = 0.52 \pm 0.02$$

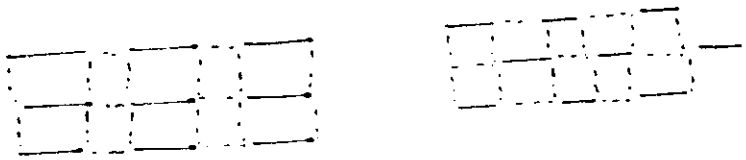
$$Z_{c_s} = c_s/\sqrt{2}J = 1.18 \pm 0.02$$

Thermodynamic Parameters of the Heisenberg Model (Ising Expansion)

Quantity	Extrapolated Estimate	SWT ($O(1/s)$)	Other Estimates
$2M^+$	0.605 ± 0.015	.60	$.60 \pm .04$ [1]
$4E_0/J$	$-2.6785 \pm .0010$		$-2.680 \pm .00$[1] < -2.675 [2]
$Z_\chi = 8\chi_1 J$	$0.52 \pm .02$	.45	.52 [3] $.53 \pm .01$ [4] .75 [5]
$Z_{\rho_s} = 4\rho_s/J$	$0.72 \pm .04$		1.16 [4]
$Z_{c_s} = c_s/\sqrt{2}J$	1.18 ± 0.02	1.16	1.2 [5]

1. Reger and Young
2. Liang, Doucot and Anderson
3. Lines
4. Auerbach and Arovas
5. Gross, Velasco and Siggia

DIMER EXPANSIONS (CLUSTER)



$$H = H_0 + \lambda H_1$$

expand in powers of λ.

For $\lambda = 0$: Ground state is a valence-bond singlet

What happens as λ is increased

Encounter Quantum Phase Transition

$$S(\pi,\pi) = \sum_r (-1)^r \langle \vec{S}_0 \vec{S}_r \rangle$$

$$\xi^2 = \frac{\sum_r (-1)^r r^2 \langle \vec{S}_0 \cdot \vec{S}_r \rangle}{\sum_r (-1)^r \langle \vec{S}_0 \cdot \vec{S}_r \rangle}$$

$$\chi(\pi,\pi) = -\frac{\partial^2 E}{\partial h_a^2}$$

$$S = \sum_n a_n \lambda^n \qquad \xi^2 \sim |\lambda_c - \lambda|^{-2\nu}$$

$$\chi \sim |\lambda_c - \lambda|^{-\gamma}$$

$$S \sim |\lambda_c - \lambda|^{-(\gamma - 2\nu)}$$

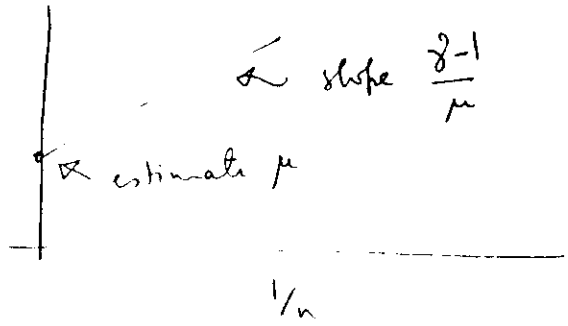
$$(1-\mu x)^{-\gamma} \to \sum_n a_n x^n$$

$$a_n \to n^{\gamma-1} \mu^n$$

then the ratio

$$r_n \equiv \frac{a_{n+1}}{a_n} \to \mu \left[\frac{n+1}{n}\right]^{\gamma-1}$$

$$\sim \mu \left[1 + \frac{\gamma-1}{n} + O\left(\frac{1}{n^2}\right)\right]$$



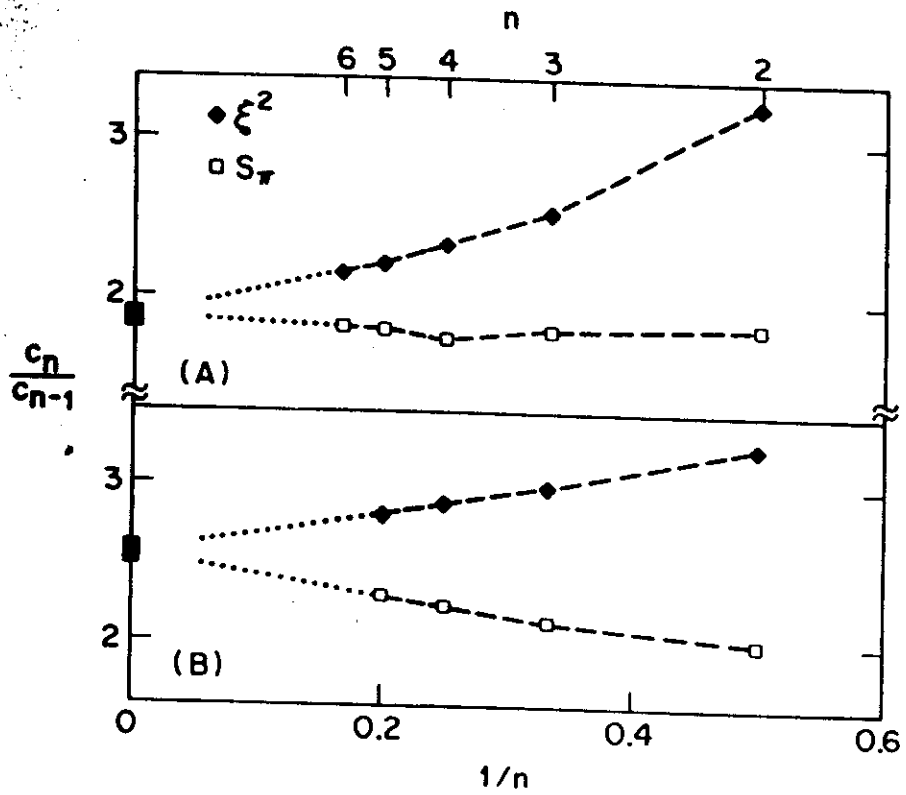
Not accurate to determine exponents to high accuracy. Consistent with 3d Heisenberg

(A) $2\nu = 1.7 \pm 0.3$, $\gamma = 1.7 \pm 0.3$, $\gamma_0 - 2\nu = 0.8 \pm 0.2$

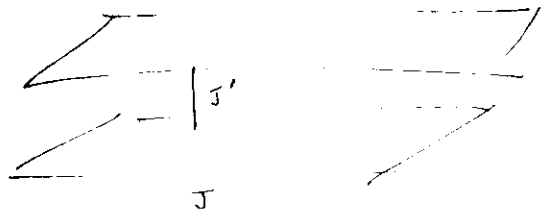
(B) $2\nu = 1.5 \pm 0.4$, $\gamma = 1.3 \pm 0.3$, $\gamma - 2\nu = 0.5 \pm 0.2$

3DCHM

$\nu \approx 0.7$, $\gamma \approx 1.4$, $z = 1$



Dimer-Expansions by Hida



Two coupled planes.

$J' >> J$

Ground state is $\perp$ dimers

[ ] [ ] [ ]

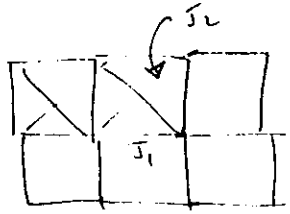
Expand in J/J'

$\Rightarrow$ critical point at $\frac{J}{J'} \sim \frac{1}{2 \cdot 5}$

critical on $S_{\pi,\pi}$, $\chi_{\pi,\pi}$, $\xi^2_{\pi,\pi}$ } exponents consistent with 3D c HM

[Quantum critical behavior at finite T]

$J_1 - J_2$ model



Study by Diner expansions

Calculate $S(\vec{q})$

Classically (π, π) ⟶ $(\pi, 0)$

Order by disorder

↑↓
↓↑

↑ ↗ ↕ ↗
↙ ↓ ↙ ↕
classically free

↑ ↑ ↑ ↑ Quantum
↓ ↓ ↓ ↓ selection

Intermediate phase evidence for spontaneous dimerization (Read + Sachdev)
Berry phase

= || = ||
= || = ||

= || = ||
|| = || =

different starting configuration (Gelfand)
Diner susceptibility.

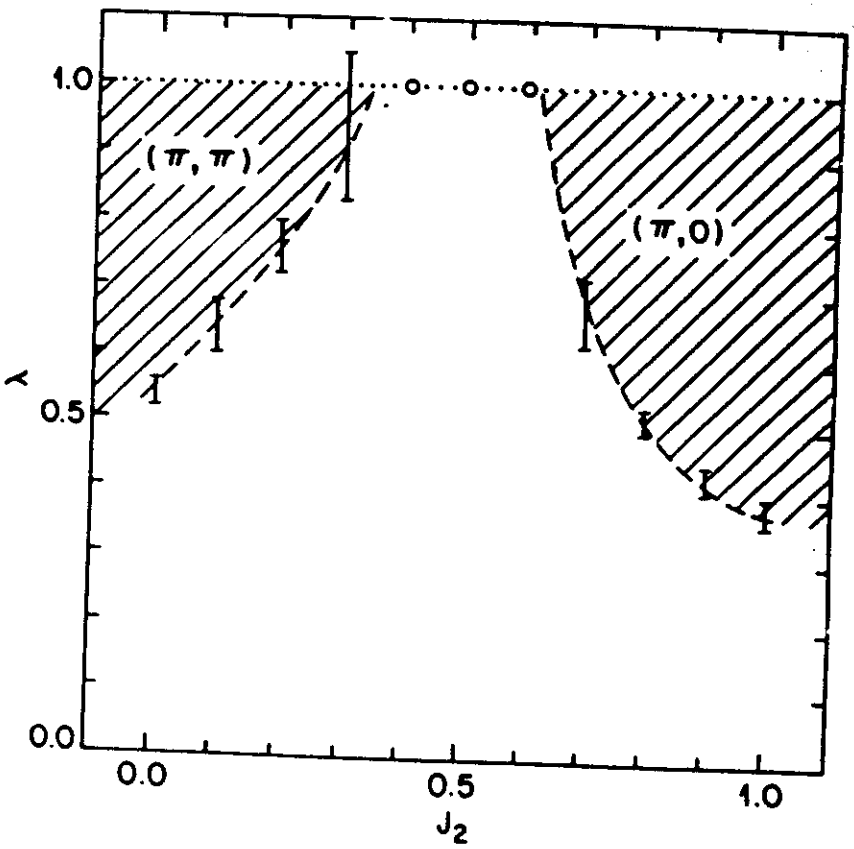
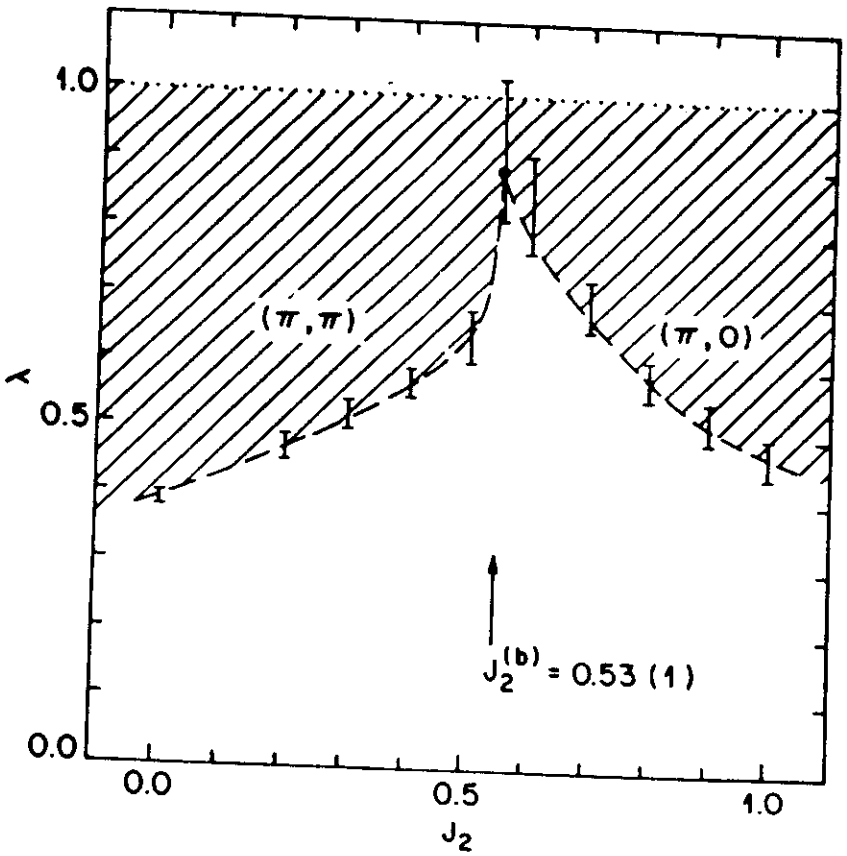


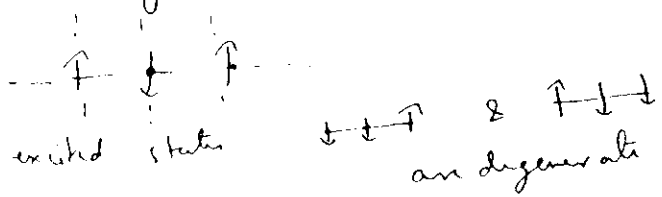
Fig. 2



Can we use our cluster expansion technique to calculate excited states perturbatively

Need to introduce $\vec{k}$? $S(k,\omega)$

Degenerate perturbation theory



More and more degeneracies have to be broken in higher orders!

