Spin-Disordered States: An Overview

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Interacting spin systems: spins interact via Heisenberg exchange interaction

Heisenberg Exchange Interaction Hamiltonian:

$$H=\sum_{(i,j)} J_{ij}\, \mathbf{S}_i . \mathbf{S}_j \qquad S=1/2,1,\ldots$$

Lattice dimensionality: d
Spin dimensionality: n
Ising model (n =1)
XY model (n =2)
Heisenberg model (n =3)

Interaction: may be ferromagnetic or antiferromagnetic

Fully anisotropic Heisenberg Hamiltonian in 1d:

$$H_{XYZ} = \sum_{i=1}^{N} \left[J_x S_i^x S_{i+1}^x + J_y S_i^y S_{i+1}^y + J_z S_i^z S_{i+1}^z \right]$$

In most cases, ground state and low-lying excitation spectrum are known

Ferromagnetic ground state: simple, all spins parallel

Excitations: spin waves

Linear chain Heisenberg ferromagnet:

$$H = -J \sum_i \vec{S}_i . \vec{S}_{i+1}$$

$$H = -J \sum_{i=1}^{N} \left[S_i^Z S_{i+1}^Z + \frac{1}{2}\left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ \right) \right]$$

$$S^Z|\alpha\rangle = \frac{1}{2}|\alpha\rangle,\ S^Z|\beta\rangle = -\frac{1}{2}|\beta\rangle$$

$$S^+|\alpha\rangle = 0,\ S^+|\beta\rangle = |\alpha\rangle, S^-|\alpha\rangle = |\beta\rangle, S^-|\beta\rangle = 0$$

Eigenvalue problem: $H|\psi\rangle = E|\psi\rangle$

$\varepsilon = E + \frac{JN}{4}$, energy of excited state measured with respect to ground state energy $E_g = -\frac{JN}{4}$

$$\varepsilon = J(1 - \cos(k))$$

$$k = 2\pi\frac{\lambda}{N}, \lambda = 0,\ 1,\ 2, \ldots\ldots,\quad N$$

Antiferromagnetic ground state: more complex, exact state known using the Bethe Ansatz

Exact ground state energy = NJ (- ln2 + ¼)

Two-spin correlation function in the ground state:

$$\langle 0|\boldsymbol{S}_n \cdot \boldsymbol{S}_0|0\rangle \propto (-1)^n \frac{1}{(2\pi)^{\frac{3}{2}}} \frac{\sqrt{\ln n}}{n}.$$

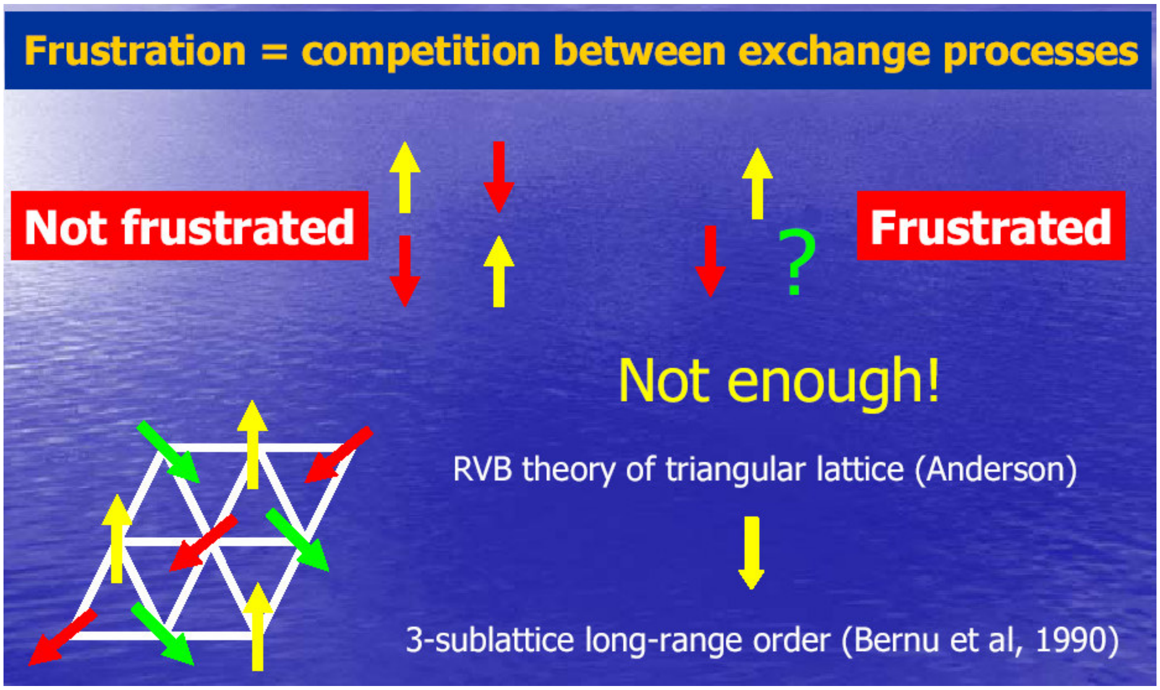
(No long range order)

Ground state: spin disordered

Ground states likely to be spin-disordered in low dimensions and in the presence of frustrating interactions

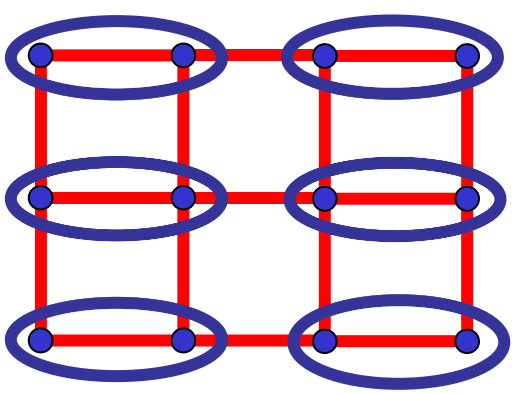
In low d: the effect of quantum fluctuations prominent, melting of spin order

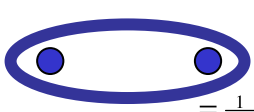
Frustration arises due to conflict in the minimization of spin-spin interaction energies



Valence bonds (VBs) provide a pictorial representation of spin disordered states

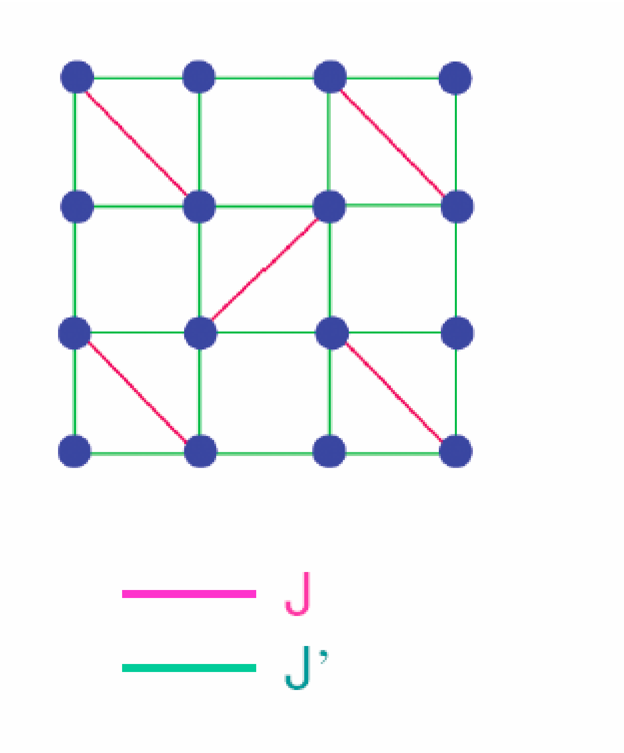
Valence Bond state (frozen VBs):





$$= \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

Shastry-Sutherland model

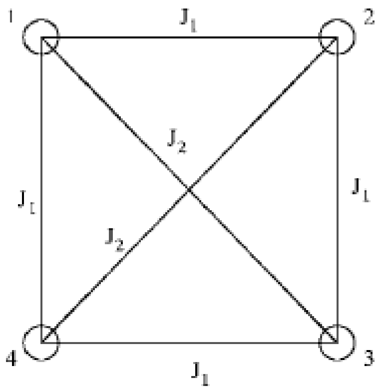


VBs along dimers for $J'/J < 0.7$

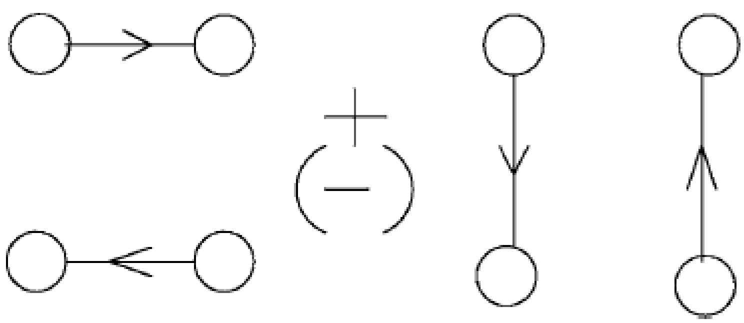
At the critical point transition from gapful disordered state to AFM ordered gapless state

