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Quantum Phase Transitions

A VIGRE[1] Research Focus Group, Fall 2011–Spring 2012

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See the RFG webpage for more information:
http://www.math.ucdavis.edu/~bxn/rfg_quantum_phase_transitions.html
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Outline

- Classic Phase Transitions
- Phase Transitions Without Temperature
- Quantum Phase Transitions
- What is a Phase?

Classic Phase Transitions

A physical system is described by a space of states, X, (e.g., phase space) and a function $H : X \to \mathbb{R}$ (the Hamiltonian). $H(x)$ is the energy of the system in state x. In general, the state of the system is described by a probability measure, $\mu(dx)$, on X. The mean energy is then $E(\mu) = \int H(x)\mu(dx)$.
States of thermal equilibrium are the minimizers of the free energy F:

$$F(\mu) = E(\mu) \ - \ TS(\mu)$$

S: entropy; T temperature measured in units of k_B, the Boltzmann constant (approx. $1.38 \times 10^{23} J/K$.)
Phase transitions arise from the competition between the energy and the entropy term in F, with T controlling their relative importance.

Example: Ising model
$d = 1, 2, 3, \ldots,,\ X = \{-1, 1\}^{\mathbb{Z}^d} = \{\sigma : \mathbb{Z}^d \to \{-1, 1\}\}$.
For each finite $\Lambda \subset \mathbb{Z}^d$, define

$$H_\Lambda(\sigma) = -J \sum_{\substack{x,y \in \Lambda \\ |x-y|=1}} \sigma_x \sigma_y .$$

$$\begin{matrix} 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 & 1 \\ -1 & 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & 1 \end{matrix} \quad \text{versus} \quad \begin{matrix} 1 & -1 & -1 & -1 & 1 \\ 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 & -1 \end{matrix}$$

Phase Transitions Without Temperature

The notion of phase transition, the existence of a critical value of a parameter where the behavior undergoes a qualitative change, has found broad application, including in situations where the temperature is not the controlling parameter. What is required: two competing trends and a parameter that changes the relative strength of the two trends; and a phenomenon, observable, or effect to make the question interesting.

- Phase transitions without energy. Example: Percolation (probability versus degeneracy (entropy)).
- Phase transitions without (obvious) entropy: Random Matrices.
- Phase transitions in the ground states on the Hamiltonian: quantum phase transitions (competing, non-commuting, contributions to the energy).

Quantum Phase Transitions

Transitions in qualitative behavior of the ground states (minimum energy), of Hamiltonians of the form

$$H = A + \lambda B, \quad \lambda \in \mathbb{R}.$$

E.g., Ising model in transverse field:

$$H_\Lambda(\sigma) = -J \sum_{\substack{x,y\in\Lambda \\ |x-y|=1}} \sigma_x^3 \sigma_y^3 + \lambda \sum_{x\in\Lambda} \sigma^1.$$

where

$$\sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

all considered as operators acting on $\mathcal{H}_\Lambda = \bigotimes_{x\in\Lambda} \mathbb{C}^2$. For large λ, the long-range order in the Ising model is destroyed, even in the ground state of the $d = 1$ model ($\lambda_c = 1$).

This can be understood as a consequence of the Heisenberg uncertainty relations: for two s.a. observables, $A, B \in \mathcal{B}(\mathcal{H})$, and $\psi \in \mathcal{H}$, one has

$$\mathrm{Var}(A)\mathrm{Var}(B) \geq \frac{1}{4}\langle \psi, (i[A, B])^2 \psi \rangle^2$$

where, for $C = A, B$, $\mathrm{Var}(C) = \langle \psi, (C - \langle \psi, C\psi \rangle \mathbb{1})^2 \psi \rangle$ is the variance of the observable C.
At $T = 0$, thermal fluctuations do not play a role, but quantum fluctuations can have a similar effect.

Did a 1-Dimensional Magnet Detect a 248-Dimensional Lie Algebra?

Title of a recent expository article [1] about a remarkable experiment [2].

At the critical point ($\lambda_c = 1$ for the one-dimensional Ising model in a transverse field), the delicate balance of the competing terms often leads to new symmetries in the state of the system. In this case, Alexander Zamolodchikov, predicted an E_8 symmetry on theoretical grounds in 1989, and evidence for it was found experimentally last year (cobalt niobate).

[1]See D. Borthwick and S. Garibaldi, Notices of the AMS, **58** (2011) Number 8, 1060.
http:www.ams.org/notices/201108/rtx110801055p.pdf

[2]R. Coldea etal., Science, 8 January 2010, 327 (no. 5962), 177-180

What is a Phase?

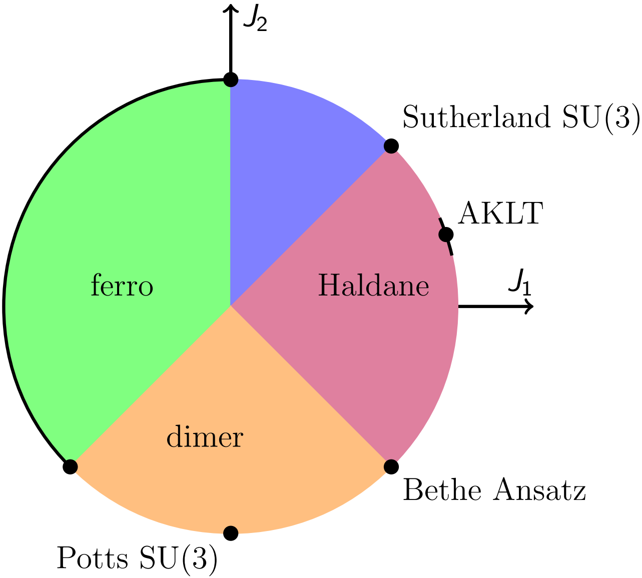
In order to be able to identify phase transitions, we need to understand when different states are in the same phase. We made progress on this question in a recent work with Sven Bachmann, Spyridon Michalakis, and Robert Sims (*Automorphic Equivalence within Gapped Phases of Quantum Lattice Systems*, arXiv:1102.0842, to appear in Commun. Math. Phys.)