We can calculate the dispersion $\omega(k)$ (estimate) in the SMA (single mode approximation)

$$S(k,\omega) = A\,\delta(\omega-\omega_k)$$

$|\Psi_g\rangle \Rightarrow$ the ground state

Variational ansatz for excited state at $\vec{k}$

$$|k\rangle = S_k^+ |\Psi_g\rangle$$

then

$$\omega(k) = \frac{\langle k|H|k\rangle}{\langle k|k\rangle} - E_g$$

$$= \frac{\langle\Psi_g|S_{-k}^- H S_k^+|\Psi_g\rangle}{\langle\Psi_g|S_{-k}^- S_k^+|\Psi_g\rangle} - \frac{\langle\Psi_g|H S_{-k}^- S_k^+|\Psi_g\rangle}{\langle\Psi_g|S_{-k}^- S_k^+|\Psi_g\rangle}$$

$$= \frac{\langle \psi_g | [S^-_{-k}, \mathcal{H}] S^+_k | \psi_g \rangle}{\langle \psi_g | S^-_{-k} S^+_k | \psi_g \rangle}$$

$$\omega(k) = \frac{\tilde{\epsilon}(k)}{S(k)}$$

$$\tilde{\epsilon}(k) = -2J(1-\gamma_k)\langle S_i^x S_j^x + S_i^y S_j^y + 2 S_i^z S_j^z \rangle$$

$$\gamma_k = \frac{1}{2}[\cos k_x + \cos k_y]$$

- $\Rightarrow$ SMA leads to linear modes near
  - $k = (0,0)$ and (π, π)

$S(k) \sim A k$ as $k \to 0$ [Singlet]
also true in SWT

$\epsilon(k) \sim k^2$

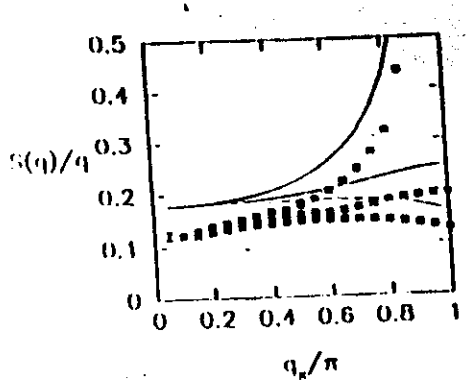
$\omega(k) \sim c_1 k$

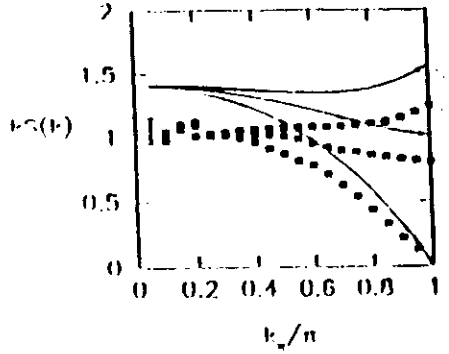
near $k = (\pi, \pi)$ $\quad q = k - (\pi, \pi)$

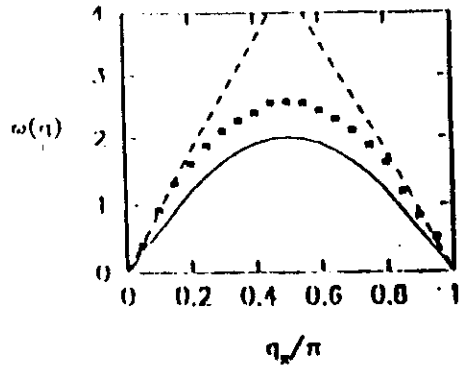
$\epsilon(q) \sim$ const

$S(q) \sim \frac{B}{q}$

$\omega(k) \sim c_1 k$

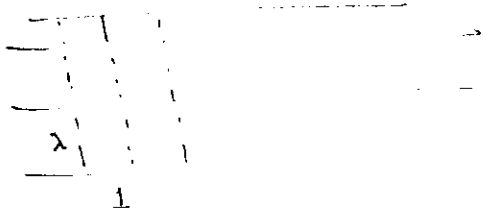






Affleck + Gelfand + RRP's

Weakly coupled $S = 1/2$ chain



Ising / Dimer expansions

Mean field arguments : always ordered

Spin-wave " : disordered for small λ

$$S - \int \frac{d^2k}{\omega_k}$$ when 2nd term equals S (Parola et. al.)

Within NLσ model (Fantoni) what is

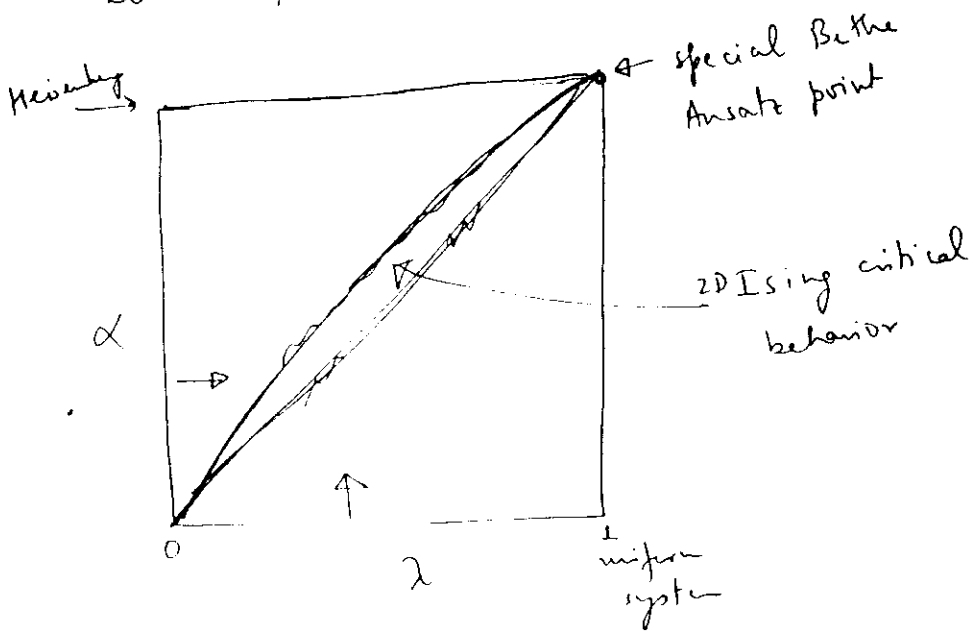
Evidence suggests it remains ordered

$\lambda_c < 0.3$

$d = 1$ $S = 1/2$

What can we get.

Both expansions converge upto $\lambda = 1$ $\alpha = 1$



Energy etc. estimated

$$\langle S_0 S_r \rangle \sim \frac{(-1)^r}{r} (\log r)^{1/2}$$ ⟸ can be seen numerically

staggered structure factor

$$\sum_r (-1)^r \langle S_0^+ S_r^- \rangle \sim \int^{\xi} \frac{1}{r} (\log r)^{\lambda}$$

$$\xi \sim e^{\frac{1}{\sqrt{t}}} \Rightarrow t^{\frac{1+\lambda}{2}}$$

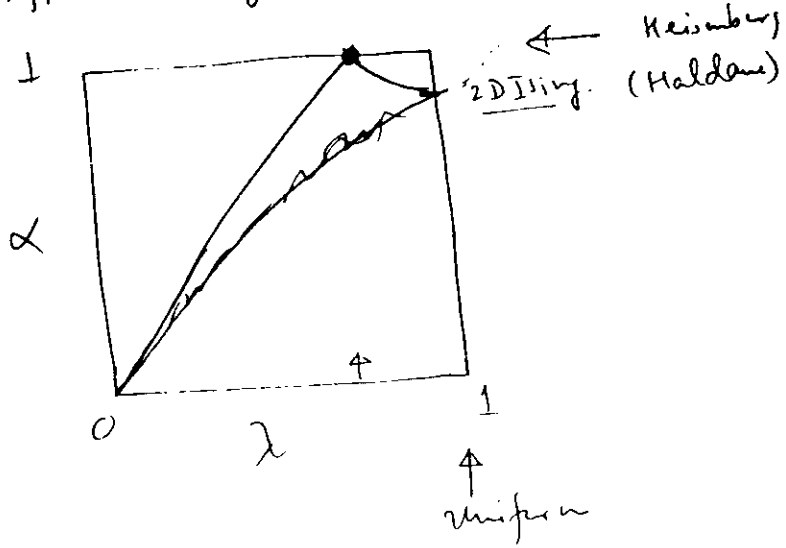
$t = 1 - \alpha$

sensitive to logarithms

Shankar, Affleck et. al.

Spin-one

Difficult to get to Haldane phase



Special point for $\alpha = 1$

Same universality class as $S = 1/2$ Bethe ansatz model

θ term irrational for dimerization

$\Rightarrow$ special value it scales to π (for spin-one)

Haldane phase remains inaccesible

One can also expand around $D S_i^{z\,2}$ 00000

still inaccessible. Special type order

Disordered flat

Triangle/Kagome magnets

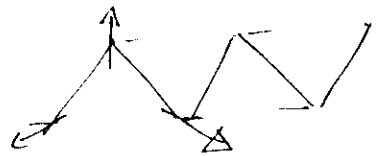
$$\mathcal{H} = 4 \sum S_i \cdot S_j$$

$$\mathcal{H}' = \mathcal{H}_0 + J_\perp (\mathcal{H} - \mathcal{H}_0)$$

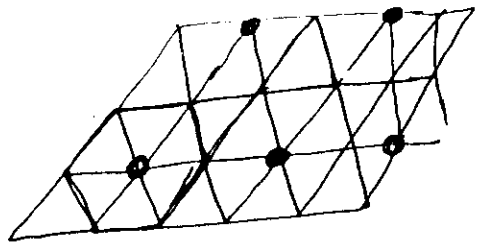
rotating axis of quantization of 3 sublattices to point at 120°

$$\mathcal{H} = \sum_{i \to} \left[-\frac{1}{2} \left[\sigma_i^z \sigma_j^z + \sigma_i^x \sigma_j^x \right] + \frac{\sqrt{3}}{2} \left[\sigma_i^z \sigma_j^x - \sigma_i^x \sigma_j^z \right) + \sigma_i^y \sigma_j^y \right]$$

$A \to B$ $\quad B \to C$ $\quad C \to A$



Kagome



Kagome is disordered

~~Heisenberg~~ Triangular is weakly ordered (may be disordered)

Hubbard Model (t-J model)

Ising expansion at half filling

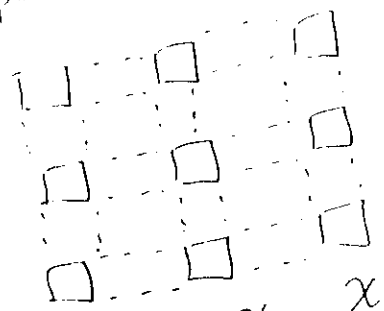
$$H = U \sum_i n_{i\uparrow} n_{i\downarrow} \pm \lambda t \sum (c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.})$$
$$+ \underbrace{J_z (1-\lambda) \sum_i S^z_i S^z_j}_{\text{breaks symmetry}}$$

expand in λ to get $\langle n_{i\uparrow} n_{i\downarrow} \rangle$, E_g, etc.

also M^+ starts to break down when $U \lesssim t$

Away from half filling $\frac{1}{4}$ filling

expand around squares



Can calculate $\chi_{\cdots}$, χ_{sc} etc

Ground States of Low-Dimensional Quantum Antiferromagnets

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We have developed a general scheme for carrying out systematic perturbation expansions for ground-state properties of quantum lattice models. As an application, we study the onset of spontaneous Néel order in $S=\frac{1}{2}$ Heisenberg antiferromagnets by expanding around dimerized Hamiltonians. In one dimension (1D) we recover accurately the known exact results. On the square lattice we find novel critical points separating Néel ordered and disordered phases; the estimated critical exponents are consistent with those of the 3D classical Heisenberg model.

