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Quantum frustration, entanglement, and frustration-driven quantum phase transitions

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Overview

1) Frustrated systems

2) Toulouse criteria: classical

3) Universal measure of total frustration

4) Toulouse criteria: quantum

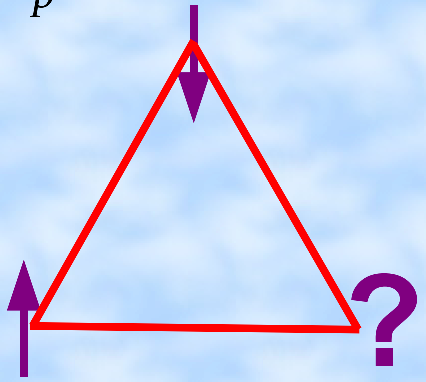
5) Frustration and entanglement

6) Valence bonds: frustration-driven transitions

Defining and characterizing frustration

Many body systems: global H sum of local terms

$$H = \sum_p h_p$$



Frustration: impossibility to satisfy simultaneously all local terms h_p

Sources of frustration: Classical World

Nontrivial geometry of the underlying physical space, e.g.: Heisenberg antiferromagnet on the 2-d Kagomé lattice

Competing interactions on different length scales, e.g. spin chains with antiferromagnetic n.n. and n.n.n. Interactions.

Sources of frustration: Quantum World

Entanglement: Non-commutativity of the different local interaction terms

Classical Toulouse criteria for frustration

[Formulation 1]: A classical Hamiltonian system is frustrated iff it is impossible to transform it in a fully ferromagnetic model only by means of local spin inversions

[Formulation 2]: A classical Hamiltonian is frustrated iff there exists at least one closed loop for which :

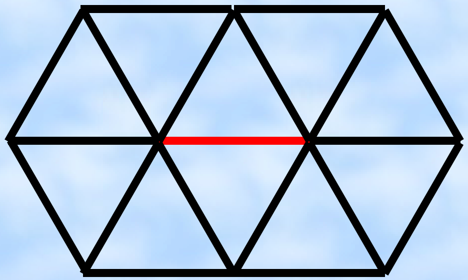
$$(-1)^{N_{af}} = -1$$

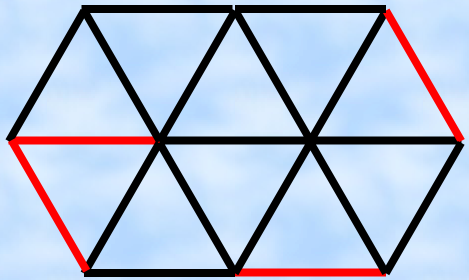
where N_{af} is the number of antiferromagnetic bonds.

Dicotomic: only two possible answer: **yes** or **no**

Ferromagnetic Links

Anti-ferromagnetic Links





Limitations of the Toulouse criteria in the quantum regime

Entanglement: T.C. do not detect quantum frustration

Classical Ising ferromagnet
All local terms commute

$$H = -J\left[S_1^z S_2^z + S_2^z S_3^z\right]$$

Minimum of the local energy terms: each pair of spins aligned.
Global ground state: all spins aligned. **No frustration.** ***T.C. ok!***

Quantum XX Hamiltonian
Local terms do not commute

$$H = -J\left[\left(S_1^z S_2^z + S_1^x S_2^x\right) + \left(S_2^z S_3^z + S_2^x S_3^x\right)\right]$$

The ground state of each pair “in vacuum” is a maximally entangled Bell state.
But spin 2 cannot be maximally entangled symultaneously with spins 1 and 3.
Monogamy of entanglement **--->** **Frustration.**

However, according to the T.C., there is no frustration!

Universal measure of total frustration

Measure of frustration: the degree of incompatibility between the local "vacuum" ground space and the "dressed" one, namely, the space of the reduced local density matrices in the presence of the many-body interactions.

$$f_p = 1 - Tr\left(\rho_p \Pi_p\right)$$

Π_p : projector onto the local ground space (local GS in "vacuum")

ρ_p : projection of the global GS on the local GS

$$f_p \geq \epsilon_p^{(d)}$$

$$\epsilon_p^{(d)} = 1 - \sum_{k=1}^{d} \lambda_k^{\downarrow}$$

Frustration-free

$$f_p = \varepsilon_p^{(d)} = 0$$

INES (INEquality Saturating): Quantum Frustration

$$f_p = \varepsilon_p^{(d)} > 0$$

Non-INES: quantum and geometric frustration

$$f_p > \varepsilon_p^{(d)}$$

Quantum Toulouse Criteria

If the global ground space has degeneracy > 1, the measure of local frustration can depend on the choice of the particular ground state

Maximally Mixed Ground State: convex combination with equal weights of all degenerate ground states. The MMGS preserves the same symmetries of the Global Hamiltonian

Quantum Touluse Criteria:

A model is prototype if
1) there exists at least one local ground state common to all local terms;
2) all coupling vectors are ferromagnetic.