$SrCu_2(BO_3)_2$: magnetic properties captured by the SS model

Consider a square plaquette of spins interacting via the AFM Heisenberg exchange interaction

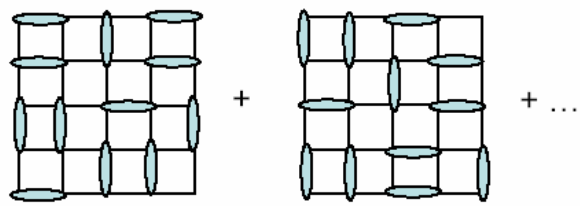


Ground states: resonating valence bond (RVB) states

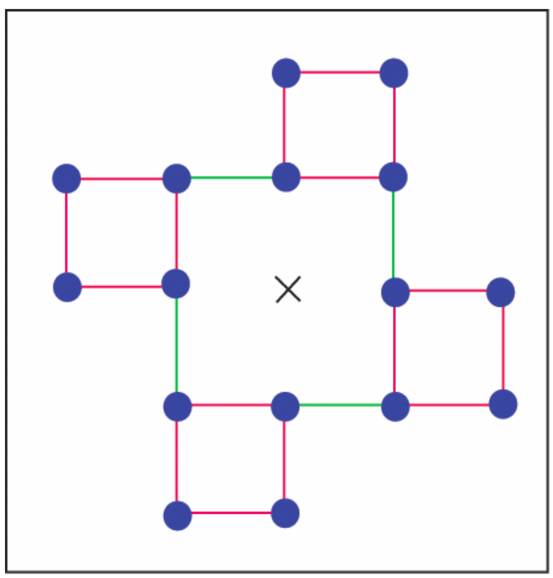


Spin Liquids?

- Anderson: proposed RVB states of quantum antiferromagnets

$$|\Psi\rangle =$$ 

CaV_4O_9

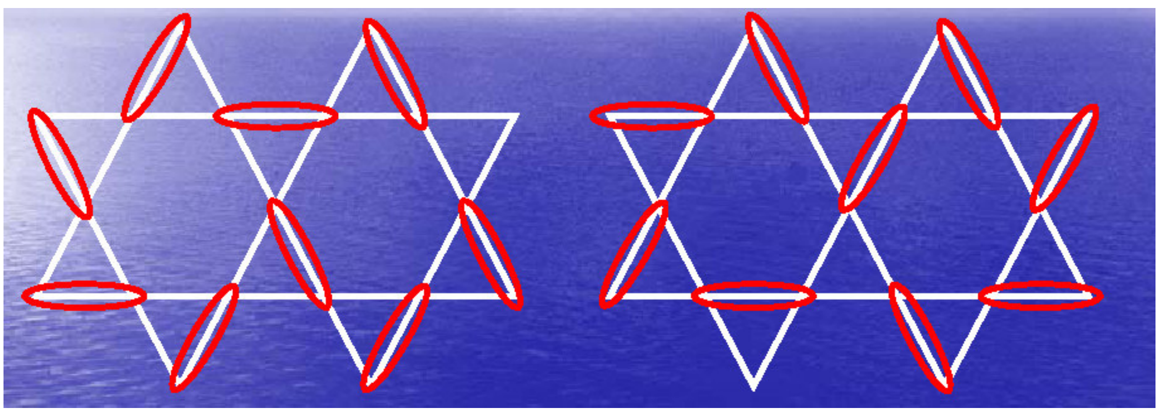


Plaquette spins in RVB states

S = ½ HAFM on kagomé lattice: a singlet-triplet gap (numerical simulations)

Large number of low-lying singlets within gap ~ $(1.15)^N$

Possible explanation: low-lying singlets are RVB states, linear combinations of singlet dimer coverings



Singlet excitations could lead to power-law dependence $C_v \sim T^{\alpha}$

Candidate ground state: VB crystal or spin liquid (RVB)

Herbertsmithite $ZnCu_3(OH)_6$: a possible physical realization

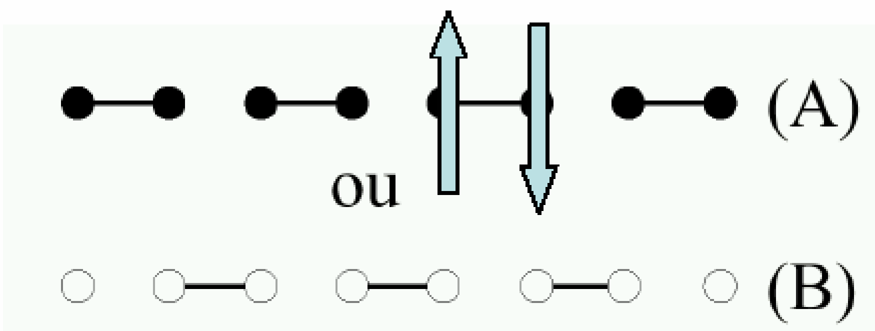
Majumdar – Ghosh chain:

Prototype of frustrated model in 1d

Competition between different couplings leads to frustration

$$H = J \sum_{i=1}^{N} \left[\vec{S}_i \cdot \vec{S}_{i+1} + \alpha \, \vec{S}_i \cdot \vec{S}_{i+2} \right]$$

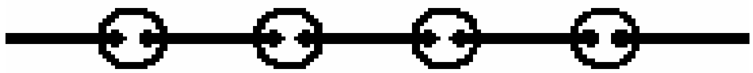
α = ½ : ground state known exactly, doubly degenerate VB states



Translationally symmetric ground states: RVB states

AKLT model (1987): ground state known exactly, valence bond solid state

A chain with spin S = 1 at each site
Each spin-1 is a symmetric combination of two spin-1/2's



S = 1 states:

$$S^Z = +1, |\psi_{++}\rangle = |\uparrow\uparrow\rangle$$

$$S^Z = -1, |\psi_{--}\rangle = |\downarrow\downarrow\rangle$$

$$S^Z = 0, |\psi_{+-}\rangle = |\psi_{-+}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)$$

VBS state: each spin-1/2 forms a singlet (valence bond) with a spin-1/2 at a neighbouring site.

Antisymmetric tensor $\varepsilon^{\alpha\beta}$:

$$\varepsilon^{++} = \varepsilon^{--} = 0, \varepsilon^{+-} = -\varepsilon^{-+} = 1$$

Singlet state: $\frac{1}{\sqrt{2}}\varepsilon^{\alpha\beta}\left|\alpha\beta\right\rangle$, summation over repeated indices

$$\left|\psi_{VBS}\right\rangle = 2^{-\frac{N}{2}}\psi_{\alpha_1\beta_1}\varepsilon^{\beta_1\alpha_2}\psi_{\alpha_2\beta_2}\varepsilon^{\beta_2\alpha_3}.....\psi_{\alpha_N\beta_N}\varepsilon^{\beta_N\alpha_1}$$

$\left|\psi_{VBS}\right\rangle$: contains configurations which look like (in the S^Z representation)
……0 + 0…..0 – 0…0 + 0….0 – 0
(each + followed by a – with an arbitrary number of zero states in between),
floating Néel order

VBS ground state does not have conventional LRO but long range string order (quantum paramagnet)
String operator

$$\sigma_{ij}^{\alpha} = -S_i^{\alpha}\exp\left(i\pi\sum_{l=i+1}^{j-1}S_l^{\alpha}\right)S_j^{\alpha}$$

String order parameter:

$$O^{\alpha}_{string} = \lim_{|i-j|\to\infty} \left\langle \sigma^{\alpha}_{ij} \right\rangle, \alpha = x, y, z$$