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The zero-temperature properties of quantum many-body systems and the location and character of ground-state instabilities (critical points) under changes of parameters in the Hamiltonian represent fundamental problems in condensed matter theory. Unlike classical statistical mechanics, where our understanding of critical phenomena and phase transitions is quite extensive, there have been few concrete developments in quantum criticality.[1] A notable exception is the case of one-dimensional systems.[2] Recent experimental[3] and theoretical[4] advances in high-temperature superconductivity have led to a resurgence of interest in some of these problems, in particular, to the question of long-range order in 2D Heisenberg antiferromagnets. We discuss here a general calculational scheme that addresses the topic of zero-temperature quantum criticality, and apply it to low-dimensional Heisenberg antiferromagnets. For 1D, we recover accurately the known exact results for alternating spin chains. In 2D we find that introducing bond alternation in the square lattice Heisenberg antiferromagnet leads to novel quantum critical points. These critical points, which separate Néel ordered and disordered phases, have critical exponents consistent with those of the 3D classical Heisenberg model, given proper interpretation of the 2D-3D correspondence.

The basic idea behind our work is that there are well defined phases in the parameter space of quantum Hamiltonians. Within a given phase the ground-state properties of one Hamiltonian can be accessed from that of another by adiabatic continuation, i.e., by following the evolution of the ground state under continuous variation in parameters. Adiabatic continuity of the ground state breaks down at phase boundaries, where singularities or crossings of energy levels occur. In order to implement this idea of adiabatic continuation in a concrete manner and investigate these quantum phase transitions, we shall borrow tools and techniques from classical critical phenomena, namely, series expansions and analysis.

We consider, specifically, spin-$\frac{1}{2}$ Heisenberg models on the linear chain and the square lattice with nearest-neighbor antiferromagnetic exchange J. Let us partition the infinite lattice into nearest-neighbor dimers and let H_0 be the part of the Hamiltonian containing the exchanges within dimers, while H_1 contains the remainder of the exchanges. We then consider the one-parameter family of models with Hamiltonian $H=H_0+\lambda H_1$. For $\lambda=0$ the spectrum of $H=H_0$ is trivial, the ground state is a product of singlets for each dimer and the energy gap to the lowest excited states is J. Turning on λ then couples the dimers; the full symmetries of the lattice are restored at $\lambda=1$. Note that we have chosen H_0 to be dimers primarily because this appears to be the simplest way to have a trivially diagonalizable system with a disordered ground state while maintaining rotational invariance in spin space. Our purpose is not primarily to study dimerized models *per se*, but rather to illustrate what are presumably more general properties of Heisenberg models.

We perform the adiabatic continuation *via* a high-order perturbation calculation in powers of λ, which is analyzed by means of standard series extrapolation methods developed for critical phenomena.[5] Since the ground state and the perturbation H_1 are both rotationally invariant in spin space, that symmetry cannot be broken in any order of the perturbation theory: One remains in the total-spin-zero subspace, with no sublattice magnetization. However, the symmetry can be spontaneously broken at some critical point, λ_c, where the perturbation expansion diverges. One cannot adiabatically continue past such a critical point to higher values of λ.[6] For the linear chain $\lambda_c=1$, while for the square lattice we find $0<\lambda_c<1$.

We obtain expansions in λ for the ground-state energy per site, E_0, the equal-time, antiferromagnetic (AF) structure factor, S_π (in 2D this is actually $S_{\pi,\pi}$), the correlation length, ξ, and the AF susceptibility, χ_π

defined by

$$H\Psi_0 = NE_0\Psi_0,$$
$$S_\pi = \frac{1}{N}\sum_{i,j}\epsilon_{ij}\langle\Psi_0|\mathbf{S}_i\cdot\mathbf{S}_j|\Psi_0\rangle/\langle\Psi_0|\Psi_0\rangle, \quad (1)$$
$$S_\pi\xi^2 = \frac{1}{N}\sum_{i,j}\epsilon_{ij}r_{ij}^2\langle\Psi_0|\mathbf{S}_i\cdot\mathbf{S}_j|\Psi_0\rangle/\langle\Psi_0|\Psi_0\rangle,$$
$$\chi_\pi = -\frac{\partial^2}{\partial(h^+)^2}E_0(h^+),$$

in the $N\to\infty$ limit, where N is the number of spins. Note that H, Ψ_0, E_0, S_π, χ_π, and ξ all implicitly depend on λ. Here h^+ is a staggered field, ϵ_{ij} is 1 if sites i and j lie on the same sublattice and -1 otherwise, while r_{ij} is the distance between i and j.

We have developed a general technique for carrying out systematic, high-order perturbation expansions for lattice-based quantum many-body systems. At $T=0$, these expansions require a perturbative diagonalization of infinite-dimensional matrices. Following the strategy of classical cluster methods,[7] we reduce the expansion for the infinite system to a sum of terms each of which involves only a finite cluster and hence a finite-dimensional Hilbert space. For a given cluster, one constructs the matrices for H_0 and H_1 in a basis in which H_0 is diagonal. Expressions for the ground-state energy and wave function are obtained through elementary recursion relations, and the wave function is then used to evaluate expansions for ground-state expectation values. The method is systematic enough that it can be carried out entirely on the computer. It is also general enough to study any quantum lattice model around a point where there is a gap in the spectrum[8] and the eigenstates are infinite direct products over states, each involving only a finite set of points in real or reciprocal space. Practical limitations are forced by considerations of computer storage and time. Recently, we have used these methods to generate expansions for the AF Heisenberg-Ising $S=\frac{1}{2}$ chain[9] to order $(J_{xy}/J_z)^{22}$ and a variety of expansions for the $S=1$ chain.[10] Application to Hubbard models is currently under consideration. Details of the method will be given elsewhere.

For the 1D linear chain there is only one type of nearest-neighbor dimerized configuration, and the problem reduces to the alternating spin chain.[11] The expansions have been developed to order λ^{15} for E_0 and to order λ^7 for S_π, ξ^2, and χ_π. Unbiased analysis of the energy series by inhomogeneous differential approximants[5] shows a critical point at $\lambda_c = 1.001 \pm 0.002$. Since the critical point is known to be exactly at $\lambda_c = 1$, a biased analysis helps in accurately determining various properties of the Heisenberg chain. We estimate the ground-state energy to be $E_0 = -0.443\,14 \pm 0.000\,01$ (the exact result being $\simeq -0.443\,147$). We estimate that S_π diverges with an exponent $\lambda_s = 0.05 \pm 0.15$, χ_π diverges with an exponent $\gamma = 0.79 \pm 0.05$, and ξ diverges with an exponent $\nu = 0.66 \pm 0.02$, which compare well with the conjectured exact answers of $O(\log)$, $\frac{2}{3}$ and $\frac{2}{3}$, respectively.[12] The details of the analysis will be presented elsewhere.[13]

For the square lattice there are infinitely many dimer configurations which can be used to specify H_0. A random dimerization would introduce quenched disorder into H, and so we consider only regular (periodic) dimerizations. One expects that the universal properties of the model, such as the topology of the phase diagram and the critical exponents, should not depend on the specific regular dimerization chosen. We have used two such dimer configurations as starting points for the expansions, namely, (A) and (B), shown in Fig. 1. Note that we have chosen (A) and (B) because they are the simplest cases, not because they have any particular physical significance (although they could be viewed as models of lattice distortions). The expansion coefficients, c_n, for E_0, S_π, χ_π, and ξ^2 are given in Table I; the expansions have been performed to orders 6 and 5, respectively. The energy series are ill behaved and are not used in the extrapolations reported here. The ratio of successive terms in the series for S_π, ξ^2, and χ_π are plotted versus $1/n$ in Fig. 2. These ratio plots[5,13] indicate critical points at $\lambda_c = 0.54 \pm 0.02$ for (A) and at $\lambda_c = 0.39 \pm 0.01$ for (B). [Note that (A) and (B) are distinct dimerizations and need not have the same λ_c.] The divergences of χ_π, S_π, and ξ^2 suggest strongly that the ground states are unstable towards Néel ordering beyond these points: Néel order for the uniform square lattice ($\lambda = 1$) has been found by many authors.[14-17]

Let us now consider the criticality at λ_c. Based on the symmetries of the problem at long wavelengths, Chakravarty, Halperin, and Nelson[17] have argued that criticality in the 2D quantum Heisenberg models at $T=0$ should lie in the universality class of the 3D classical Heisenberg model,[18] which has critical exponents for variation in temperature given by $\gamma = 1.40 \pm 0.02$ and $2\nu = 1.42 \pm 0.04$.[19] This correspondence implies that the critical point should be "Lorentz invariant"; i.e., the critical exponents for correlations in the spatial and temporal directions should be equal. Quite generally one can

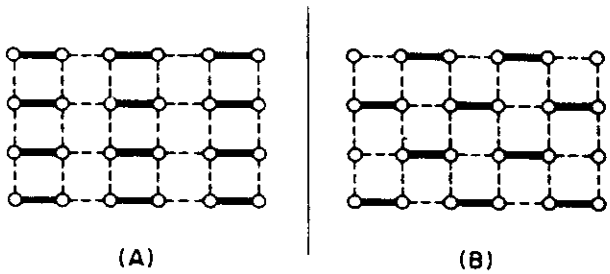

FIG. 1. Dimer configurations (A) and (B). The solid bonds represent the terms in H_0, while the dashed bonds represent the terms in H_1.

(57)

TABLE I. Expansion coefficients, c_n, for E_0, S_π, ξ^2, and χ_π as power series in λ, on the square lattice for dimer configurations (A) and (B).

	(A)				(B)			
n	$8E_0$	$4S_\pi$	ξ^2	χ_π	$8E_0$	$4S_\pi$	ξ^2	χ_π
0	−3	6	0.5	1	−3	6	0.5	1
1	0	9	3	3	0	9	4	3
2	−1.875	16.5	9.75	7.375	−1.125	18	13	8.625
3	−0.84375	29.625	25.042	17.063	−0.84375	38.313	38.833	23.937
4	−0.33789	51.751	58.969	37.402	−0.75586	85.783	111.90	65.171
5	0.24333	93.256	131.82	79.690	−0.76383	198.34	314.20	175.24
6	0.24172	168.77	284.65	165.96				

define a dynamic exponent z for the quantum problem by requiring that the gap, Δ, which gives the inverse correlation length in the time direction, vanish as $\Delta \sim \xi^{-z}$ as $\lambda \to \lambda_c$. Thus $z=1$ corresponds to Lorentz-invariant criticality.