We proposed automorphic equivalence as a characterization of states belonging to "the same phase" and proved that, under general assumptions, that this equivalence holds along curves of Hamiltonians along which there is a non-vanishing gap in the spectrum above the ground state (i.e., the smallest eigenvalue is separated by a finite distance from the rest of the spectrum).

The Spin-1 Chain

$$H_{[1,L]} = \sum_{x=1}^{L-1} J_1 \mathbf{S}_x \cdot \mathbf{S}_{x+1} + J_2 (\mathbf{S}_x \cdot \mathbf{S}_{x+1})^2.$$

The parameter λ can be thought of as the angle θ in the parametrization $J_1 = \cos\theta, J_2 = \sin\theta$.
There are multiple phase transitions in this model, most of which are not mathematically well-understood.



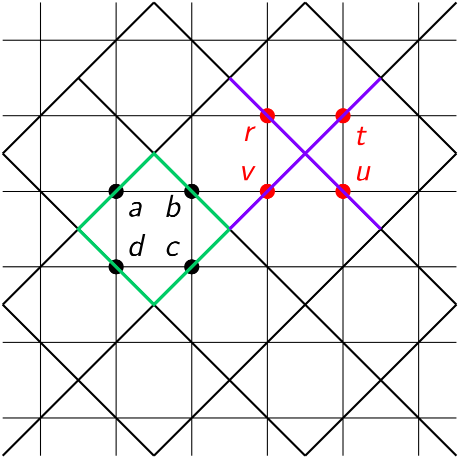
$$H = \sum_x J_1 \mathbf{S}_x \cdot \mathbf{S}_{x+1} + J_2 (\mathbf{S}_x \cdot \mathbf{S}_{x+1})^2$$

The AKLT model (Affleck-Kennedy-Lieb-Tasaki, 1987).
$\Lambda \subset \mathbb{Z}$, $\mathcal{H}_x = \mathbb{C}^3$;

$$H_{[1,L]} = \sum_{x=1}^{L} \left(\frac{1}{3}\mathbb{1} + \frac{1}{2}\mathbf{S}_x \cdot \mathbf{S}_{x+1} + \frac{1}{6}(\mathbf{S}_x \cdot \mathbf{S}_{x+1})^2 \right) = \sum_{x=1}^{L} P^{(2)}_{x,x+1}$$

In the limit of the infinite chain, the ground state is unique, has a finite correlation length, and there is a non-vanishing gap in the spectrum above the ground state (Haldane phase). Exact ground state is "frustration free" (Valence Bond Solid state (VBS), Matrix Product State (MPS), Finitely Correlated State (FCS)).

Toric Code model (Kitaev, 2003, 2006). $\Lambda \subset \mathbb{Z}^2$, $\mathcal{H}_x = \mathbb{C}^2$.



$H = -\sum_p h_p - \sum_s h_s$

$h_p = \sigma_a^3 \sigma_b^3 \sigma_c^3 \sigma_d^3$

$h_s = \sigma_r^1 \sigma_t^1 \sigma_u^1 \sigma_v^1$

all terms commute

On a surface of genus g, the model has 4^g frustration free ground states. Example of "topological insulator".

What about the so-called topological phases?

The space of ground states of Kitaev's Toric Code model, and other models introduced depends crucially on the topology of the lattice on which it is defined. Such models are better described as a family of models defined by interactions Φ^g on lattices Γ^g, which are identical in the bulk, i.e., away from boundaries and on a scale too short to detect the topology, which is labeled by $g \in \mathcal{G}$. The different topologies of interest are represented by $\{\Gamma^g\}_{g\in\mathcal{G}}$.

To express the equivalence of members of one "topological phase", we then need to consider paths of interactions Φ^g_s, $0 \leq s \leq 1$, for all g.

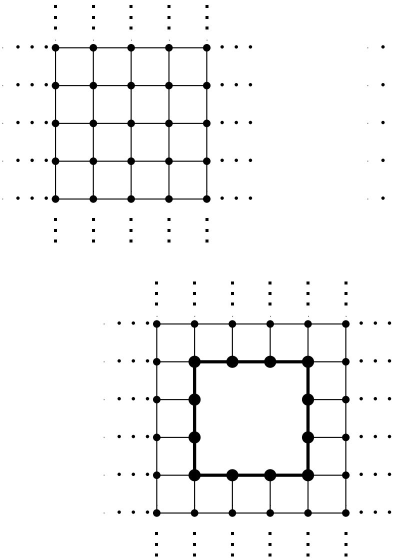
So, in one dimension, we need to consider at least two types of infinite systems:

The bold site denotes a boundary. Other “large” but finite systems can be pieced together from these two. So a classification of one-dimensional gapped phase would involve a bulk phase together with a boundary phase (essential for non-trivial topological phase in higher dimensions, cfr Klich's talk).

With Bachmann we are working out explicit examples. E.g., for the AKLT model, we can construct a gapped path of frustration free models showing that AKLT is connected to

- a bulk phase that is a unique product state
- a boundary phase (class of edge states) with a two-dimensional space of edge states: the product state and an exponentially localized excitation of it.

The simplest examples in two dimensions are:



etc.

Conclusions