= 4/9 in the AKLT state

> 0 in the Haldane phase

AKLT Hamiltonian:

$$H_{AKLT} = \sum_i P_2\left(\vec{S}_i + \vec{S}_{i+1}\right)$$

P_2: projection operator onto spin 2 for a pair of n. n. spins

Total spin of each pair cannot be two

AKLT (VBS) state: exact ground state of AKLT Hamiltonian with energy zero

Projection operator (j = 2)

$$P_j\left(\vec{S}_i + \vec{S}_{i+1}\right) = \prod_{l=0,1} \frac{\left[l(l+1) - \vec{S}^2\right]}{[l(l+1) - j(j+1)]}$$

$$\vec{S} = \vec{S}_i + \vec{S}_{i+1}$$

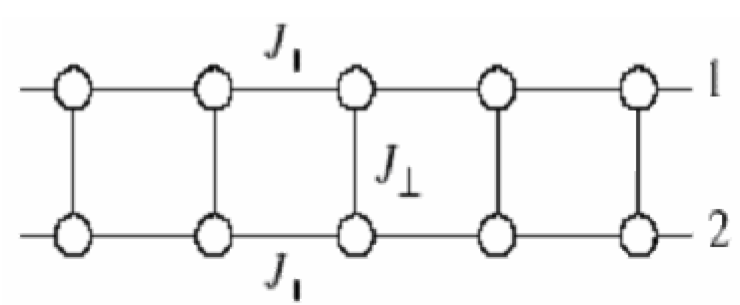
$$H_{AKLT} = \sum_i \left[\frac{1}{2} \vec{S}_i . \vec{S}_{i+1} + \frac{1}{6} \left(\vec{S}_i . \vec{S}_{i+1} \right)^2 + \frac{1}{3} \right]$$

AKLT model smoothly connected to spin-1 Heisenberg chain (same physical properties)

Examples of spin-1 AFMs:

$CsNiCl_3$, $RbNiCl_3$,
$Ni(C_2H_8N_2)_2NO_2(ClO_4)$ (NENP),
Y_2BaNiO_5 etc.

Spin Ladders:



$$\mathcal{H} = \sum_{j=1}^{L} [J_{\|}(\mathbf{S}_{1,j} \cdot \mathbf{S}_{1,j+1} + \mathbf{S}_{2,j} \cdot \mathbf{S}_{2,j+1}) + J_{\perp}\mathbf{S}_{1,j} \cdot \mathbf{S}_{2,j}] - H\sum_{j=1}^{L} (S^z_{1,j} + S^z_{2,j}),$$

Examples: $Cu_2(C_5H_{12}N_2)_2Cl_4$
$(C_5H_{12}N)_2CuBr_4$
$(5IAP)_2CuBr_4.2H_2O$

Excitation spectrum is gapped

Family of ladder compounds

$Sr_{n-1}Cu_{n+1}O_{2n}$ planes of weakly-coupled ladders of (n + 1)/2 chains

Odd-even effect :

Excitation spectrum gapped (gapless) for n even (odd)

Doped ladder models: toy models of strongly correlated systems

Ladder compound: $Sr_{14-x}Ca_xCu_{24}O_{41}$, exhibits superconductivity under pressure (hole doped)

$T_c \sim 12$ K at a pressure of 3 GPa

Spin-disordered states: quantum paramagnets, characterized by the existence of novel order parameters

MG model:

No LRO in the two-spin correlation function in the ground state

$$K^2(i, j) = \langle S_i^Z S_j^Z \rangle = \tfrac{1}{4}\,\delta_{ij} - 1/8\ \delta_{|i-j|,1}$$

Four-spin correlation function has ODLRO

$$K^4(ij, lm) = \langle S_i^x S_j^x S_l^y S_m^y \rangle$$

$$= K^2(i, j)\, K^2(l,m) + 1/64\ \delta_{|i-j|,1}\ \delta_{|l-m|,1}\ \exp\left(i\pi((i + j)/2 - (l+m)/2)\right)$$

Quantum information theoretic (QIT) concepts and tools provide new ways to characterize the states

$$\frac{1}{\sqrt{2}}\left(|0\rangle|1\rangle - |1\rangle|0\rangle\right)$$

Cannot be written as a product of individual qubit states

$\frac{1}{\sqrt{2}}\left(|0\rangle|0\rangle + |0\rangle|1\rangle\right)$: unentangled, i.e., separable state

More general definitions:
Quantum states: pure or mixed

Pure state: can be described by a single ket vector or a sum of basis states

$$|\Psi_1\rangle = |a\rangle, |\Psi_2\rangle = \frac{1}{\sqrt{2}}|a\rangle + \frac{1}{\sqrt{2}}|b\rangle$$

Mixed state: statistical mixture of pure states

Represented by density operator

$$\rho = \sum_k p_k |\Psi_k\rangle\langle\Psi_k|$$

p_k : probability that the system is in state $|\Psi_k\rangle$, $\sum_k p_k = 1$

Pure state: $\rho = |\Psi\rangle\langle\Psi|$

Pure state: $tr(\rho^2) = 1$

Mixed state: $tr(\rho^2) < 1$

Mean value of observable A:

$\langle A \rangle = Tr\ (\rho\ \ A\ )$

Pure state:

$|\Psi\rangle = |\Phi_1\rangle|\Phi_2\rangle|\Phi_3\rangle......|\Phi_N\rangle \Rightarrow$ separable

$|\Psi\rangle$ cannot be written in product form

$\Rightarrow$ entangled

Mixed state:

$\rho = \sum_k p_k |\Psi_k\rangle\langle\Psi_k|$

Separable: if each $|\Psi_k\rangle$ can be written in product form

Entangled: non-separable

Ground states of quantum many body states: entangled

Entanglement can be

created
destroyed
manipulated
quantified

Entanglement acts as a resource in quantum computation, teleportation and cryptography protocols

Can be of different types

Bipartite: between two subsystems

Multipartite: between more than two subsystems

Localizable, zero temperature, finite temperature etc.

Appropriate quantification measures are available in some cases
Magnetic solids: interacting spin systems
Ground and thermal states are entangled
Amount of entanglement: can be changed by changing temperature T and external magnetic field h

Measures of Entanglement

N identical S = ½ spins on a lattice

State $|\Psi\rangle \rightarrow$ density matrix $\rho = |\Psi\rangle\langle\Psi|$
One-body reduced density matrix

$$\rho_i^{(1)} = Tr_{j \neq i}\,\rho$$

λ_1, λ_2 : eigenvalues of $\rho_i^{(1)}$

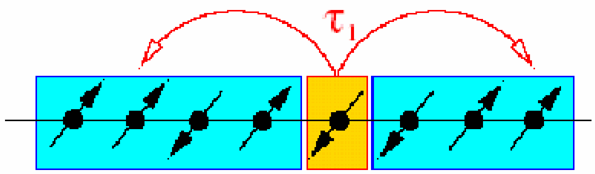
Von-Neumann entropy

$E = -\lambda_1 \log \lambda_1 - \lambda_2 \log \lambda_2$

One-tangle $\tau_1 = 4 \det \rho_i^{(1)} = 4 \lambda_1 \lambda_2$

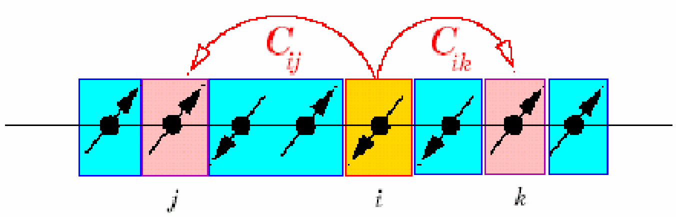
E, τ_1: measure the entanglement of the i-th particle with the rest

(measure of global entanglement)



$E = \tau_1 = 0$ (for each particle i) $\Leftrightarrow$ $|\Psi\rangle$ is a factorised state, i.e., separable

PAIRWISE ENTANGLEMENT



Two – body reduced density matrix

$\rho_{ij}^{(2)} = Tr_{k \neq i,j}\, \rho$

$\rho_{ij}^{(2)}$: 4×4 matrix

$$R = \rho_{ij}^{(2)} \left(\sigma_i^y \otimes \sigma_j^y\right) \rho_{ij}^{(2)*} \left(\sigma_i^y \otimes \sigma_j^y\right)$$

$\lambda_1, \lambda_2, \lambda_3, \lambda_4$: decreasing eigenvalues of R

CONCURRENCE:

$$C_{ij} = 2 \max\left(\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0\right)$$