We can estimate the exponents γ, ν, and γ_s in the present problem and obtain z through a simple scaling relation. The AF susceptibility, χ_π, is related to the frequency-dependent AF structure factor, $S_\pi(\omega)$, via[20] $\chi_\pi \sim \int d\omega S_\pi(\omega)/\omega$, while the equal-time structure factor $S_\pi \sim \int d\omega S_\pi(\omega)$. Thus by scaling one expects near criticality $S_\pi \sim \Delta \chi_\pi$; this yields the exponent relation $\gamma_s = \gamma - z\nu$. Dlog Padé analyses and ratio tests indicate that $2\nu = 1.7 \pm 0.3$, $\gamma_s = 0.8 \pm 0.2$, and $\gamma = 1.7 \pm 0.3$ for (A), and that $2\nu = 1.5 \pm 0.4$, $\gamma_s = 0.5 \pm 0.2$, and $\gamma = 1.3 \pm 0.3$ for (B). Furthermore, by scaling we get $z = 1.0 \pm 0.4$ for both (A) and (B). Thus, our results are consistent with a criticality that is Lorentz invariant, and

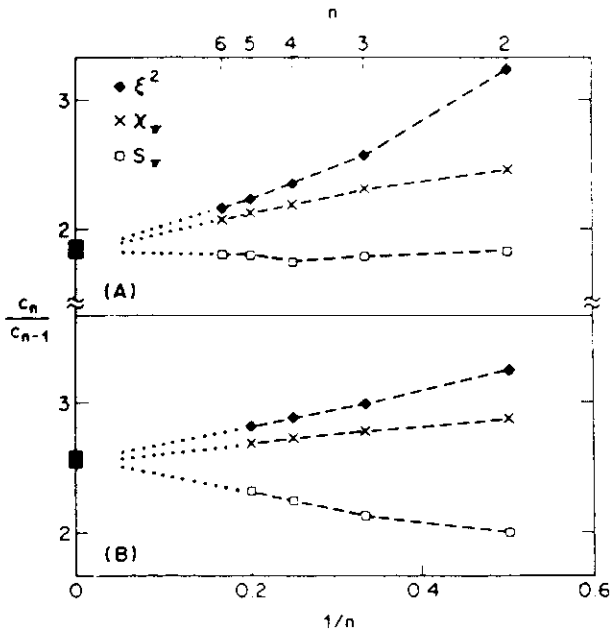

FIG. 2. Ratios of expansion coefficients for S_π, χ_π, and ξ^2 plotted vs $1/n$ for cases (A) and (B). The estimated values of $1/\lambda_c$ are indicated on the vertical axis.

furthermore, in the universality class of the 3D classical Heisenberg model (with . playing the role of inverse temperature). For $\lambda > .$ we thus expect long-range Néel order in the ground state.

Direct evidence for Néel ordering for $\lambda > \lambda_c$ can be obtained by expanding the sublattice magnetization $m^\dagger$ around the Ising limit ($J_{xy}=0$) for general values of λ, as is done for $\lambda = 1$ in Ref. 14. This gives

$$m^\dagger = \frac{1}{2} - \frac{J_{xy}^2}{36\lambda^2 J_z^2}\left(\frac{27\lambda^4+4\lambda^2+4\lambda+1}{4\lambda^2+4\lambda+1}\right) + O\left(\left[\frac{J_{xy}}{J_z}\right]^4\right). \quad (2)$$

Notice that to the displayed order, $m^\dagger$ is the same for cases (A) and (B)—the difference arises in the next order. The leading two terms give a reasonable estimate of $m^\dagger$ at $\lambda = 1$ and $J_{xy} = J_z$ if we remove the expected spin-wave singularity by changing to a new variable δ defined by[14] $[1-(J_{xy}/J_z)^2]^{1/2} = 1-\delta$. After the change of variable, one finds

$$m^\dagger = \frac{1}{2} - \frac{\delta}{18\lambda^2}\left(\frac{27\lambda^4+4\lambda^2+4\lambda+1}{4\lambda^2+4\lambda+1}\right) + O(\delta^2). \quad (3)$$

For $\lambda \to 0$, the coefficient of δ diverges; this is expected because disconnected Ising dimers are always disordered. We can estimate λ_c at $\delta = 1$ by setting $m^\dagger = 0$ in (3), which gives $\lambda_c \simeq 0.36$, a value not far from the critical points estimated earlier. This further strengthens the case that the observed critical points separate the Néel ordered and disordered phases.

To conclude, we have developed a general technique to carry out high-order perturbation expansions in quantum spin systems and applied it to the $S = \frac{1}{2}$ Heisenberg antiferromagnet on the linear chain and square lattice. The method accurately reproduces the ground-state properties of the alternating spin chain. For the square-lattice Heisenberg antiferromagnets we have found novel quantum critical points as a function of dimerization. These critical points appear Lorentz invariant, and their critical exponents are consistent with those of the 3D

(58)

classical Heisenberg model.

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Three-Sublattice Order in Triangular- and Kagomé-Lattice Spin-Half Antiferromagnets

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We study the possibility of $\sqrt{3}\times\sqrt{3}$ antiferromagnetic order in the $S=\frac{1}{2}$ triangular- and Kagomé-lattice Heisenberg models. An Ising-like anisotropy is introduced into the Hamiltonian, which picks a pair of ground states out of the manifold of the classically ordered states. To study properties of the Heisenberg model, we develop series expansions around one ordered state. We find that the Kagomé-lattice model is disordered whereas the triangular-lattice model is very close to the critical point for antiferromagnetism; if ordered, the latter has an order parameter much smaller than that predicted by spin-wave theory.

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The magnetic properties of two-dimensional frustrated quantum-spin Hamiltonians have been of considerable interest for a long time. Early work goes back to Anderson and co-workers [1], who proposed that the ground state of the spin-half triangular antiferromagnet should have no long-range order. They proposed a special type of ground state due to strong quantum fluctuations which was called a resonating valence bond state. Several numerical studies including exact diagonalizations [2] were interpreted in favor of this picture. Another notable work is the proposed mapping by Kalmeyer and Laughlin [3] between the triangular-lattice Heisenberg model and a two-dimensional electron gas in a strong magnetic field. On that basis they suggested a disordered ground state with an excitation gap. Huse and Elser [4] carried out a variational wave-function study of the triangular antiferromagnet. They found that they could construct wave functions which had energy substantially lower than that of Kalmeyer and Laughlin. Within their variational scheme the ground-state energy was minimized by a wave function that had a large (about 68% of the classical value) antiferromagnetic order parameter.

One technique for studying magnetic order in the presence of quantum fluctuations is the spin-wave or large-S expansion [5]. Recent numerical studies [6] of the square-lattice Heisenberg model found that the spin-wave expansion was quantitatively accurate even for $S=\frac{1}{2}$. For example, the estimated sublattice magnetization and spin-wave velocity agree with the spin-wave answer truncated at order $1/S$ [7]. Such $1/S$ expansions have also been developed [8] for the triangular lattice, and predict an order parameter about 48% of the classical value.

Another approach that has provided a lot of insight into the magnetically ordered and disordered phases of these systems is the large-N expansion of Read and Sachdev [9]. For the square lattice, they predicted the existence of Néel and dimer ordered phases. Numerical evidence for such phases was also obtained by series expansions [10] and by exact diagonalization studies [11]. For the triangular and Kagomé lattices, where the classical order is noncollinear, these large-N expansions predict a nondimerized quantum disordered ("spin liquid") phase for sufficiently small S. However, this theory cannot predict accurately the value of the spin where the transition from magnetic order to disorder takes place.

The Kagomé-lattice antiferromagnet has generated tremendous interest lately from both an experimental [12,13] and a theoretical point of view [14–18]. A simple way to visualize the Kagomé lattice is to regard the triangular lattice as consisting of four sublattices and remove the spins on one of the sublattices. As shown, e.g., by Broholm *et al.* [12], the classical ground state is highly degenerate in this case, with nonzero entropy of the degeneracy per spin. However, the entropy of classical zero-point fluctuations gives different relative Boltzmann weights to the various ground states such that the classical Heisenberg model on the Kagomé lattice apparently has true long-range antiferromagnetic order in the limit of vanishing temperature [18]. Thus the question naturally arises as to whether this order survives the strong quantum fluctuations of the spin-half system. The spin correlations found in exact ground states of small clusters suggest that the spin-half system does not have magnetic order [19], but a more systematic approach to address this question is clearly called for.

In this Letter we study the spin-half models by series-expansion methods. We introduce an Ising-type anisotropy, which allows us to develop systematic series expansions for the ground-state properties. The series are extrapolated by standard methods. The results of the extrapolations indicate that the Kagomé antiferromagnet is not antiferromagnetically ordered. Thus this system may well have a true spin-liquid ground state. For the triangular antiferromagnet, on the other hand, we can only conclude that it is very close to its critical point. If long-range ordered, it has an order parameter much smaller than given by spin-wave theory; if disordered it has a large correlation length. Given the length of our series we cannot resolve whether or not it is ordered. However, we do obtain a significantly improved estimate of the

60

ground-state energy.

The spin-half Heisenberg models are defined by the Hamiltonian

$$\mathcal{H} = 4 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j , \tag{1}$$

where the sum is over all nearest-neighbor pairs of spins. In order to develop Ising-type expansions around a classical ground state, which is noncollinear, we need to introduce an anisotropy parameter in the Hamiltonian that selects a pair of ground states out of the classical ordered states. For the triangular lattice and for the Kagomé lattice, this corresponds to the three-sublattice 120° order (also called $\sqrt{3} \times \sqrt{3}$ order). Let us choose a ground state with the spins on the A sublattice pointing along the z axis, and the spins on the B and C sublattices rotated 120° either way in the x-z plane from the z axis. We choose new variables $\sigma_i = 2\mathbf{S}_i$ on A, $2R_+\mathbf{S}_i$ on B, and $2R_-\mathbf{S}_i$ on C, where the operator $R_\pm$ is a rotation around the y axis by $\pm 120°$. In these new variables our reference classical ground state has all the σ_i pointing along the z axis (ferromagnetic order). The transformed Hamiltonian is

$$\mathcal{H} = \sum_{i \to j} \left[-\frac{1}{2}(\sigma_i^z \sigma_j^z + \sigma_i^x \sigma_j^x) + \frac{\sqrt{3}}{2}(\sigma_i^z \sigma_j^x - \sigma_i^x \sigma_j^z) + \sigma_i^y \sigma_j^y \right] . \tag{2}$$

Here $i \to j$ goes from sublattice A to B, B to C, and C to A. Taking as the unperturbed Hamiltonian

$$\mathcal{H}_0 = -\tfrac{1}{2} \sum_{i \to j} \sigma_i^z \sigma_j^z , \tag{3}$$

and writing the full Hamiltonian as

$$\mathcal{H}' = \mathcal{H}_0 + J_\perp (\mathcal{H} - \mathcal{H}_0) , \tag{4}$$

we can generate power-series expansions in the variable $J_\perp$. The Heisenberg antiferromagnet corresponds to $J_\perp = 1$.

We generate the expansions by the cluster method [20,21]. As in a low-temperature expansion, we define our clusters as sets of sites. A cluster of N sites only contributes in Nth or higher order. To calculate the contribution of a given cluster, we include all terms in the Hamiltonian which flip spins only in the cluster. All clusters which are related to each other by a symmetry of the lattice can be grouped together; because of the directionality of the bonds in (2) we cannot group clusters together by their topology. For the triangular lattice we find 182 510 clusters in eleventh order. For the Kagomé lattice we consider the decomposition of the triangular lattice into four sublattices and keep only the clusters which do not fall on all four sublattices. The lattice constants of the clusters for the Kagomé lattice can be obtained from the triangular ones. Straight, linear clusters have their lattice constant reduced to $\frac{1}{3}$ of the triangular value while all other permitted clusters have it reduced t $\frac{1}{2}$. In twelfth order we find only 26 079 clusters for th Kagomé lattice. This allows us to carry out the expan sions for the Kagomé lattice to higher order than for th triangular case [22]. Let us define the order paramete M and the structure factor S by the relations

$$M = \langle \sigma_0^z \rangle , \quad S = \sum_i (\langle \sigma_0^z \sigma_i^z \rangle - \langle \sigma_0^z \rangle \langle \sigma_i^z \rangle) , \tag{5}$$

where the brackets denote ground-state expectatio values. The expansion coefficients are presented in Tabl I.

We first consider the extrapolation of the order parameter series assuming long-range order at th Heisenberg point. In this case, there will be a square-roo singularity at $J_\perp = 1$. If there were no other singularitie in the complex plane within the unit circle, the partia sum of the first n terms in the series should asymptotically converge as $1/\sqrt{n}$, allowing for a systematic estimate of the sum of the infinite series [6]. However, this is not true if there are other singularities in the complex plane with $|J_\perp| < 1$. From the Hamiltonian, we expect an additional singularity on the negative real axis near $J_\perp = -0.5$, where the system may order ferromagnetically along the y axis. Such a singularity is clearly present, causing the partial sums to alternate and diverge before $J_\perp = 1$. To move this singularity away, we use Euler transforms to change variables from $J_\perp$ to $x = J_\perp / [a + (1-a)J_\perp]$. For very small a the series coefficients become extremely small, making extrapolations harder. For a close to unity, the coefficients are hardly changed from the untransformed series. Good compromises appear to be $a = \frac{1}{2}$ and $a = \frac{1}{3}$, which map $J_\perp = -1$ and $J_\perp = -\frac{1}{2}$ to infinity, respectively. The resulting plots of the partial sums are shown in Fig. 1. The Kagomé antiferromagnet is clearly extrapolating to a negative value

TABLE I. Expansion coefficients for the ground-state energ E_0, the order parameter M, and the structure factor S.

