Emergent structures in statistical mechanics and quantum systems

Michael Aizenman
Princeton Univ.

André Aisenstadt Lecture (II)
CRM, Montreal
Sept. 24, 2018
As is well known, ground states of quantum systems with local interactions can be presented in terms of stat. mech. systems\(^\ast\) in \(d + 1\) dimensions.

As a demonstration of this approach I shall present an application of statistic mechanical analysis to the question of dimerization in the ground states of a family of \(SU(2S + 1)\) spin chains, introduced by I. Affleck. The case \(S = 1/2\) corresponds to the Heisenberg anti-ferromagnetic spin chain.

To get there, I would comment on the role of emergent structures in the phase structure, and phase transitions of statistic mechanical systems.

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*My works on a range of related topics were carried in collaborations with:* R. Graham, D. Barsky, R. Fernandez, B. Nachtergaele, S. Warzel, H. Duminil-Copin, V. Tassion, M. Bahri ...

*Related recent results on the questions discussed here were presented in works of:* B. Nachterchale and D. Ueltschi and H. Duminil Copin, M. Gagnebin, M. Harel, I. Manolescu and V. Tassion.
An example of an emergent structure (reminder from lecture 1)

The power laws observed in the correlation functions at $T_c$ are related to the Hausdorff dimensions of the critical clusters and of their boundaries.

Figure 2: Simulations of three-state planar Potts model at subcritical, critical and supercritical temperatures.

The figure, generated by V. Befara, is further discussed in lecture notes by H. Duminil-Copin.
Quantum spin operators

Spin operators $S = \left( S^{(1)}, S^{(2)}, S^{(3)} \right)$  

($= \text{Generators of SU(2)}$)

- Commutation relations: $\left[ S^{(1)}, S^{(2)} \right] = iS^{(3)}$  
  (& cyclically)

- Irreducible representation on $\mathbb{C}^{2s+1}$: $S^2 = s(s + 1)$  
  $s \in \frac{1}{2} \mathbb{N}$

Square of total spin $S^2 = S \cdot S = \sum_{\alpha=1}^{3} \left( S^{(\alpha)} \right)^2$  

($= \text{Casimir operator}$)

Example $s = \frac{1}{2}$:  
$S = \frac{1}{2} \left( \sigma^{(1)}, \sigma^{(2)}, \sigma^{(3)} \right)$ in terms of Pauli matrices

$\sigma^{(1)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$,  
$\sigma^{(2)} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$,  
$\sigma^{(3)} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.  

Classical analogue
The question of dimerization under an $SU(2S + 1)$ invariant hamiltonian

For a system of quantum spins $S_u = (S_u^{(1)}, S_u^{(2)}, S_u^{(1)})$, of magnitude $S \ (= 1/2, 1, 3/2, ...)$, on $u \in \mathbb{Z} \cap (-L_1, L_2]$, consider the hamiltonian:

$$H = - \sum_u P(|S_u + S_{u+1}| = 0)$$

with $P$ – the projection on the singlet state.

A simplified picture of the ground state’s possible structure:

- either

- or

In the limit $L \to \infty$: degenerate ground state, and spectral gap to the rest.

An alternative:

Unique ground state and no spectral gap. Question: which is it?
The ground states’ \((d + 1)\) functional integral representation

For a finite system \((L \leq \infty)\) the ground state expectation value of an observable \(Q\) can be presented as

\[
\langle Q \rangle = \lim_{\beta \to \infty} \frac{\text{tr} \ Q \ e^{-\beta H}}{\text{tr} \ e^{-\beta H}} = \frac{\sum_{\sigma} \langle \sigma | Q \ e^{-\beta H} | \sigma \rangle}{\sum_{\sigma} \langle \sigma | e^{-\beta H} | \sigma \rangle}.
\]

With \(H(t) \equiv H\) (a special case of time ordered exponential)

\[
e^{-\beta H} = \sum_{n=0}^{\infty} (-1)^n \int_{0 < t_1 < \ldots < t_n} dt_1 \ dt_2 \ldots dt_n \ H(t_n) \ldots H(t_2) \ H(t_1)
\]

For an extensive Hamiltonian, \(H = -\sum_b A_b\) this yields

\[
\langle \sigma' | e^{-\beta H} | \sigma \rangle = \sum_{n=0}^{\infty} \int_{0 < t_1 < \ldots < t_n} dt_1 \ dt_2 \ldots dt_n \langle \sigma' | \prod_{n}^* A_{(b,t)n} | \sigma \rangle
\]
Example: 

\[ H = -\sum_u P(|S_u + S_{u+1}| = 0) \]

with

\[ P(|S_u + S_{u+1}| = 0)_{u,u+1} = (2S+1)^{-1} \sum_{a,b=-S}^S (-1)^{a-b} \langle b, -b | a, -a \rangle \]

\[ \langle \sigma' | e^{-\beta H} | \sigma \rangle = \int \mu(d\omega) \]

Quasi-state decomposition

\[ \langle Q \rangle = \int \mu(d\omega) \langle Q \rangle_\omega \]

\[ \langle \sigma_u^{(3)} \sigma_v^{(3)} \rangle_\omega = \left[ \frac{(-1)^{u-v}}{2S+1} \sum_{m=-S}^S m^2 \right] \langle 1 | u \leftrightarrow v \rangle_\omega \]
These 1D quantum spin chains are related to the 2D classical Potts model with $Q = (2S + 1)^2$.

The equivalence was conjectured by Affleck '90, and established on the level of the spectrum of the transfer matrices by Batchelor - Barber '90, and Klümper '90. The relation was further clarified in:

Aiz. - Nachtergaele “Geometric Aspects of Quantum Spin States” ('94) where a general results on dense loop-soup measures was used for:

**Theorem:** (Spectral dichotomy) In the limit $L \to \infty$, for the above spin chain at any given $S$ there is either a unique ground state in which the correlation decay slow enough so that

$$\sum_{u \in \mathbb{Z}} |u \langle S_0 \cdot S_u \rangle| = \infty$$

or else the system has a pair of distinct ground states, each of period 2, with

$$\langle S_n \cdot S_{n+1} \rangle = A \pm (-1)^n B, \quad B \neq 0$$

(a generalized form of dimerization).

(This is reminiscent of, but different than, Haldane’s spectral gap conjecture and Affleck-Lieb dichotomy).
The actual behavior depends on $S$:

For $S = 1/2$ option 2 holds, based on H. Bethe analysis of the Heisenberg anti-ferromagnet (‘31).

Recently, D. Ueltschy and B. Nachtergaele (‘17) have established that for $S \geq 8$ dimerization (option 1) takes place.

The more complete result, which was expected and is now proven in a joint ongoing work:

**Theorem:** (Aiz. and H. Duminil-Copin, in prep)

Dimerization takes place for all $S > 1/2$.

**Remark:** this corresponds to $Q = (2S + 1)^2 > 4$, and relies on a recent proof of the discontinuity over that range of the order parameter in $Q$ state Potts models


**Question:** Can the quasi state decomposition be improved into a proper quantum state decomposition?
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Thank you for your attention.