CKW inequality for three particles

$$\tau_1 \geq \tau_2 = \sum_{j \neq i} C_{ij}^2$$

$$\tau_{A(BC)} = C_{AB}^2 + C_{AC}^2 + \tau_{ABC}$$

Pairwise entanglement does not exhaust the global entanglement

OUR TOOLS TO STUDY ENTANGLEMENT

$T = 0$: one tangle τ_1 , concurrence C_{ij}

Some idea of n-wise entanglement through CKW conjecture

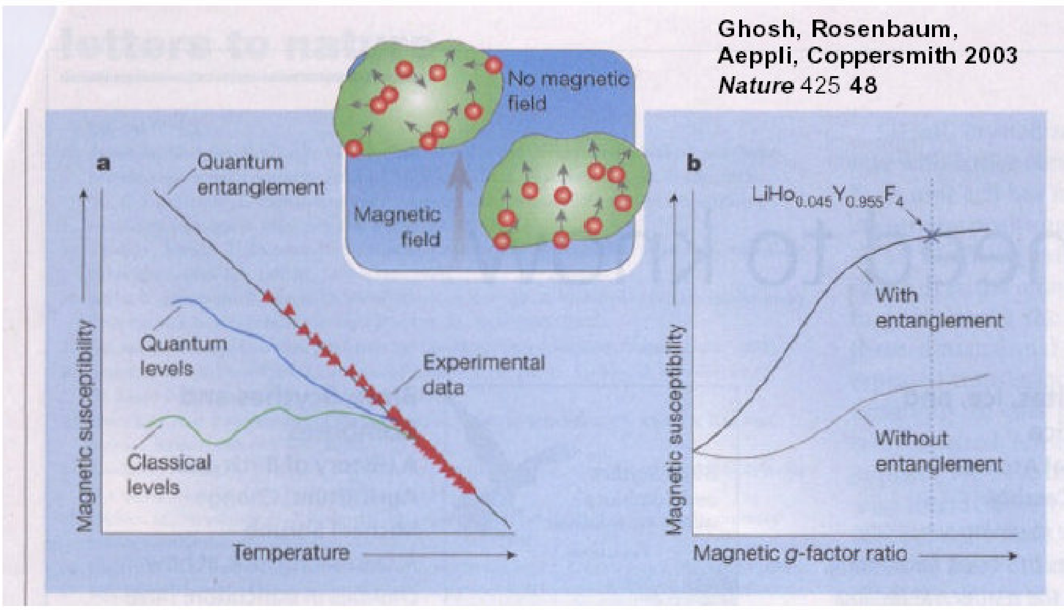
T > 0 : concurrence C_{ij} only

Good news: τ_1, C_{ij} are easy to calculate

Experimental demonstrations of entanglement : mostly confined to the microworld

Ghosh, Rosenbaum, Aeppli and Coppersmith (Nature 425, 48 (2003) : Entanglement can affect the magnetic properties of solids

Macroscopic properties of $LiHo_{0.045}Y_{0.955}F_4$ showing effects of entanglement



Thermodynamic properties can serve as macroscopic entanglement witnesses

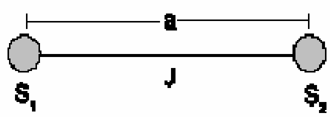
Brukner, Vedral, Zeilinger (2004): Susceptibility as enanglement witness in antiferromagnetic spin dimer system

Thermal entanglement properties of small spin clusters (Bose + Tribedi, Phys. Rev. A 72, 022314 (2005))

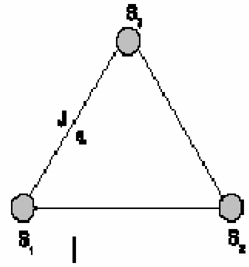
Molecular and nanomagnets: dominant interactions are confined to small spin clusters like dimers, trimers, tetramers etc.

Examples:

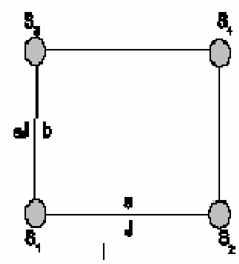
Dimers (S = ½) :
$Cu(NO_3)_2$ 2.5 D_2O, VO (HPO_4).0.5 H_2)



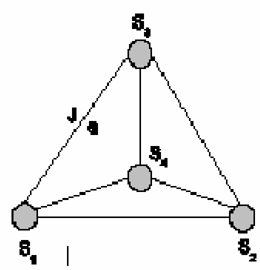
Symmetric trimers (S = ½):
Na_9 [$Cu_3Na_3(H_2O)_9$ (α- AsW_9 $O_{33})_2$].26H_2O
[Cu_3(cpse)$_3$ ($H_2O)_3$].8.5 H_2O

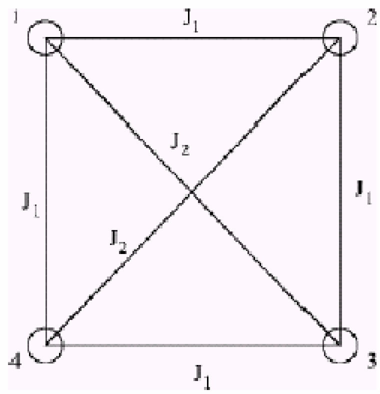


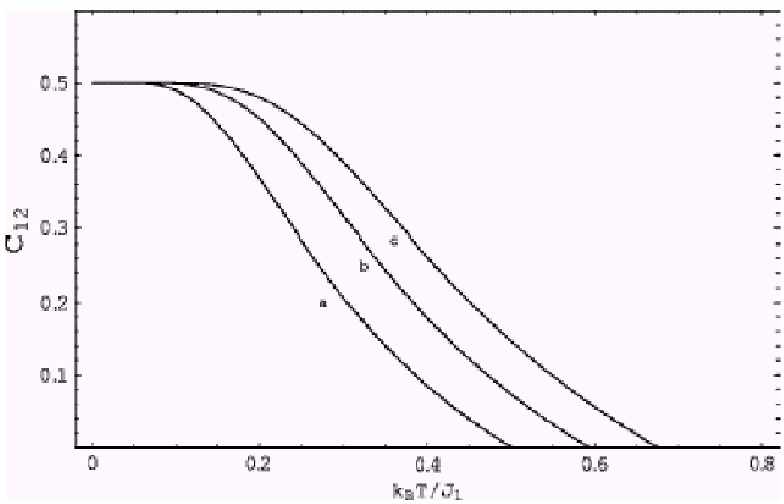
Tetramer ($S = ½$)
Polyoxovanadate compound
$(NHEt)_3[V_8^{IV} V_4^{V} As_8O_{40}(H_2O)].H_2O$
Finite temperature entanglement
properties:



Tetrahedron:







$\frac{J_2}{J_1} = 0.5$, T_C : temperature above which entanglement as measured by concurrence is zero

Calculation of C_{ij}'s : requires knowledge of both eigenvalues and eigenvectors of Hamiltonian

Macroscopic thermodynamic observables can serve as EWs

Experimental data can provide evidence for entanglement

Entanglement witness Z_{EW} :

ρ is entangled $\Rightarrow tr(Z_{EW}\,\rho) < 0$

ρ is separable $\Rightarrow tr(Z_{EW}\,\rho) \geq 0$

Internal energy U, Magnetization M, Susceptibility χ : serve as Ews

Suceptibility χ_α along direction α

$\alpha = x, y, z$:

$$\chi_\alpha = \frac{(g\mu_B)^2}{k_B T}\left[\left\langle (M_\alpha)^2 \right\rangle - \left\langle M_\alpha \right\rangle^2\right]$$

$$M_\alpha = \sum_j S_j^\alpha$$

Magnetic field = zero $\Rightarrow \langle M_\alpha \rangle = 0$

Isotropy $\Rightarrow \chi_x = \chi_y = \chi_z = \chi$

$$\chi = \frac{(g\mu_B)^2}{k_B T}\left[\frac{N}{4} + \frac{2}{3}\sum_{i<j}\langle S_i . S_j \rangle\right]$$