		Triangular			Kagome	
m	E_0	M	S	E_0	M	S
0	-1.5	1	0	-1	1	0
1	0	0	0	0	0	0
2	-0.675	-0.27	1.08	-0.75	-0.5	2
3	0.135	0.108	-0.432	0.125	0.1666667	-0.6666667
4	-0.1773482	-0.2726916	1.4341347	-0.08020833	-0.3245833	1.7695833
5	0.0817034	0.1717951	-0.9583433	0.02412326	0.1749051	-1.0925162
6	-0.1133163	-0.3315263	2.0593548	-0.02719836	-0.2906697	1.9306204
7	0.1261394	0.4110737	-2.7696352	0.06731218	0.4679179	-3.6055473
8	-0.1906393	-0.7382203	5.2916370	-0.1751062	-1.1833128	8.9968224
9	0.2740349	1.1781303	-8.9566042	0.1891826	1.5674260	-12.925980
10	-0.4101784	-2.0109889	16.0740098	-0.2419287	-2.5738747	21.789716
11	0.6262086	3.4012839	-28.4769501	0.3815669	4.3229068	-39.288456
12				-0.6701061	-8.0770009	76.5639246

(61)

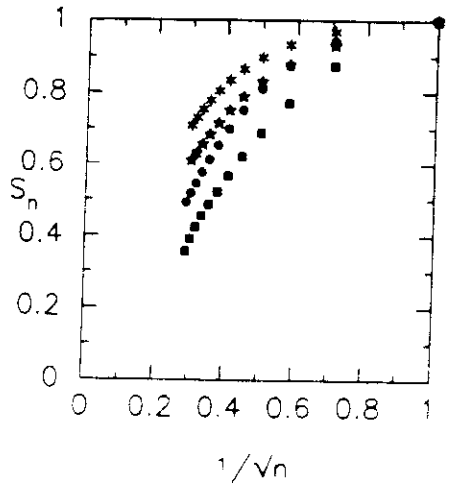

FIG. 1. Partial sums for the order-parameter series. The five- and six-point stars are for the triangular lattice with Euler transform parameters $a=\frac{1}{2}$ and $a=\frac{1}{3}$, respectively. The squares and the circles are for the Kagomé lattice with $a=\frac{1}{2}$ and $a=\frac{1}{3}$, respectively.

suggesting that it is disordered, while the triangular-lattice model appears to extrapolate to a value of about 20% of the classical moment. This should be compared with the spin-wave estimate of 48%.

Since the order-parameter estimate for the triangular lattice is so small, the analysis assuming long-range order cannot be fully relied upon. Unfortunately, unbiased analysis shows poor convergence. Hence we look for consistency with different scenarios. If the system disorders before reaching the Heisenberg point, we expect the critical point to be in the classical 3D Ising universality class. On the other hand, if it disorders right at the Heisenberg point we expect it to have the universality of the classical Heisenberg antiferromagnet on the stacked triangular lattice [23]. In the first case we expect to see the magnetization vanish at the critical point with the exponent $\beta_I \approx \frac{1}{3}$, while in the latter case it should be $\beta_{HI}=\beta_H/\phi_I$, where β_H is the exponent for the stacked triangular Heisenberg model for disordering with temperature, and ϕ_I is the crossover exponent for Ising anisotropy. Kawamura quotes [23] $\beta_H \approx 0.3$, $\phi_I < \gamma \approx 1.1$. Alternative scenarios for the stacked triangular lattice give similar estimates [24]. Thus β_{HI} is not far from $\frac{1}{3}$. To investigate these different possibilities we raise the magnetization series to different powers, such that the resulting series may have a simple zero. We then use Padé extrapolations to estimate the location of the zero. These estimates of the zeros of $M^{\frac{1}{3}}$ are shown in Table II. The closeness of the estimates to Table I shows just how near the Heisenberg system is to the critical point. For the Kagomé lattice we find that all high order ($N+M>8$), near diagonal ($|N-M|<6$) estimates of the zero are in the range 0.83–0.94, showing that it disorders well before the Heisenberg point.

We also studied the order-parameter series by biased differential approximants. We constructed d-log Padé approximants for the series which were biased to have a power-law singularity at $J_\perp=1$. The approximants can then be used to estimate the exponent and the value of the function at that point. For the triangular lattice, we found that those approximants which gave exponent estimates around $\frac{1}{3}$ gave an order-parameter estimate around 20%, as in our previous analysis. However, an equal number of approximants gave exponent estimates in the range 0.3 to 0.4. These had values very close to zero. For the Kagomé lattice these biased approximants did not give sensible results, as might be expected if the singularity really occurs well before $J_\perp=1$.

TABLE II. $[N/M]$ Padé estimate for the zero of $(M^{\frac{1}{3}})$ for the triangular lattice. A value of 1 corresponds to the Heisenberg model.

M/N	2	3	4	5	6	7	8
1	1.385	1.205	1.062	1.019	1.015	1.003	1.002
2	1.004	0.955	0.910	1.015	1.019	1.001	1.003
3	0.960	0.827	0.949	1.001	0.997	1.008	1.014
4	0.923	0.954	0.974	0.998	1.000	1.012	
5	1.125	1.005	1.005	1.020	0.978		
6	0.875	1.005	1.005	0.999			
7	1.191	1.016	0.997				
8	0.863	1.037					
9	1.337						

As long as the triangular system does not disorder much before $J_\perp=1$, the ground-state energy per spin E_I for the Heisenberg model can be estimated from the series. Since the singularity in the ground-state energy is weak (a $\frac{1}{2}$ power in spin-wave theory), a reasonable estimate can be obtained by direct Padé approximants. Different approximants showed excellent agreement with each other for the triangular lattice. From these we would estimate $E_I=-2.204\pm0.005$, where the uncertainties reflect the spread in the Padé estimates. However, we expect a systematic error in this estimate. If the Heisenberg model is disordered, there is a singularity at $J_\perp<1$, and we cannot reliably predict this systematic error. However, if the singularity is at the Heisenberg point (which will occur for long-range ordered and critical cases), we can also estimate the energies by biased differential approximants. We find that a number of approximants show a very weak singularity (exponent ≥ 3), and they have energy estimates in the range quoted earlier. However, a few approximants which give exponent values close to $\frac{1}{2}$ suggest an energy estimate slightly lower. If the Heisenberg model is critical, we expect the exponent to be larger than $\frac{1}{2}$. Thus our best overall estimate for the ground-state energy of the triangular-lattice Heisenberg model is

$$E_I=-2.21\pm0.01. \tag{6}$$

This can be compared with the results from exact diago-

nalizations [2] of $E_t = -2.20 \pm 0.04$. On the other hand, the extrapolations for the Kagomé-lattice energy series are ill-behaved as expected. A similar extrapolation was done for the structure factor to ascertain its location and power of divergence. The convergence was not as good, but the results were consistent with earlier conclusions.

To summarize, in this Letter we have developed systematic Ising-type expansions for the $S = \frac{1}{2}$ Kagomé- and triangular-lattice antiferromagnets. We find that the Kagomé-lattice Heisenberg model is magnetically disordered, while the triangular-lattice Heisenberg model is very close to its critical point: If ordered it has an order parameter much smaller than predicted by spin-wave theory; if disordered it has a large correlation length.

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Microscopic calculation of the spin-stiffness constant for the spin-$\frac{1}{2}$ square-lattice Heisenberg antiferromagnet

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We discuss a systematic, microscopic calculation of the spin-stiffness constant ρ_s for the spin-$\frac{1}{2}$ square-lattice Heisenberg antiferromagnet. An infinitesimal twist is imposed upon the system by gradually rotating the direction of antiferromagnetic ordering. The difference in the ground-state energy of this system with respect to the uniformly ordered ground state can be related to the spin-stiffness constant ρ_s. Series expansions and extrapolation for the energy of the twisted system lead to the estimate $Z_{\rho_s}(=4\rho_s/J)=0.72\pm0.04$. The ratio of the series for ρ_s and perpendicular susceptibility $\chi_\perp$ leads to an estimate for the spin-wave velocity c_s of $Z_{c_s}(=c_s/\sqrt{2}J)=1.18\pm0.02$. The experiments on La_2CuO_4 are quantitatively consistent with a nearest-neighbor Heisenberg model when one takes into account these quantum renormalizations.

Recently there has been much interest in understanding the low-temperature static[1] and dynamic[2,3] properties of Heisenberg antiferromagnets. Underlying any macroscopic description of these systems are the questions of long-range order and the microscopic determination of the parameters such as the sublattice magnetization M^+, the spin-stiffness constant ρ_s, the transverse susceptibility $\chi_\perp$, and the spin-wave velocity c_s. In previous papers[4-7] we have shown that series expansions and extrapolations around various ordered and disordered exactly soluble Hamiltonians provide a systematic way of understanding the ground-state properties of these systems. In particular, expansions around the disordered ground states of dimerized Hamiltonians suggest a spontaneous development of Néel order for the uniformly coupled square-lattice nearest-neighbor (NN) spin-$\frac{1}{2}$ Heisenberg antiferromagnet.[5] In complete agreement with this conclusion, the expansion around the ordered ground state of the Ising Hamiltonian suggests that for the Heisenberg model M^+ is reduced but not eliminated by quantum fluctuations.[4,6] Thus, the Ising expansions are convergent up to the Heisenberg point, and, hence, provide a basis for a systematic determination of the above parameters. The power series thus obtained are, however, singular due to the existence of gapless spin-wave excitations at the Heisenberg point. Nevertheless, borrowing series extrapolation techniques from the study of classical critical phenomena they can be used to estimate these parameters accurately.

It is the purpose of this paper to explain how the spin-stiffness constant ρ_s, and hence the spin-wave velocity c_s, can be estimated by series expansions around the Ising limit. The extrapolated estimates have been reported previously.[6] ρ_s is defined in terms of the energy required to impose an infinitesimal twist on the system. Our calculation involves rotating the direction of antiferromagnetic ordering gradually in space and calculating the energy of the imposed twist. In order to obtain this energy, we rotate the axis of quantization, and thus the direction of ordering, gradually in space and express the Heisenberg Hamiltonian in terms of the rotated spin variables. We can now perform Ising expansions for the ground-state energy of this system in the variable $J_\perp/J_\parallel$, where $J_\parallel$ is the coupling parallel to the direction of ordering, and $J_\perp$ the coupling perpendicular to it. Our calculation, thus, illustrates a general principle that can be used to develop Ising-type expansions for systems which may have noncolinearly ordered ground states, such as the triangular-lattice Heisenberg model. Finally, the ratio of the series for ρ_s and $\chi_\perp$ is used to estimate the spin-wave velocity c_s.

The summation of these series, to estimate the parameters of the Heisenberg model, is guided by the spin-wave theory.[8] This theory not only gives us the exact values for the exponents of the singularities in ρ_s and c_s at the Heisenberg point $(J_\perp/J_\parallel=1)$, but also some suitably defined universal amplitude ratios.[6] These turn out to be very useful in an accurate determination of these parameters.