Conjectures:

Quantum Toulouse criterion I - All prototype models are INES.

Quantum Toulouse criterion II – All models obtained from prototype models by local unitary operations and partial transpositions are INES.

No rigorous proof yet. Supported by vast numerical evidence.

Frustration and Entanglement

Pure Ground state → $\varepsilon_p^{(d)}$ → **Bipartite entanglement monotone** on states with Schmidt rank > *d.* Vanishing on states with Schmidt rank < *d*.

↓

$\varepsilon_p^{(1)}$ → **Bipartite GS Entanglement** between the local subsystem p and the rest of the system R. Distance from the set of biseparable pure states.

Mixed Ground State → Sum of the (convex-roof) bipartite **entanglement** between p and R and of the **classical correlations** established by a local measurement performed on p by an ancillary system A.

$$\varepsilon_p^{(d)} = E_{p|R}^{(d)} + C_{p|A}^{(d)}$$

Frustration and Entanglement: generic Heisenberg models (spin ½) - I

$$H=\sum_p h_p \qquad h_{p=(i,j)}=\alpha^x_{i,j} S^x_i S^x_j + \alpha^y_{i,j} S^y_i S^y_j + \alpha^z_{i,j} S^z_i S^z_j$$

H preserve parity along the three spin directions x, y and z

$$\rho_p = \begin{pmatrix} \frac{1}{4}+g_p^{zz} & 0 & 0 & g_p^{xx}-g_p^{yy} \\ 0 & \frac{1}{4}-g_p^{zz} & g_p^{xx}+g_p^{yy} & 0 \\ 0 & g_p^{xx}+g_p^{yy} & \frac{1}{4}-g_p^{zz} & 0 \\ g_p^{xx}-g_p^{yy} & 0 & 0 & \frac{1}{4}+g_p^{zz} \end{pmatrix}$$

ρ_p admits as eigenstates the maximally entangled Bell states

⇓

If all h_p admit a common ground state with d>1 the system is frustration free

⇓

Absence of quantum frustration

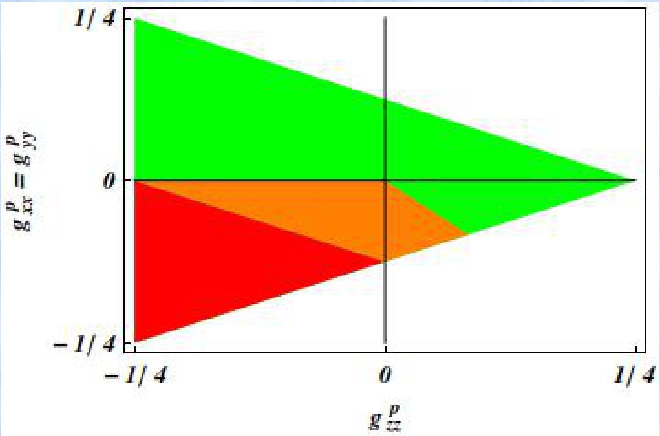
Frustration and Entanglement: generic Heisenberg models (spin ½) - II

$$\rho_p = \begin{pmatrix} \frac{1}{4}+g_p^{zz} & 0 & 0 & g_p^{xx}-g_p^{yy} \\ 0 & \frac{1}{4}-g_p^{zz} & g_p^{xx}+g_p^{yy} & 0 \\ 0 & g_p^{xx}+g_p^{yy} & \frac{1}{4}-g_p^{zz} & 0 \\ g_p^{xx}-g_p^{yy} & 0 & 0 & \frac{1}{4}+g_p^{zz} \end{pmatrix}$$

ρ_ij has as eigenstates the Bell states, and d=1 (nondeg. antiferr. local GS)

Local-term concurrence C_ij

$$C_{ij} = max\left(0, 1-2\varepsilon_{ij}^{(1)}\right) \geq max\left(0, 1-2f_{ij}\right)$$