N = number of interacting spins

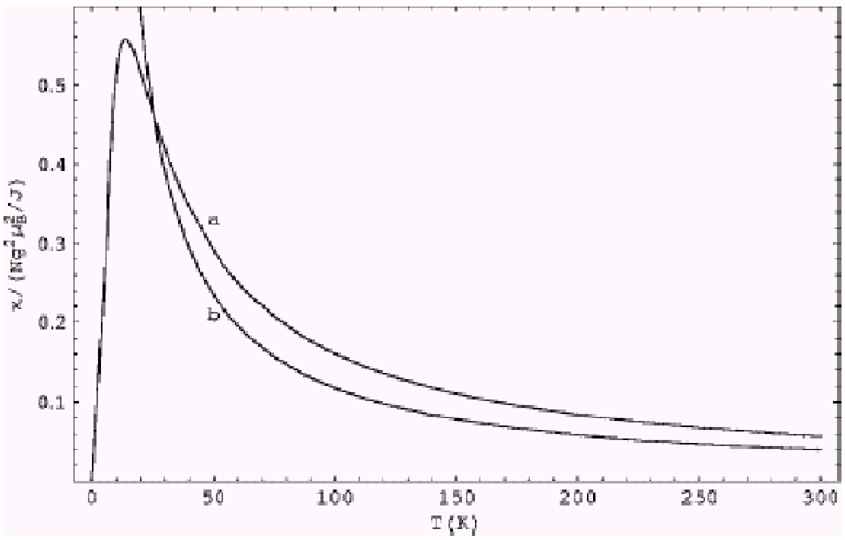
$\sum_{i<j}\langle S_i . S_j \rangle = \langle H_S \rangle$, where H_S is Hamiltonian with all-to-all spin couplings

$\langle H_S \rangle < 0$ because of AFM correlations

For separable states, $\langle H_S \rangle_{\min}$ = ground state energy of equivaent classical Hamiltonian

$$N = 4, \langle H_S \rangle_{\min} = -\frac{1}{2}$$

$$\chi \geq \frac{(g\mu_B)^2}{k_B T}\frac{2}{3}$$ for separable states



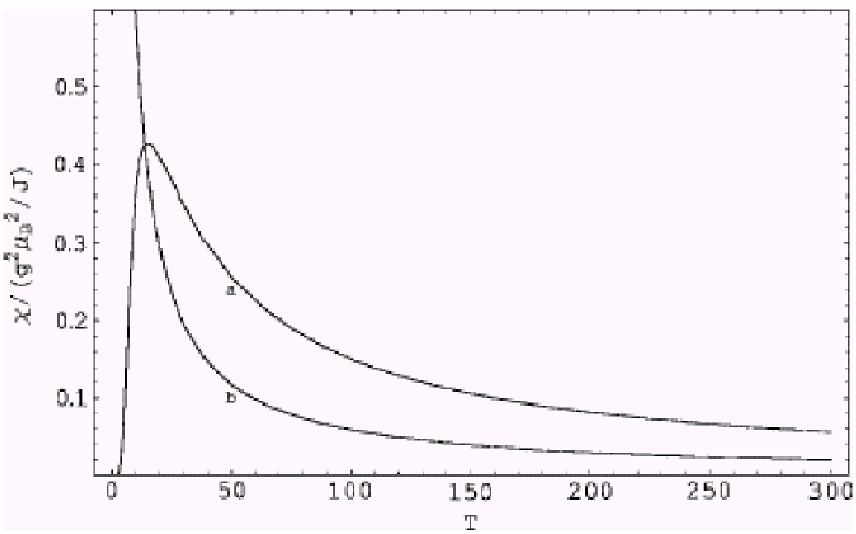
Susceptibility curve for V12

$\frac{J_1}{k_B} \approx 17.6\,K$, $T_C \approx 25.4\,K$: the critical entanglement temperature (lower bound) below which entanglement is present in V12

T_C^{pair} : critical temperature for pairwise entanglement $\approx 15.2\,K$

$T_C > T_C^{pair} \Rightarrow$ entanglement other than pairwise entanglement present for $T_C^{pair} < T < T_C$

Result for tetrahedron:



When $\chi_x = \chi_y = \chi_z = \chi$,

separability criterion for a single cluster of N spins is

$$\chi \geq [(g\mu_B)^2 / k_B T] N/6$$

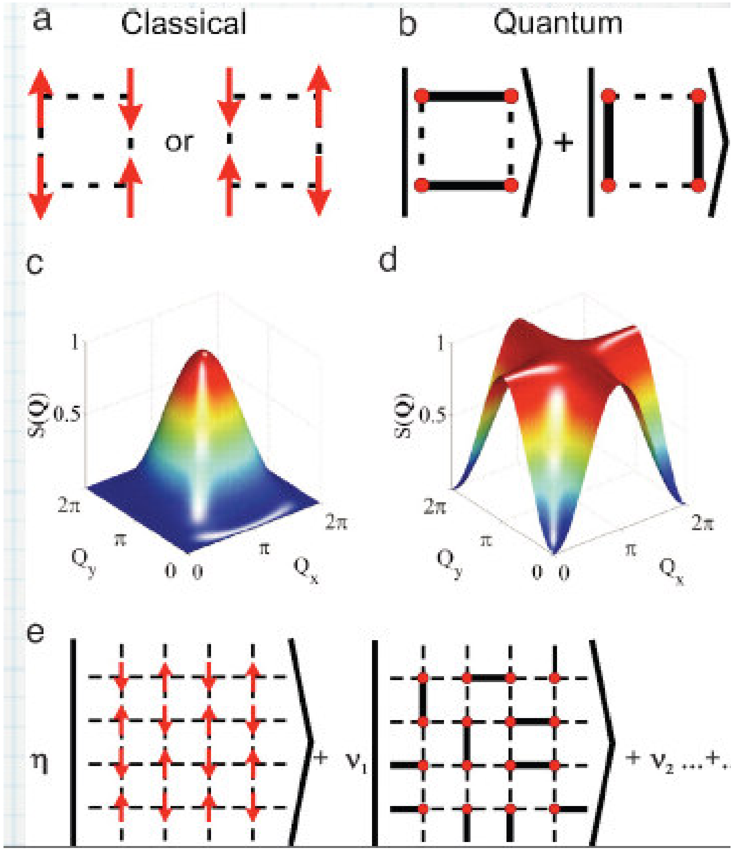
More general inequality:

$$\chi_x + \chi_y + \chi_z \geq NS / k_B T$$

Brukner et al. (2004, 2006) analysed susceptibility data of cupric nitrate trihydrate with $T_C \sim 5$ K

Tribedi and Bose (2005): for polyoxovanadate compound
$T_C \sim 25.4$ K

Vértesi and Bene (2006): for NaV_3O_7,
$T_C \sim 365$ K!



Christensen et al., PNAS (2007)

Neutron scattering cross-section:

$$\frac{d^2\sigma}{d\Omega \; dE} \approx \left| \langle f \,|\, S_Q \,|\, i \rangle \right|^2$$

Structure factor

$$S_Q = \sum_j S_j \exp(i Q . r_j)$$

Entanglement properties of spin-disordered states:

For rotationally invariant states, reduced density matrix of two spins describes a Werner state:

$$\rho_2 = p\left|\psi^-\right\rangle\left\langle\psi^-\right| + (1-p)/4\, I$$

$(-1/3 \leq p \leq 1)$

Concurrence

$$C(\rho_2) = \max(0, 3/2\, p - 1/2)$$

Two-site von Neumann entropy

$$S(\rho_2) = -\sum_j \lambda_j \log \lambda_j$$

$$= 2 - (1 + 3p)/4 \log(1 + 3p) - 3(1 - p)/4 \log(1 - p)$$

Examples of rotationally-invariant states:

Ground state of MG chain, RVB states

Ground state of MG chain: the VB spins are maximally entangled, concurrence has non-zero value only if the two spins form a singlet

One-site, two-site von Neumann entropies can be calculated

RVB state on a bipartite lattice:

$$\left|\Psi\right\rangle = \sum h\left(i_1,\ldots\ldots,i_N, j_1,\ldots\ldots,j_N\right)\left|\left(i_1, j_1\right)\ldots\ldots\left(i_N, j_N\right)\right\rangle$$

Chandran et al. (PRL 2007):

RVB states are genuine multipartite entangled with a negligible amount of two-site entanglement

Dhar and Sen (De) (2010) : RVB state on a spin ladder, bipartite entanglement on rungs (chains) significant (not substantial)
Genuine multipartite entanglement negligible

Sen (De), Sen et al., PRL (2010)
Area law:

Block entanglement in a gapped ground state is proportional to the area of block boundary

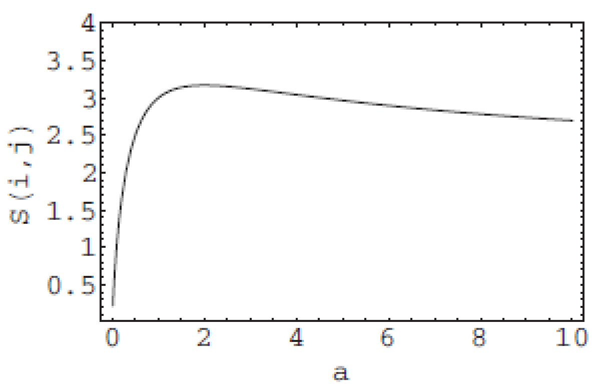
At criticality: more complex relations

Highly frustrated systems: area law not obeyed

AKLT VBS state:

Single-site von Neumann entropy has maximum possible value log 3

Two-site von Neumann entropy has maximum value in the AKLT state for a one-parameter family of S = 1 Hamiltonians (Tribedi + Bose, PRA 2007)



a = 2 corresponds to AKLT model

Signatures of quantum phase transitions in spin systems using QIT measures:

Quantum phase transitions (QPTs) in many body systems: occur at T = 0, brought about by tuning a non-thermal parameter (pressure, chemical composition, magnetic field etc.)