Let us begin with the definition of the spin-stiffness constant or helicity modulus ρ_s. If we rotate the order parameter of a magnetically ordered thermodynamic system by an angle θ per unit length then the ground-state energy of the system, per lattice site, is increased to

$$E(\theta)=E(\theta=0)+\tfrac{1}{2}\rho_s\theta^2+O(\theta^4)\ . \tag{1}$$

For example, let us first consider the classical Heisenberg Hamiltonian with spin S on a square lattice,

$$H=J\sum_i \mathbf{S}_i\cdot[\mathbf{S}_{i+\hat{\mathbf{x}}}+\mathbf{S}_{i+\hat{\mathbf{y}}}]\ , \tag{2}$$

where $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ are unit distances to the nearest neighbors in the x and y directions. Applying a twist θ per lattice constant along the y direction (so $\mathbf{S}_i=-\mathbf{S}_{i+\hat{\mathbf{x}}}$ and $\mathbf{S}_i\cdot\mathbf{S}_{i+\hat{\mathbf{y}}}=-S^2\cos\theta$), the energy per lattice site becomes

$$E(\theta)=J(1+\cos\theta)(-S^2)\ , \tag{3}$$

so that the spin-stiffness constant is

$$\rho_s = JS^2 . \tag{4}$$

To estimate ρ_s for the $S=\frac{1}{2}$ quantum system we rotate the axis of quantization by a relative angle θ for the neighboring sites along the y direction. (The rotation being about the y axis in spin space.) In terms of the rotated spin variables, $\{\sigma_i\}$, the Hamiltonian becomes

$$H = J\sum_{\langle ij\rangle} \mathbf{S}_i\cdot\mathbf{S}_j = \frac{J}{4}\sum_i [\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_{i+\hat{x}} + \sigma_i^y\sigma_{i+\hat{y}}^y + \sigma_i^x[\sigma_{i+\hat{y}}^x\cos\theta + \sigma_{i+\hat{y}}^z\sin\theta] + \sigma_i^z[-\sigma_{i+\hat{y}}^x\sin\theta + \sigma_{i+\hat{y}}^z\cos\theta]]$$

$$= \frac{J}{4}\left[\sum_i \boldsymbol{\sigma}_i\cdot[\boldsymbol{\sigma}_{i+\hat{x}} + \boldsymbol{\sigma}_{i+\hat{y}}] + (\cos\theta - 1)\sum_i (\sigma_i^x\sigma_{i+\hat{y}}^x + \sigma_i^z\sigma_{i+\hat{y}}^z) + \sin\theta\sum_i (\sigma_i^x\sigma_{i+\hat{y}}^z - \sigma_i^z\sigma_{i+\hat{y}}^x)\right] , \tag{5}$$

where the $\{\sigma_i\}$ are Pauli spins (normalized so $\sigma_i^2=3$). We would like to compute the energy of this system with the spins σ ordered antiferromagnetically along the z axis, the original spins S are twisted when the spins σ are uniform. Since the definition of ρ_s requires the computation of the ground-state energy only to order θ^2, we expand the cosine and sine in powers of θ to get

$$H = \frac{J}{4}\left[\sum_i \boldsymbol{\sigma}_i\cdot(\boldsymbol{\sigma}_{i+\hat{x}} + \boldsymbol{\sigma}_{i+\hat{y}}) - \tfrac{1}{2}\theta^2\sum_i (\sigma_i^x\sigma_{i+\hat{y}}^x + \sigma_i^z\sigma_{i+\hat{y}}^z) + \theta\sum_i (\sigma_i^x\sigma_{i+\hat{y}}^z - \sigma_i^z\sigma_{i+\hat{y}}^x)\right] + O(\theta^3) . \tag{6}$$

The second term is already of order θ^2 so it can be replaced by its expectation value in the ground state of the $\theta=0$ Hamiltonian. The contribution of the third term to the ground-state energy in order θ^2 can be obtained by treating it in second-order perturbation theory. Thus we consider the Hamiltonian

$$H_\theta = \frac{J}{4}\left[\sum_{\langle ij\rangle} \boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j + \theta\sum_i \sigma_i^z(\sigma_{i-\hat{y}}^x - \sigma_{i+\hat{y}}^x)\right] , \tag{7}$$

where the first term runs over all nearest-neighbor pairs, and we have rearranged the θ term from the previous expression.

Let the ground-state energy per site of the Hamiltonian H_θ be

$$E_\theta = E(\theta=0) + \tilde{E}_0\theta^2 + O(\theta^3) . \tag{8}$$

Then ρ_s is given by the expression

$$\tfrac{1}{2}\rho_s = -\tfrac{1}{2}J\sum_i \langle S_i^x S_{i-\hat{y}}^x + S_i^z S_{i+\hat{y}}^z\rangle + \tilde{E}_0 . \tag{9}$$

Here the angular brackets represent the expectation value in the unperturbed ground state with the spins ordered along the z axis. Our aim now is to develop perturbation expansions for the terms on the right-hand side of this expression. In order to do this we add another parameter to H_θ, defining

$$H'_\theta = \sum_{\langle ij\rangle}\left[\frac{J_\parallel}{4}\sigma_i^z\sigma_j^z + \frac{J_\perp}{4}\boldsymbol{\sigma}_i^\perp\cdot\boldsymbol{\sigma}_j^\perp\right] + \frac{J_\parallel\theta}{4}\sum_i \sigma_i^z(\sigma_{i-\hat{y}}^x - \sigma_{i+\hat{y}}^x) , \tag{10}$$

where $\sigma^\perp$ constitutes the x and y components of σ. The Heisenberg model is $J_\perp = J_\parallel$, while $J_\perp = 0$ is an Ising model for which the ρ_s defined by (9) is simply calculated. We then develop a perturbation expansion for this ρ_s in powers of $x \equiv J_\perp/J_\parallel$.

The expansions are developed by the method of Singh, Gelfand, and Huse.[5] The only new feature is that the 90° rotational symmetry of the lattice is broken by the imposed twist in the Hamiltonian. This leads to additional diagrams compared to those needed in Ref. 6 for $\chi_\perp$ or M^+.

It is common to express ρ_s and c_s in terms of a multiplicative renormalization of the classical answer. Thus, we obtain the expansions (giving four significant digits)

$$Z_{\rho_s} = \left[\frac{4\rho_s}{J}\right] = 1 - \tfrac{1}{18}x^2 - \tfrac{1}{18}x^3 - 0.016\,85x^4 - 0.004\,394x^5 - 0.013\,06x^6 - 0.007\,554x^7 . \tag{11}$$

Furthermore, a similar renormalization for $\chi_\perp$ is given by[6]

$$Z_\chi = 8\chi_\perp J = 2 - \tfrac{4}{3}x + \tfrac{17}{9}x^2 - \tfrac{82}{27}x^3 + 3.068x^4 - 3.145x^5 + 3.167x^6 - 3.223x^7 . \tag{12}$$

From these two, and the assumption of standard antiferromagnetic hydrodynamics in the Heisenberg model, a series that extrapolates to the spin-wave velocity at $x=1$ can be obtained through the relation $Z_c^2 = Z_{\rho_s}/Z_{\chi_\perp}$.

Before we analyze these series, we need to consider the structure of the singularity at the Heisenberg point $x=1$. We know from spin-wave theory[8] that the quantities Z_{ρ_s}, Z_χ, Z_{c_s}, etc., have singularities at $x=1$ caused by the closing of the gap for the Goldstone mode (spin waves). Furthermore, the form of the singularities has to be of the type $(1-x)^{m+1/2}$ with $m=0,1,2,\ldots$, etc. The amplitude for the leading (square-root) singularity should be universal if appropriate dimensional factors are scaled out. Thus, if we separate the singular parts at $x=1$ via

$$\rho_s = \rho_s^0 + \rho^{\text{sing}}, \quad \chi_\perp = \chi_\perp^0 + \chi_\perp^{\text{sing}} , \tag{13}$$

then

$$R = \lim_{x\to 1}(\rho_s^{\text{sing}}/\rho_s^0)/(\chi_\perp^{\text{sing}}/\chi_\perp^0) , \tag{14}$$

should be universal, independent of short-distance properties such as spin, etc.

A spin-wave estimate can be obtained for the expression in Eq. (14) through the Holstein-Primakoff transformation. The $S \to \infty$ limit for ρ_s and its leading (square-root) singularity comes entirely from the first term in a $1/S$ expansion. It then follows from a straightforward calculation that $R = 1$. That $\chi_\perp$ and ρ_s have the same relative singularities is not surprising since they play essentially identical roles as coefficients of the gradient-squared terms in the $(2+1)$-dimensional nonlinear σ-model description of this system.[1]

Since the series for c_i^2 is the ratio of the series for ρ_s and $\chi_\perp$ it follows that the amplitude for the square-root singularity in c_i^2 must vanish identically. Thus, the leading singularity that needs to be taken into account in extrapolating c_i^2 should be of the form $(1-x)^{3/2}$. This is a definite prediction from the hypothesis of universal (independent of S) amplitude ratios, which can, in principle, be checked through the series.

Since the quantities $Z_\perp$ and Z_{ρ_s} have competing singularities at $x = \pm 1$, we go to a new variable which moves the singularity at $x = -1$ to infinity. This new variable is

$$z = 2x/(1+x) .$$

In this variable, the series become

$$Z_{\rho_s} = 1 + 0z - 0.013\dot{8}z^2 - 0.020\,83z^2 - 0.021\,89z^4 - 0.019\,60z^5 - 0.016\,20z^6 - 0.012\,93z^7 ,$$

$$(Z_c)^2 = \tfrac{1}{2} + \tfrac{1}{3}z + 0.2049z^2 + 0.1204z^2 + 0.069\,08z^4 + 0.039\,75z^5 + 0.023\,73z^6 + 0.015\,25z^7 + \cdots .$$

In order to sum these series at the Heisenberg point, we construct the sums S_N given by[6]

$$S_N = \sum_{n=0}^{N} a_n x^n .$$

Then, asymptotically (as $N \to \infty$)

$$S_N \approx S_\infty + \frac{C}{(N+\alpha)^\lambda} + O(N^{-(2+\lambda)}) ,$$

where S_∞ is the sum of the infinite series, λ the exponent, C the amplitude of the leading singularity, and α depends on the amplitude of the next to leading singularity. The ratio of C to S_∞ for two different quantities, such as ρ_s and $\chi_\perp$ is determined by the criterion of universal amplitude ratios. Hence, to estimate these quantities we plot the partial sum S_N versus $1/(N+\alpha)^\lambda$ for different α and choose a value of α such that $R = 1$ to get the best estimate for ρ_s. The plot is shown in Fig. 1, while that for $\chi_\perp$ is in Ref. 6. We obtain

$$Z_{\rho_s} = 0.71 \pm 0.04 .$$

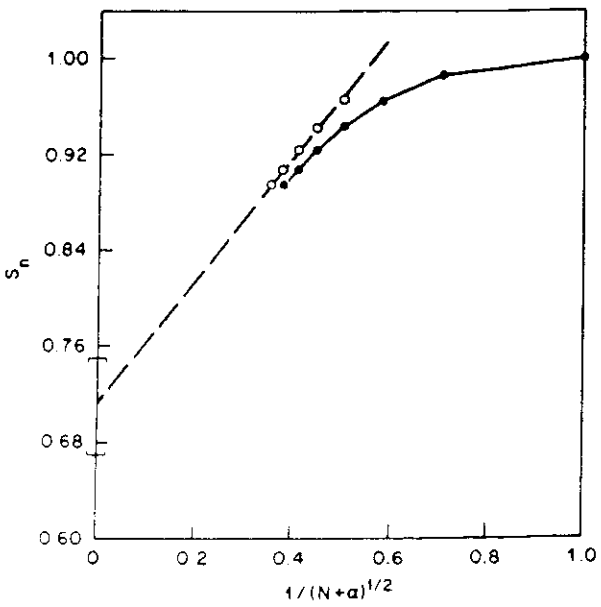

FIG. 1. Plots of partial sum S_N for Z_{ρ_s} vs $1/(N+\alpha)^{1/2}$ where N is the number of terms in the series. The solid circles correspond to $\alpha = 0$, while the open circles correspond to $\alpha = 1$. The latter is chosen to get the ratio R in Eq. (14) equal to unity. The dashed line is a least-squares fit to the points. The extrapolated estimate (S_∞) is shown by brackets.

Alternatively, ρ_s can also be estimated by employing the change of variables (Ref. 4) $1-\delta = \sqrt{1-z}$ to get a series in δ which is free of singularities at the Heisenberg point ($\delta = 1$). We can then use ordinary Padé approximants to sum the series. The Padé estimates are shown in Table I. From these we estimate

$$Z_{\rho_s} = 0.73 \pm 0.04 ,$$

where the uncertainties reflect the spread in the Padé es-

TABLE I. Padé estimates for Z_{ρ_s} in the variable δ. An asterisk indicates a singularity on the real axis in the range $0 < \delta < 1$.

M/N	0	1	2	3	4	5	6	7
0	1.0	1.0	0.94	0.83	0.72	0.67	0.69	0.76
1	1.0		1.06*	5.12*	0.62	0.69	0.65*	
2		1.06*	0.94	0.87	0.79	0.76		
3	0.86	−1.01*	0.87	2.39*	0.70			
4	0.78	0.70	0.80	0.70				
5	0.74	0.74	0.77					
6	0.74	0.74*						
7	0.76							

timates. Thus the two different methods lead to estimates which are consistent with each other.