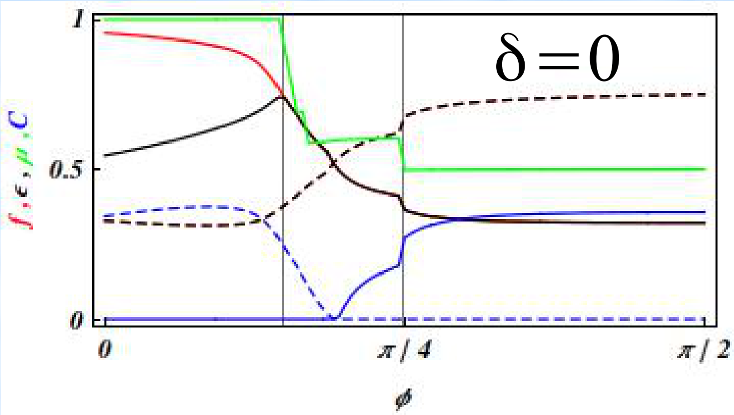


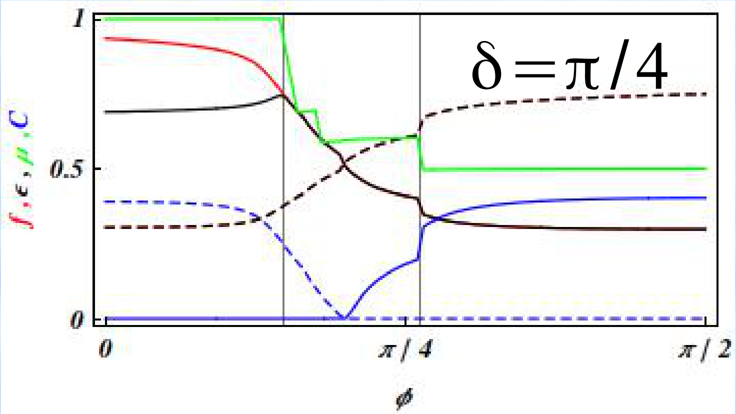
$$\sum_j max\left(0, 1-2f_{ij}\right)^2 = \sum_j C_{ij}^2 \leq \tau_i = 1$$

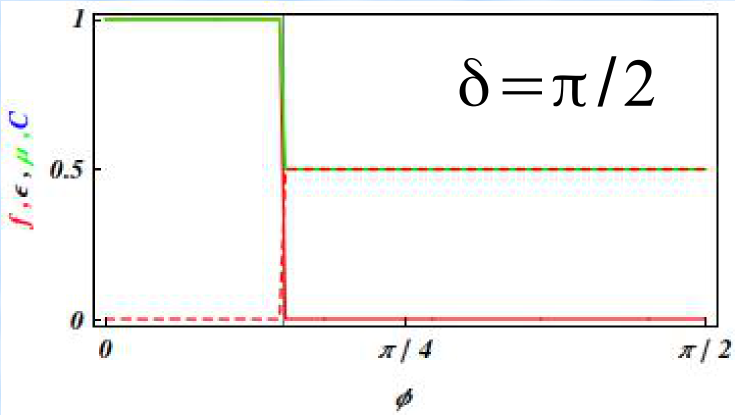
General relation between frustration and monogamy of entanglement!

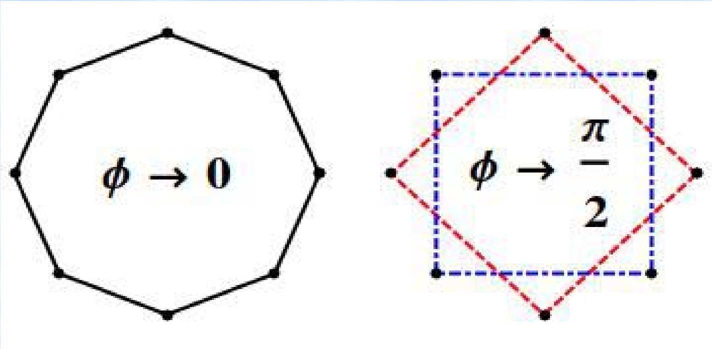
VBS (dimerized GS): transition to QF (INES)

$$\begin{aligned} H &= J\cos\phi \sum_i \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \sin\delta\, S_i^z S_{i+1}^z\right) \\ &+ J\sin\phi \sum_i \left(S_i^x S_{i+2}^x + S_i^y S_{i+2}^y + \sin\delta\, S_i^z S_{i+2}^z\right) \end{aligned}$$