QPTs: first order, second order….

Classical critical point: thermal fluctuations, scale invariance, divergent correlation length. Free energy is a non-analytic function at $T = T_c$

Quantum critical point: quantum fluctuations at $T = 0$, scale invariance, divergent correlation length.
Ground state energy: non-analytic function of tuning parameter $g = g_c$

Quantum Information Theoretic (QIT) measures like entanglement and fidelity provide signatures of QPTs

First order QPT: discontinuity in first derivative of ground state energy

Discontinuity in bipartite entanglement measure (Bose et al 2002, Wu et al 2004)

Second order QPT: discontinuity/divergence in second derivative of ground state energy

Discontinuity/divergence in first derivative of bipartite entanglement measure

How does entanglement evolve at a QPT ?

Osterloh et al. Nature (2002)

Osborne et al. PRA (2002)

$$H = -\lambda \sum_{i=1}^{N} (1+\gamma) S_i^x S_{i+1}^x + (1-\gamma) S_i^y S_{i+1}^y - \sum_{i=1}^{N} S_i^z$$

$\gamma = 0$: isotropic XY model

$\gamma = 1$: transverse Ising model

QCP at $\lambda_c = 1$

Order parameter: $\langle S^x \rangle \neq 0$ for $\lambda > \lambda_c$

$= 0$ for $\lambda \leq \lambda_c$

$\langle S^z \rangle \neq 0$ for any value of λ

Is entanglement between distinct subsystems extended over macroscopic regions ?

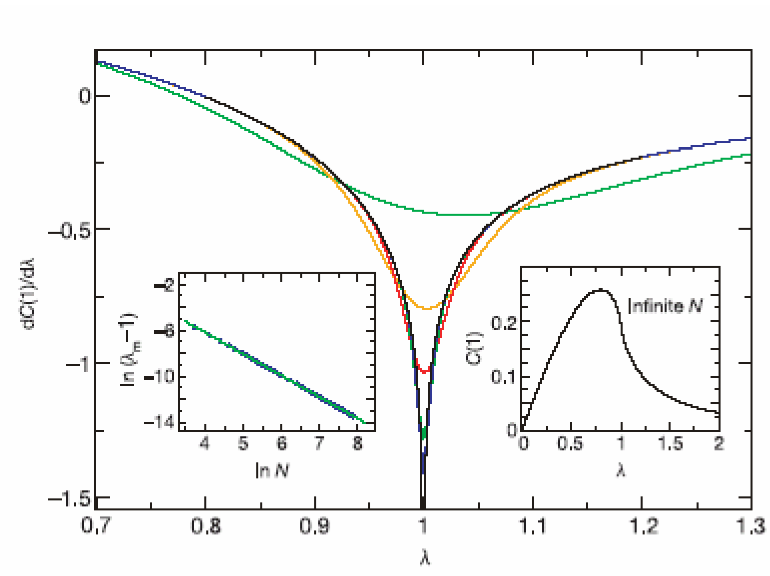
Concurrence: measure of pairwise entanglement

Transverse Ising model: at $\lambda_c = 1$,

$C(n) = 0$ for $n > 2$

Pairwise entanglement is not long-ranged

$$\partial_\lambda \, C(1) = \frac{8}{3\pi^2} \ln|\lambda - 1| + const.$$



(Osterloh et al., Nature 2002)

First derivative of concurrence: non-analytic at QCP

Vidal et al. PRL (2003): consider entanglement between a block of spins (length L) and rest of the system

Von Neumann entropy:

S_L = (c1+ c2)/6 $\log_2$ L + k

(diverges logarithmically with L)

First derivative of $S(i)$ and $S(i,j)$ w.r.t.

λ diverges at QCP $\lambda_c = 1$ (Chen 2007)

Generalised global entanglement (GGE):
measure of multipartite entanglement

$$G(2,n) = \frac{d}{d-1}\left[1 - \sum_{l,m=1}^{d^2} |[\rho(j,j+n)]_{lm}|^2\right],$$

GGE maximal at critical point
Entanglement length (EL) diverges at critical point
EL is half the correlation length

Another QIT measure: Fidelity F

$$F(\lambda,\lambda+\delta\lambda) = |\langle\psi_0(\lambda)|\psi_0(\lambda+\delta\lambda)\rangle|.$$

(Modulus of overlap of normalized ground state wave functions)

Reduced Fidelity (RF): refers to a subsystem

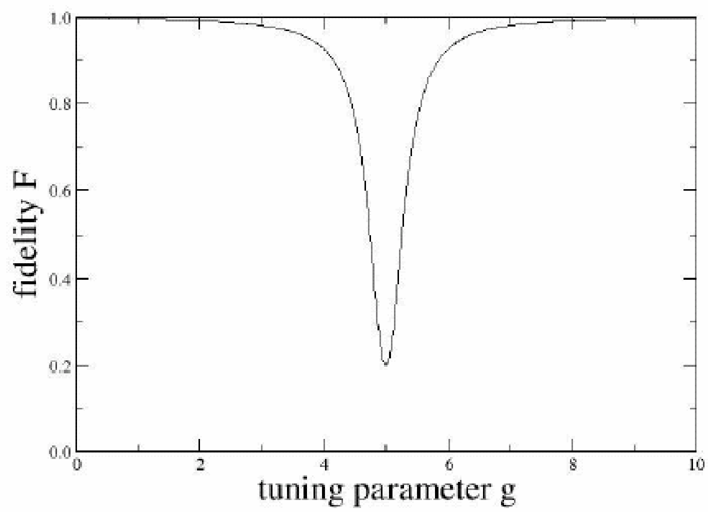
$$F_R(h, h+\delta) = \mathrm{Tr}\sqrt{\rho^{1/2}\tilde{\rho}\rho^{1/2}}.$$

(Overlap between reduced density matrices $\rho \equiv \rho(h)$ and $\tilde{\rho} \equiv \rho(h+\delta)$)

Fidelity and RF drop sharply at a QCP

Fidelity susceptibility diverges

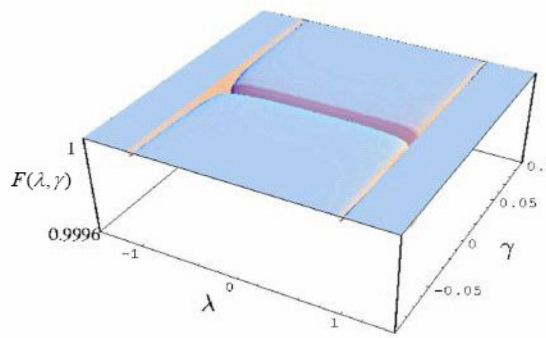
$$F(g) = \left|\langle \Psi(g) | \Psi(g+\Delta g) \rangle\right|$$



Fidelity in the quantum XY chain

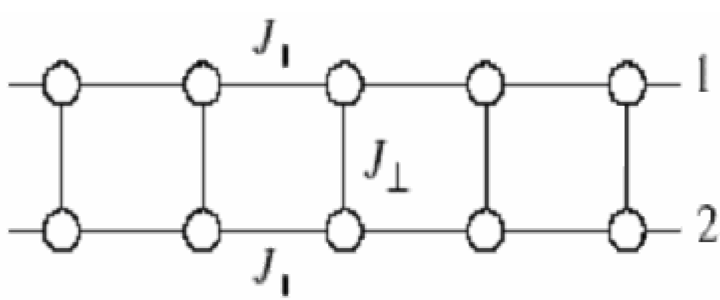
$$\hat{H}(\gamma,\lambda) = -\sum_{i=-M}^{M}\left(\frac{1+\gamma}{2}\hat{\sigma}_i^x\hat{\sigma}_{i+1}^x + \frac{1-\gamma}{2}\hat{\sigma}_i^y\hat{\sigma}_{i+1}^y + \frac{\lambda}{2}\hat{\sigma}_i^z\right)$$

- quantum phase transitions indicated by drop in fidelity.
- Ising transition at $\lambda=\pm1$.
- Anisotropy transition at $\gamma=0$.
- critical exponents in agreement with scaling theory.