To compare with other evaluations of ρ_s, we note that the order $1/S$ expansion of the spin-wave theory[1,8] gives $Z_{\rho_s} \simeq 0.60$, while the Schwinger boson mean-field theory[2] gives $Z_{\rho_s} \simeq 0.71$. Thus our results are in excellent agreement with that of Schwinger boson mean-field theory.

To get the estimate for the renormalization of the spin-wave velocity we plot the partial sums versus both $1/N^{1/2}$ and $1/N^{3/2}$ (see Fig. 2). We see that the plot versus $1/N^{3/2}$ settles down to a nice straight line, thus validating the assumption of universal amplitude ratios, which suggests that the amplitude for the square-root singularity for Z_c must vanish. Thus, we estimate

$$Z_c^2 = 1.38 \pm 0.04 .$$

This estimate is quite close to that obtained in the $1/S$ expansion by Oguchi,[8] and in Schwinger boson mean-field theory.[3] In both cases the value is $Z_c^2 \simeq 1.35$.

We are now in a position to compare these estimates against experiments on La_2CuO_4. We first note that the exchange constant J for La_2CuO_4 has been accurately obtained by comparing the frequency moments of the observed two-magnon light scattering spectra to that estimated by Ising expansions.[7] This leads to $J = 1500 \pm 75$ K. Furthermore, the slope of the spin-wave (magnon) dispersion near the antiferromagnetic zone center has been measured directly by neutron scattering,[9] leading to an estimate for the spin-wave velocity, c_s. Using the renormalization Z_{c_s} computed above, this leads to an estimate of $J = 1550 \pm 60$ K. The quantity ρ_s can also be measured directly through experiments as it controls the exponential growth of the correlation length above the three-dimensional ordering temperature

$$\xi \approx A e^{(2\pi\rho_s)/(k_B T)} \equiv A e^{(\pi Z_{\rho_s} J)/(2 k_B T)} .$$

Here, the prefactor A is a slowly varying function of temperature. Because the estimation of ρ_s requires fitting the data above the Néel temperature to this form, the uncertainties are large. For ξ deduced from the Brookhaven susceptibility data,[10] Chakravarty, Halperin, and Nelson find $J \approx 1200$ K assuming $Z_{\rho_s} \simeq 0.60$ (the spin-wave estimate). In an independent fit Gomez-Santos, Joannopoulos, and Negele[11] find the data to be consistent with $Z_{\rho_s} \approx 0.63$ and $J = 1600$ K. The latter implies that the data is also consistent with $Z_{\rho_s} = 0.7$ and $J = 1500$ K. It should be noted that the Néel temperature for the Brookhaven sample is 195 K instead of 265 K for the other two measurements, and hence it can have a somewhat smaller J value, due to sample preparation.

An interesting question that arises is: To what extent does the nearest-neighbor Heisenberg model quantitatively describe La_2CuO_4, and what role, if any, is played by frustrating further-neighbor interactions?

The comparison of various frequency moments of the inelastic light scattering spectra[7] against those computed theoretically for the NN Heisenberg model agreed to an accuracy of 10%. This suggests that short-wavelength fluctuations are quantitatively accounted for, to this accuracy, by this model. The measured long-wavelength spin-wave velocity[9] is also in excellent agreement with the renormalization expected for the NN Heisenberg model, assuming J is taken from the two-magnon light scattering experiments. Thus, the shape of the full spin-

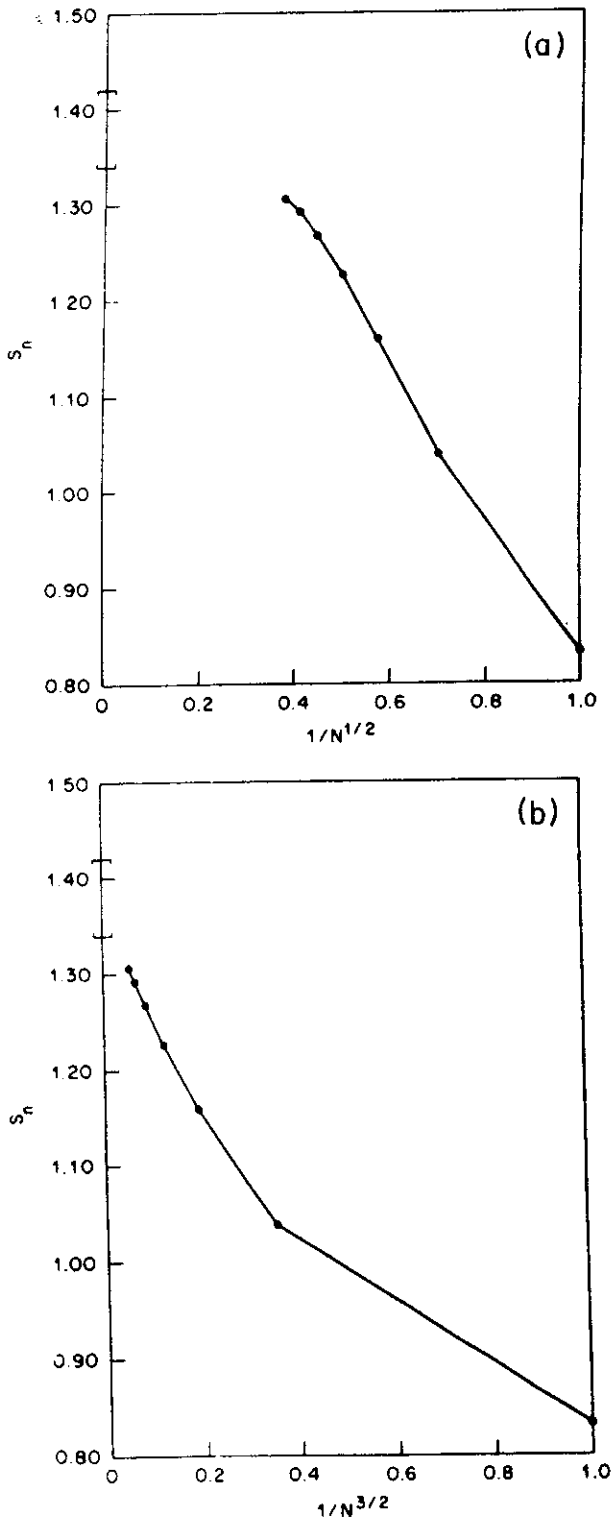

FIG. 2. Plots of partial sum S_N for Z_c^2 (a) vs $1/N^{1/2}$, (b) vs $1/N^{3/2}$. If the leading singularity for Z_c^2 goes as $(1-x)^{3/2}$ then the plot vs $1/N^{1/2}$ should approach the Y axis at 90°.

wave dispersion curve must agree reasonably well with that of a NN Heisenberg model. The estimates of Z_{ρ_s}, from the temperature dependence of ξ, are also consistent (within large uncertainties) with the estimates for the NN model. However, to the extent that one obtains a somewhat smaller Z_{ρ_s} than expected for the NN Heisenberg model, it gives us a measure of the amount of frustration in this system. Let us remember that with sufficient frustration (for example, due to second- or third-neighbor interactions) the system may be disordered at $T=0$. At this point[1] $Z_{\rho_s} \to 0$, $Z_\chi \to 0$, whereas Z_{c_s} remains finite, and presumably the entire spin-wave dispersion curve is not drastically altered. Thus the relative reduction in Z_{ρ_s} or Z_χ with respect to Z_{c_s} is a measure of the significance of further-neighbor interaction in the system. Thus a combined measurement of the $T=0$ spin-wave velocity and the temperature dependence of ξ on the same sample could, in principle, serve to constrain the amount of frustration in the system.

To summarize, we have presented here a systematic microscopic calculation of the spin-stiffness constant ρ_s, and the spin-wave velocity c_s, for the $T=0$, NN spin-$\frac{1}{2}$ square-lattice Heisenberg antiferromagnet. The estimate for Z_{ρ_s} (0.72 ± 0.04) differs from the order $1/S$ spin-wave value (0.60) by about 15%, while that for Z_{c_s} (1.18 ± 0.02) is very close to it (1.16). Both these estimates are remarkably close to the Schwinger boson mean-field theory ($Z_{\rho_s}=0.71$, $Z_{c_s}=1.16$). The estimated quantum renormalizations provide a quantitatively consistent picture for the experiments on La_2CuO_4.

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PHYSICAL REVIEW B VOLUME 47, NUMBER 18 1 MAY 1993-II

Transverse-spin correlations and single-mode approximation for the square-lattice $S=\frac{1}{2}$ Heisenberg model

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We calculate the equal-time transverse-spin correlations at zero temperature for the nearest-neighbor square-lattice spin-$\frac{1}{2}$ Heisenberg antiferromagnet by expansions around the Ising limit. To a good approximation, these correlations are proportional over the entire Brillouin zone, to the spin-wave result. If we use the single-mode approximation to estimate the spin-wave dispersion, we find linear gapless modes near both $q=(0,0)$ and $q=(\pi,\pi)$, with spin-wave velocity approximately 1.4 times the spin-wave answer of $\sqrt{2}J$. This is larger than previous estimates of $Z_c=1.18\pm0.02$, reflecting the mixing of higher magnons.

In recent years the antiferromagnetic behavior of the insulating phase of high-T_c cuprates has been studied thoroughly in terms of the two-dimensional (2D) spin-$\frac{1}{2}$ Heisenberg model.[1] Many detailed comparisons between theory and experiments show that these systems can be described by a layered Heisenberg model with an in-plane exchange constant J of order 1000 K, and a very weak coupling in the perpendicular direction. One of the surprising theoretical results[2] is that despite strong quantum fluctuations, many properties of the 2D spin-$\frac{1}{2}$ Heisenberg model are in remarkable quantitative agreement with the linear spin-wave theory.[3]

A possible exception is the spin-pair excitation spectra which have been measured in Raman scattering.[4] It was found that these spectra have a very different line shape than the two-magnon spectra derived from spin-wave theory.[5] In particular, the experimental spectra are much broader and have a pronounced shoulder at higher energies. It was recently argued that this results from enhanced quantum fluctuations in the spin-$\frac{1}{2}$ system, where multiple magnon spectra overlap to give a broad peak. The frequency moments of the spin-pair excitation spectra for the Heisenberg model, which were calculated by series expansion methods,[6] were found to be rather close to experimental values. Finite-size studies[7] also lead to frequency moments in agreement with the series expansion results. A number of other calculations,[8] based on fermionic spin excitations, also obtain a line shape similar to experiments.

On the other hand, recent spin-wave calculations by Canali and Girvin[9] show the two-magnon and four-magnon spectra to be well separated in energy, and the two-magnon peak by itself to be much narrower. They find that the spin-wave theory can still lead to a second frequency moment comparable to those obtained from series expansions due to the large separation between the two- and four-magnon peaks.[10] Since these spectra are so qualitatively different from the experiments, they raise the question of why there should be such marked deviation from spin-wave theory for some quantities, when it works so well for others. One could argue that the coupling of light to antiferromagnets is not well understood, and that the simple Raman Hamiltonian used in the calculations is inadequate.[11,12]

In contrast to light scattering, the coupling of neutrons to antiferromagnets is simpler to understand.[13] Thus one might ask what would be the contribution of multimagnon excitations to neutron scattering. Since neutron scattering measures the dynamical structure factor,[14] $S(\mathbf{q},\omega)$, at zero temperature it involves single-spin flips with respect to the ground state. However, these single-spin flips may consist of $1,3,5,\ldots$ magnons. Thus, one might expect three-magnon sidebands to the usual single-magnon spectra. Looking for these higher magnon terms can give us quantitative insight into deviations from linear spin-wave theory.

Spin-spin correlations at zero temperature are a good way of characterizing the ground-state wave function of the Heisenberg model.[15] They can be measured directly in neutron-scattering experiments, if the dynamic scattering is integrated up to high enough energies. Here we would like to calculate the transverse correlation functions by expanding around the Ising limit. Furthermore, we would like to apply the single-mode approximation (SMA) to estimate the spin-wave dispersion.[16] We find the transverse-spin correlations to be roughly proportional to those in spin-wave theory over the entire Brillouin zone. Thus, the resulting spin-wave dispersion is also similar to spin-wave theory with gapless modes near (0,0) and (π,π). However the spin-wave velocity is estimated to be approximately 1.4 times the classical spin-wave answer of $\sqrt{2}J$, which is clearly larger than previous estimates of the renormalization of spin-wave velocity $Z_c=1.18\pm0.02$.[17] Strictly speaking the single-mode approximation gives an upper bound for the spin-wave velocity, and its deviation from the actual velocity is a quantitative measure of the mixing of higher magnons.