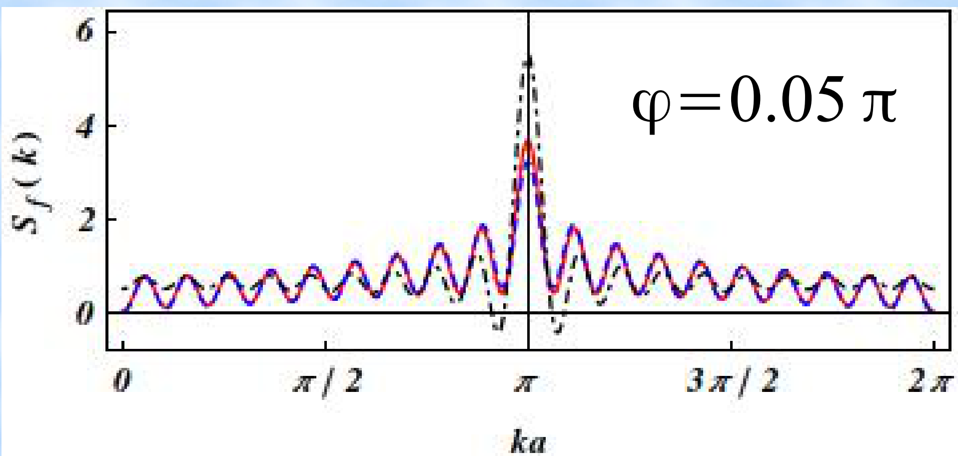


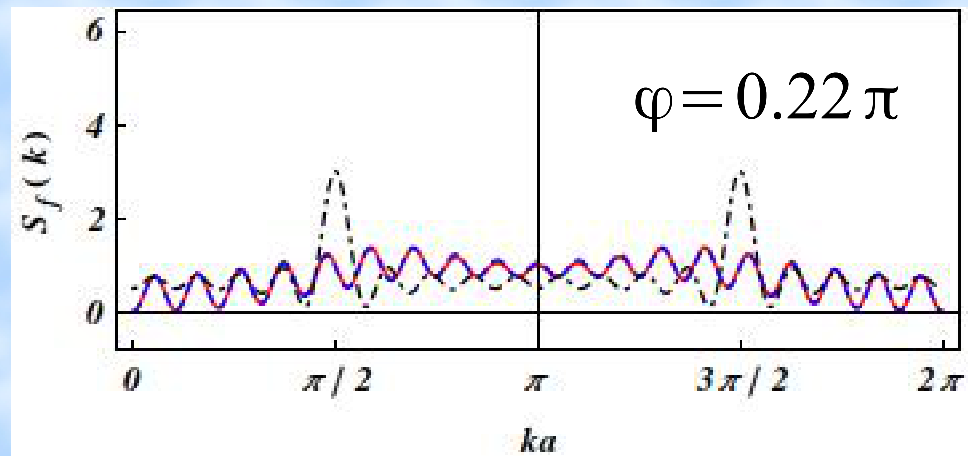


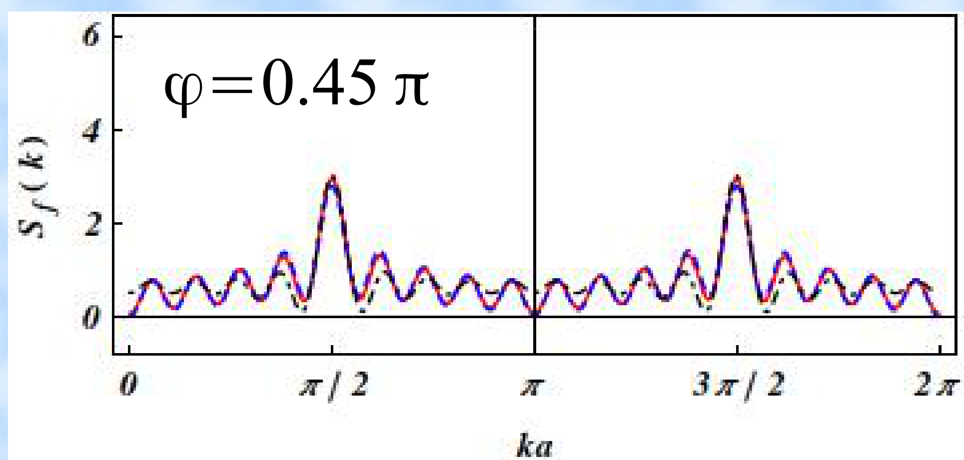
Frustration-driven transition to VBS: observable

Behavior of the static structure factor approaching the Majumdar-Ghosh point J_2/J_1 = 1/2

$$S_f(k)=\frac{1}{N}\sum_{i,j}\cos(ka|i-j|)\langle \vec{S}_i \cdot \vec{S}_j\rangle$$







Conclusions & Outlook

Summary:

1) Universal measure of total frustration

2) General relation with GS entanglement

3) QuantumToulouse criteria

4) Relation between frustration and monogamy of entanglement in generic Heisenberg models

5) VBS: transition from geometric to quantum frustration

Memos for future directions:

1) Scaling behavior, area laws, and dynamics. Existence of a “frustration length”?

2) Relations with genuine multipartite entanglement.

3) Frustration and globally ordered phases (e.g. topological order).

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