(Zanardi & Paunkovic, PRE 74, 031123 (2006).)

We use QIT measures to study QPTs in two-chain spin ladders



Ladder Hamiltonian:

$$\mathcal{H} = \sum_{j=1}^{L} [J_{\|}(\mathbf{S}_{1,j} \cdot \mathbf{S}_{1,j+1} + \mathbf{S}_{2,j} \cdot \mathbf{S}_{2,j+1}) + J_{\perp}\mathbf{S}_{1,j} \cdot \mathbf{S}_{2,j}] - H\sum_{j=1}^{L} (S^z_{1,j} + S^z_{2,j}),$$

Organic ladder compounds exhibit QPTs by varying an external magnetic field H

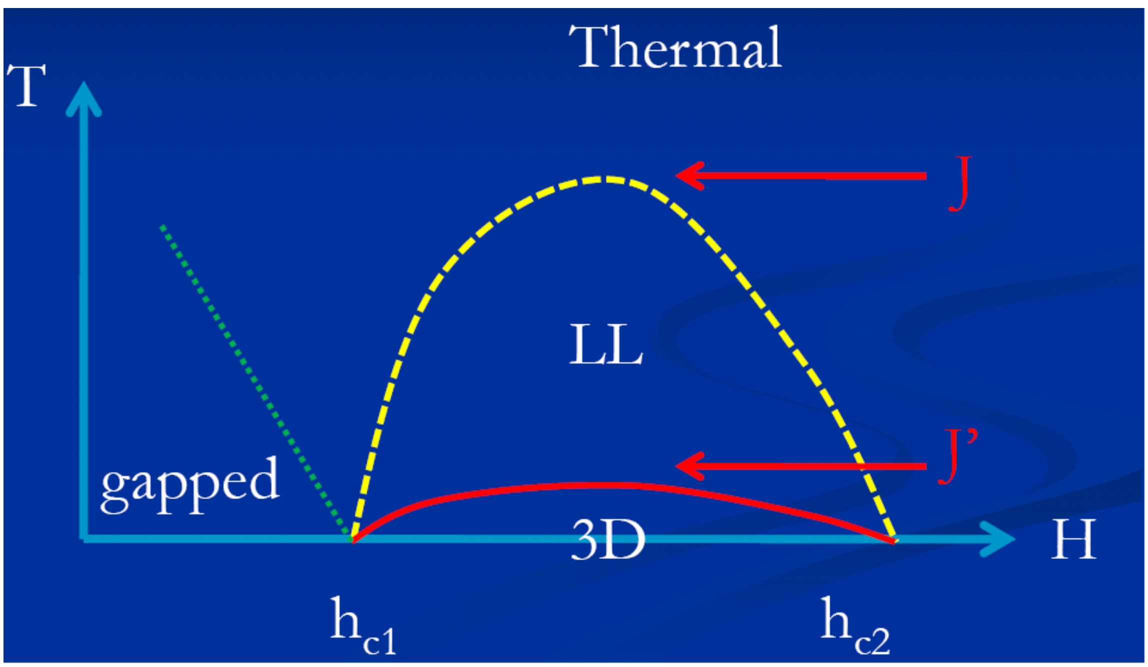
Examples: $Cu_2(C_5H_{12}N_2)_2Cl_4$

$(C_5H_{12}N)_2CuBr_4$

$(5IAP)_2CuBr_4.2H_2O$

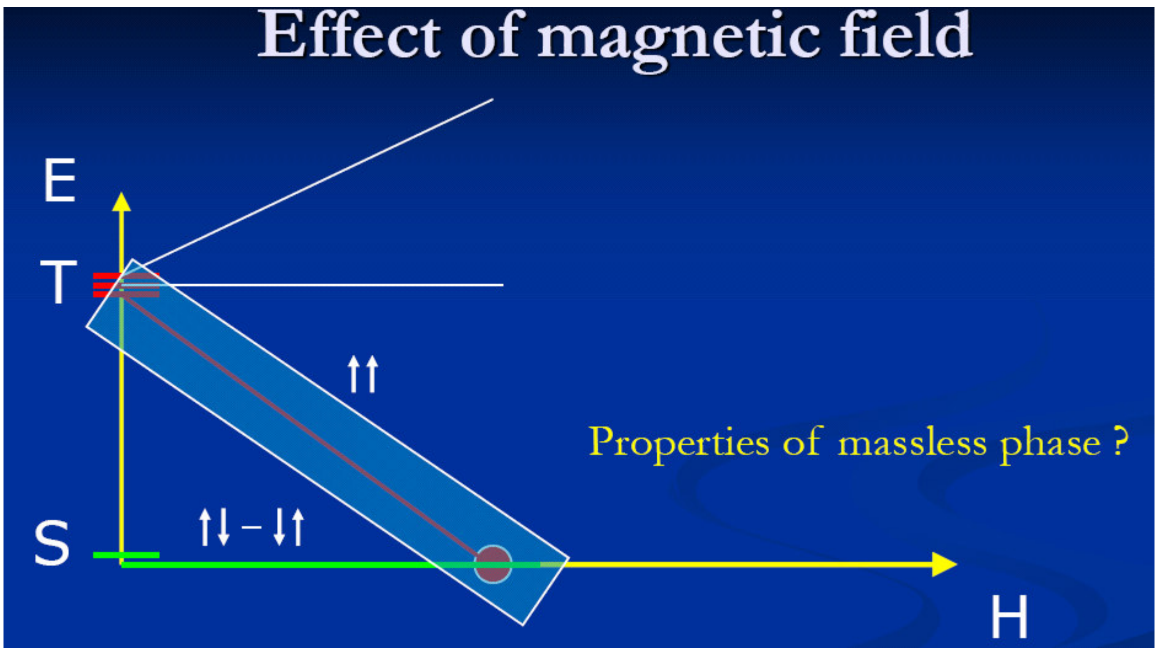
Two QCPs: at H_{C1} and H_{C2}

Generic Phase Diagram



$0 < H < H_{C1}$: spin gap phase (Δ = magnitude of spin gap)

Zeeman splitting of triplet excitation spectrum



At $H = H_{C1} = \Delta$, gap closes and QPT occurs to Luttinger Liquid (LL) phase with gapless excitation spectrum

At $H = H_{C2}$, another QPT to the fully polarized ferromagnetic (FM) state occurs

Do QIT measures provide signatures of QPTs at $H = H_{C1}$ and H_{C2} ?

Our work (Tribedi and Bose, PRA 2009)

Single-site von Neumann entropy:

$$S(i) = -Tr\ \rho(i) \log_2 \rho(i)$$

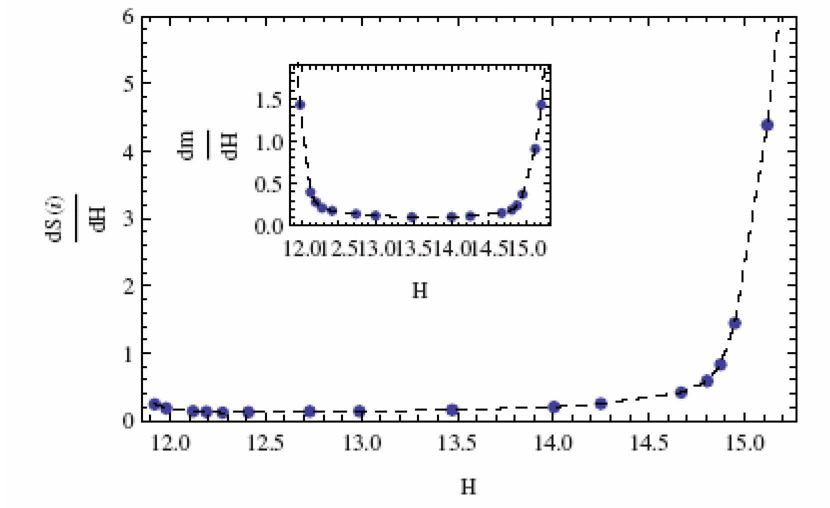
ρ (i) = single-site reduced density matrix

$$\rho(i) = \begin{pmatrix} \frac{1}{2} + \langle S_i^z \rangle & 0 \\ 0 & \frac{1}{2} - \langle S_i^z \rangle \end{pmatrix}$$

$$S(i) = -\sum_i \lambda_i \log_2 \lambda_i$$

λ_i (i = 1, 2): diagonal elements of ρ (i)