We consider the Hamiltonian

$$\mathcal{H}=\sum_{\langle i,j\rangle} J_z S_i^z S_j^z + J_{xy}(S_i^x S_j^x + S_i^y S_j^y)\ , \tag{1}$$

where the sum runs over the nearest-neighbor pair of

sites on the square lattice. We have introduced an Ising anisotropy so that the ground-state properties can be calculated by expansions around the Ising limit. We define the transverse real-space spin correlations as

$$\tilde{S}(\mathbf{r})=N(\mathbf{r})\langle S_0^x S_\mathbf{r}^x+S_0^y S_\mathbf{r}^y\rangle \ , \tag{2}$$

where the angular brackets represent ground-state expectation values. $N(\mathbf{r})$ is the number of symmetry related vectors of $\mathbf{r}$. We develop expansions for these correlations in powers of $x=J_{xy}/J_z$ by the method of Singh, Gelfand, and Huse.[18] The expansions up to ninth order in x are shown in Table I.

The equal-time structure factor can now be calculated from the expression

$$S(\mathbf{q})=\sum_\mathbf{r} \exp i\mathbf{q}\cdot\mathbf{r}\langle S_0^x S_\mathbf{r}^x+S_0^y S_\mathbf{r}^y\rangle \ . \tag{3}$$

We extrapolate the series for $S(\mathbf{q})$ to the Heisenberg point ($x=1$) by Padé approximants. We expect direct Padé approximants to work well except very near $q=0$ and $q=(\pi,\pi)$. Near $q=0$ we expect the correlations to vanish linearly with q for the Heisenberg model and at $q=0$ the series should vanish as $\sqrt{1-x}$ as $x\to 1$. On the other hand, near (π,π) we expect the correlations to diverge as $1/|\mathbf{q}-\pi|$ for the Heisenberg model and the series at $\mathbf{q}=\pi$ to have a $1/\sqrt{1-x}$ divergence as $x\to 1$. For all other $\mathbf{q}$, we expect only a weak energylike singularity at $x=1$. We are primarily interested in the behavior of the correlation functions for the Heisenberg model ($x=1$). We use Padé approximants to estimate these correlations away from $q=0$ and $\mathbf{q}=(\pi,\pi)$. We find that the spin-spin correlations are decreased nearly uniformly from the classical spin-wave result over the entire zone. Such a result was also obtained in a $1/S$ expansion by Igarashi and Watabe.[19]

TABLE I. Expansion coefficients for the transverse correlation functions of the square-lattice spin-$\frac{1}{2}$ Heisenberg model.

r	S(r)
(1,0)	$-0.666\,666\,67x+0.007\,407\,407\,4x^3$ $-0.018\,978\,836x^5-0.013\,203\,406x^7$ $-0.006\,237\,013\,0x^9$
(1,1)	$0.222\,222\,22x^2+0.029\,876\,543x^4$ $+0.020\,521\,788x^6+0.013\,168\,097x^8$
(2,0)	$0.111\,111\,111x^2+0.059\,135\,802x^4$ $+0.017\,206\,134x^6+0.014\,153\,935x^8$
(2,1)	$-0.233\,333\,33x^3-0.048\,404\,321x^5$ $-0.033\,849\,103x^7-0.023\,358\,328x^9$
(2,2)	$0.06x^4+0.020\,796\,729x^6+0.014\,603\,336x^8$
(3,0)	$-0.038\,888\,889x^3-0.040\,350\,896x^5$ $-0.014\,015\,742x^7-0.012\,184\,987x^9$
(3,1)	$0.08x^4+0.050\,104\,937x^6+0.025\,388\,254x^8$
(3,2)	$-0.069\,686\,949x^5-0.031\,957\,878x^7-0.022\,616\,142x^9$
(3,3)	$0.019\,984\,043x^6+0.011\,921\,170x^8$
(4,0)	$0.01x^4+0.020\,649\,317x^6+0.012\,522\,252x^8$
(4,1)	$-0.034\,843\,474x^5-0.034\,776\,854x^7-0.019\,276\,328x^9$
(4,2)	$0.029\,976\,064x^6+0.024\,370\,713x^8$
(4,3)	$-0.024\,311\,737x^7-0.017\,500\,727x^9$
(4,4)	$0.007\,330\,236\,3x^8$
(5,0)	$-0.003\,484\,347\,4x^5-0.010\,640\,911x^7-0.009\,006\,002\,6x^9$
(5,1)	$0.011\,990\,426x^6+0.019\,880\,711x^8$
(5,2)	$-0.014\,587\,042x^7-0.016\,531\,477x^9$
(5,3)	$0.011\,728\,378x^8$
(5,4)	$-0.009\,160\,734\,0x^9$
(6,0)	$0.000\,999\,202\,15x^6+0.004\,553\,325\,1x^8$
(6,1)	$-0.004\,862\,347\,4x^7-0.011\,101\,598x^9$
(6,2)	$0.005\,864\,189\,0x^8$
(6,3)	$-0.006\,107\,156\,0x^9$
(7,0)	$-0.000\,347\,310\,53x^7-0.002\,093\,094\,8x^9$
(7,1)	$0.001\,675\,482\,6x^8$
(7,2)	$-0.002\,617\,352\,6x^9$
(8,0)	$0.000\,104\,717\,66x^8$
(8,1)	$-0.000\,654\,338\,15x^9$
(9,0)	$-0.000\,036\,352\,119x^9$

In what follows, we are interested in the limiting form of the structure factor for the Heisenberg model near $q=0$ and $\mathbf{q}=(\pi,\pi)$. Let us define

$$A=\lim_{q\to 0} S(q)/q \ . \tag{4}$$

To estimate A we calculate $S(q)/q$ along different directions in momentum space near $q=0$. These quantities, along the directions $q_y=0$, $q_y=q_x/2$, and $q_y=q_x$, are shown in Fig. 1. The corresponding plots for the classical spin-wave theory are also shown for comparison. From these plots we estimate

$$A=0.123\pm 0.007 \ . \tag{5}$$

Near the antiferromagnetic vector, let $\mathbf{k}=(\pi,\pi)-\mathbf{q}$, and

$$B=\lim_{k\to 0} kS(k) \ . \tag{6}$$

To estimate B, we calculate $kS(k)$ along different directions in momentum space near $k=0$. These quantities, along the directions $k_y=0$, $k_y=k_x/2$, and $k_y=k_x$, are shown in Fig. 2. The corresponding plots for the classical spin-wave theory are also shown for comparison. From these plots we estimate

$$B=1.05\pm 0.10 \ . \tag{7}$$

The single-mode approximation is a variational estimate for the energy of the modes at a given $\mathbf{q}$. Within this approximation the dispersion is given by

$$\omega(\mathbf{q})=\tilde{e}(\mathbf{q})/S(\mathbf{q}) \ , \tag{8}$$

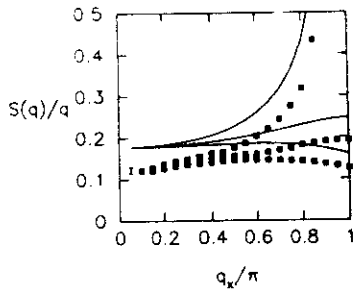

FIG. 1. Plots of $S(q)/q$ as a function of q_x along the directions $q_y=0$, $q_y=q_x/2$, and $q_y=q_x$ in momentum space. The solid lines represent the corresponding plots for classical spin-wave theory. The error bar represents the estimate of the amplitude $A=\lim_{q\to 0} S(q)/q$.

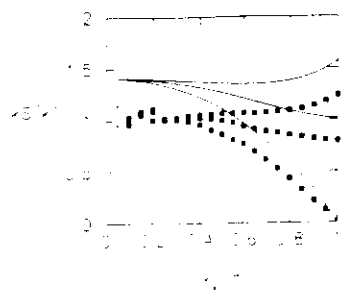

FIG. 2. Plots of $kS(k)$ as a function of k_x along the directions $k_y=0$, $k_y=k_x/2$, and $k_y=k_x$ in momentum space, where $\mathbf{k}=\pi-\mathbf{q}$. The solid lines represent the corresponding plots for classical spin-wave theory. The error bar represents the estimate of the amplitude $B=\lim_{k\to 0} kS(k)$.

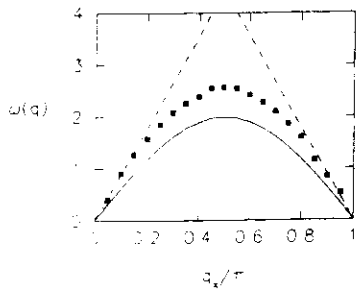

FIG. 3. The spin-wave dispersion in the single-mode approximation along the direction $q_x=q_y$. The solid lines represent the dispersion in classical spin-wave theory. The dashed lines represent an estimate for the linear dispersion at the two end points.

where

$$\tilde{\epsilon}(\mathbf{q})=\sum_r \exp(i\mathbf{q}\cdot\mathbf{r})\langle[S_0^z,H],S_r^x\rangle+\langle[S_0^x,H],S_r^y\rangle\rangle , \tag{9}$$

Here the square brackets refer to commutators. It is easily shown that this expression reduces to

$$\tilde{\epsilon}(\mathbf{q})=-2Je(1-\gamma_q) , \tag{10}$$

where

$$\gamma_q=(\cos q_x+\cos q_y)/2 \tag{11}$$

and

$$e=\langle S_i^xS_j^x+S_i^yS_j^y+2S_i^zS_j^z\rangle , \tag{12}$$

for nearest neighbor i and j. The quantity e can be estimated from Ising expansions to be approximately -0.50.

We note that the behavior of the structure factor combined with the fact that $(1-\gamma_q)$ vanishes as q as $q\to 0$ and goes to a constant as $\mathbf{q}\to\pi$ implies that we have linear gapless modes both at $\mathbf{q}=(0,0)$ and at $\mathbf{q}=(\pi,\pi)$. The estimated dispersion is shown in Fig. 3. We note that the experimentally measured dispersion for La_2CuO_4 also appears very similar to the spin-wave dispersion.[20] From the estimates of the amplitudes A and B, the renormalization of spin-wave velocity with respect to the classical answer of $\sqrt{2}J$ is estimated near $q=(0,0)$ to be 1.44 ± 0.10 and near $q=(\pi,\pi)$ to be 1.36 ± 0.13. These numbers are higher than previous estimates[17] of $Z_c=1.18\pm0.02$ by about 15% and are an upper bound on the spin-wave velocity renormalization. If we crudely estimate the three magnons to be at three times the energy of single magnons then the S^- operator creates about 10% three-magnons. These results reinforce the general validity of the spin-wave approximation. Further studies of the neutron-scattering line shapes at higher energies and the relative contribution of the single spin-wave and multiple spin-wave to the spectra will be illuminating.

This study further raises the question of why the experimental spin-pair excitation spectra deviate so much from spin-wave theory. As suggested in the introduction, a possible explanation is that the coupling of light to antiferromagnets is more complicated. The spectra for the pure Heisenberg model with the simplest form of the Raman Hamiltonian, contain well-separated but narrow peaks quite different from the experiments. These multiple peaks lead to the large frequency moments. The experimental line shape is affected by resonance effects, which change the Raman Hamiltonian,[11,12] in particular, add further neighbor terms to it. These additional terms can give rise to scattering at energies around $4J$, which is between the energy $3J$ for two-magnons and $5J$ for four-magnons, thus resulting in a single broadened spectra, without significantly affecting the first few frequency moments. It would be useful to carry out a spin-wave calculation with such additional terms in the Raman Hamiltonian.

In conclusion, in this paper we have used expansions around the Ising limit to calculate the zero-temperature spin correlations for the square-lattice Heisenberg model. The correlations are roughly proportional to the spin-wave answer over the entire Brillouin zone. The single-mode approximation leads to a spin-wave dispersion with gapless modes near $\mathbf{q}=(0,0)$ and $\mathbf{q}=(\pi,\pi)$, but with spin-wave velocity larger than those estimated by other methods, suggesting a mixing of higher magnon modes. We hope our work will stimulate further investigations of multimagnon contributions to neutron scattering.

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