$\frac{dS(i)}{dH}$ diverges only near H_{C2}



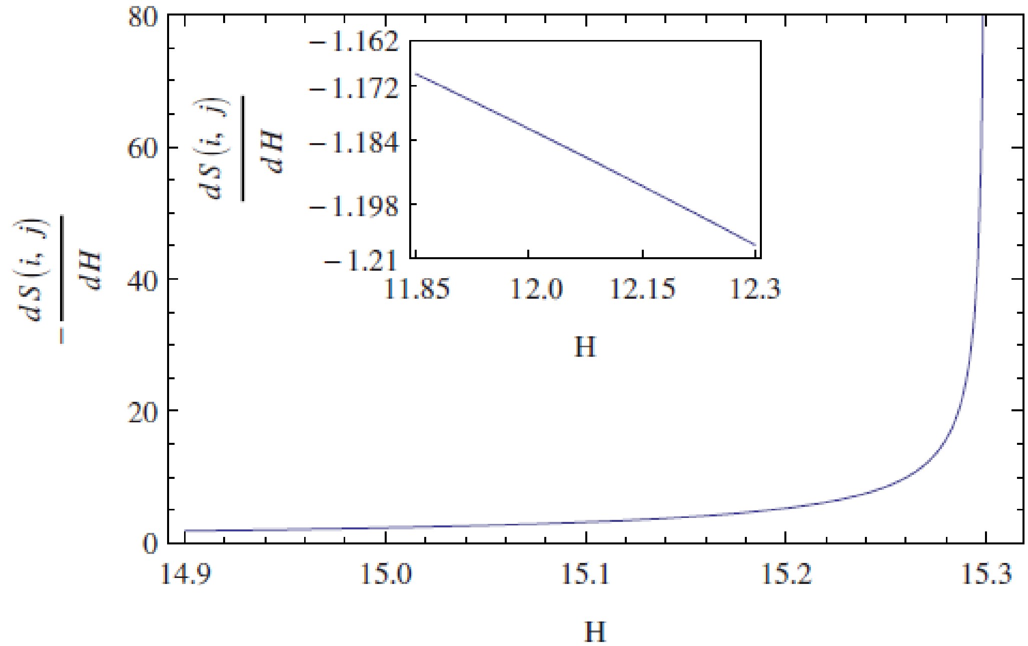
Two-site entanglement:

$$S(i, j) = -Tr\ \rho(i, j) \log_2 \rho(i, j)$$

$$= -\sum_i \epsilon_i \log_2 \epsilon_i ,$$

ε_i's: eigenvalues of ρ (i , j)

Again, first derivative of S(i, j) w.r.t. H diverges at H = H_{C2} but not at H = H_{C1}



Similar result is obtained for first derivative of nearest-neighbour concurrence w.r.t. magnetic field

Can other QIT measures detect both the QCPs ?

Reduced Fidelity (RF):

$$F_R(h, h+\delta) = \mathrm{Tr}\sqrt{\rho^{1/2}\tilde{\rho}\rho^{1/2}}.$$

Consider one-site RF

One-site reduced density matrix is

$$\rho(i) = \begin{pmatrix} \frac{1}{2} + \langle S_i^z \rangle & 0 \\ 0 & \frac{1}{2} - \langle S_i^z \rangle \end{pmatrix}$$

Another measure: RF susceptibility (RFS)

$$\chi_R(H) = \lim_{\delta \to 0} \frac{-2 \ln \mathcal{F}_R(H, H+\delta)}{\delta^2}$$

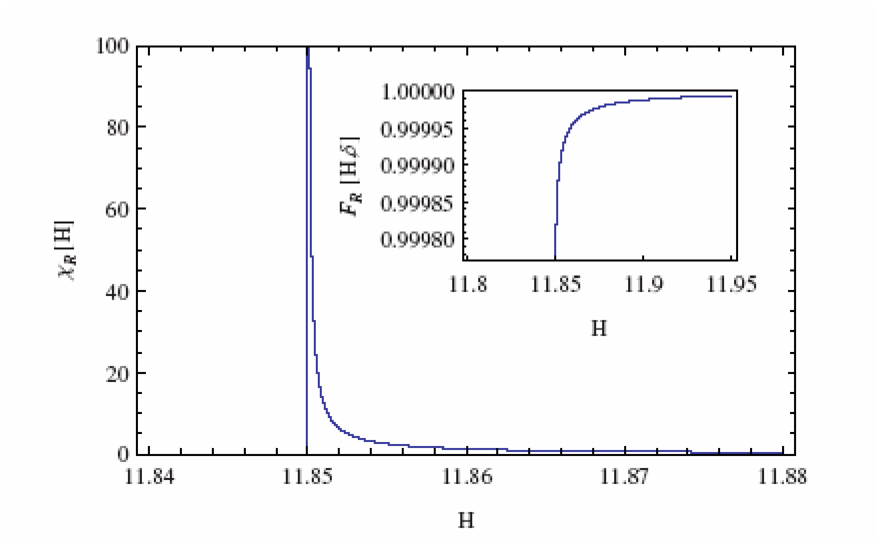
m(H) = $\langle S_i^z \rangle$ known close to QCPs

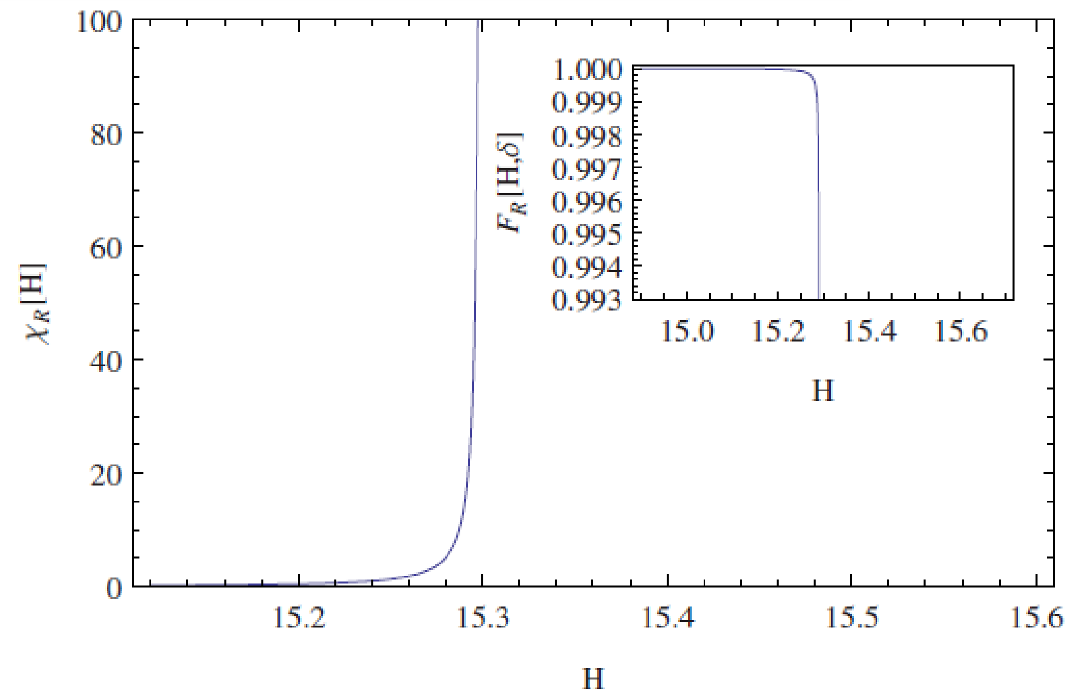
$$m(H) \sim \frac{\sqrt{2}}{\pi} \sqrt{(H - H_{c1})/J_\parallel}, \quad H > H_{c1},$$

$$m(H) \sim 1 - \frac{\sqrt{2}}{\pi} \sqrt{(H_{c2} - H)/J_\parallel}, \quad H < H_{c2}.$$

RF drops to zero at both QCPs

RFS diverges at both QCPS





A new measure of quantum correlations: Quantum Discord

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