Spectrum of Reduced Density Matrix: Bethe Ansatz vs Valence Bond Solid states

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Reduced Density Matrix

Entropy of a subsystem of a pure system

In **classical case** the following simple theorem is valid: 

*If the entropy of a system is zero, then there is no entropy in any subsystem:*

In **quantum case** the entropy of a subsystem of a pure system can be positive. This means that the subsystem is entangled with the rest of the system. It is an important resource for quantum control.
Example

Two spins 1/2: \[ |\psi^{E,B}\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle_E |\downarrow\rangle_B - |\downarrow\rangle_E |\uparrow\rangle_B) \]

Density matrix of one spin is proportional to identical matrix

\[ \rho_B = tr_E \left( |\psi^{E,B}\rangle\langle\psi^{E,B}| \right) = \frac{1}{2} I_2 \]

\[ S_{E,B} = 0 \quad \text{but} \quad S_B = \ln(2) > 0 \]

Cannot happen for classical subsystems. This is a way to distinguish quantum system from classical.
Two systems in general. One can choose the orthonormal basis in both spaces so that:

\[ |\psi^{E,B}\rangle = \sum_{j=1}^{d} a_j |\psi_j^E\rangle \otimes |\psi_j^B\rangle \quad \text{and} \quad \sum_j |a_j|^2 = 1 \]

Theorem: If \( S_B > 0 \) then \( d > 1 \).
The subsystems \( E \) and \( B \) are entangled.
Quantum Control

Measurement of subsystem $E$ can be organized to project on one of basis states $|\psi^E_{j0}\rangle$. The wave function will turn into

$$|\psi^E_B\rangle = |\psi^E_{j0}\rangle \bigotimes |\psi^B_{j0}\rangle$$

with probability $|a^2_{j0}|$. This changes the state of another subsystem $B$. $E$ and $B$ entangled: one can control one system by another. This is quantum control useful for building quantum devices.
Application to XX Model

\[ H_{XX} = - \sum_{n=-\infty}^{\infty} \sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y + h \sigma_n^z, \quad |h| \leq 2 \]

- Solved by Lieb, Schultz & Mattis 1961
- The \(|gs\rangle\) is unique
- Entanglement of a block of \(L\) sequential spins with the rest of the ground state [environment].
Entanglement

- $|gs\rangle = |B \cup E\rangle$
- Density matrix of the ground state state

$$\rho = |gs\rangle \langle gs|$$

- Density matrix of the block is the reduced density matrix.

$$\rho_B = \text{Tr}_E \rho$$

Individual entries of $\rho_B$ are correlation functions.
In each lattice site $j$ we have four 'Pauli' matrices $\sigma^a_j$, here $a = 0, x, y, z$ with $\sigma^0 = I$.

$$\rho_B = 2^{-L} \sum_{a_j} \left( \bigotimes_{j=1}^L \sigma^a_j \right) \langle gs | \prod_{j=1}^L \sigma^a_j | gs \rangle$$

For gap-full models limit of large block exists.
Quantum Entanglement

Measures of entanglement for a pure state

- **Von Neumann Entropy** of subsystem [block]:
  
  \[ S(\rho_B) = -\text{Tr}_B (\rho_B \ln \rho_B) \]

- **Rényi Entropy** of subsystem [block]:
  
  \[ S(\rho_B, \alpha) = \frac{\ln (\text{Tr}_B \rho_B^\alpha)}{1 - \alpha} \]

\( \alpha \) is a parameter.

Also known in literature as zeta function or replica trick.

Same method work for evaluation of the entropy
**Von Neumann Entropy**

- **Asymptotic** $L \to \infty$:

$$S(\rho_B) \to \frac{1}{3} \ln L + \frac{1}{6} \ln \left[ 1 - \left( \frac{h}{2} \right)^2 \right] + \frac{1}{3} \ln 2 + \gamma_1 + O \left( \frac{1}{L} \right)$$

(The $\ln L$ term was discovered Holzhey, Larsen, Wilczek 1994)

- **Sub-leading terms**: B.-Q. Jin, V.E. Korepin in 2004

$$\gamma_1 = - \int_0^{\infty} dt \left\{ \frac{e^{-t}}{3t} + \frac{1}{t \sinh^2(t/2)} - \frac{\cosh(t/2)}{2 \sinh^3(t/2)} \right\} \approx 0.495$$
Asymptotic of Rényi entropy is

\[ S(\rho_B, \alpha) \to \left( \frac{1 + \alpha^{-1}}{6} \right) \ln \left( 2L \sqrt{1 - \left( \frac{h}{2} \right)^2} \right) + \gamma \{ \alpha \} \]

Later reproduced by J. Cardy and P. Calabrese from conformal filed theory, arXiv:hep-th/0405152
XY model

Gap-full models

\[ H_{XY} = - \sum_{n=-\infty}^{+\infty} (1 + \gamma) \sigma_n^x \sigma_{n+1}^x + (1 - \gamma) \sigma_n^y \sigma_{n+1}^y + h \sigma_n^z \]

- Lieb, Schultz & Mattis 1961
- Phases
  1a. Moderate field: \( 2 \sqrt{1 - \gamma^2} < h < 2 \)
  1b. Weak field: \( 0 \leq h < 2 \sqrt{1 - \gamma^2} \)
  2. Strong field: \( h > 2 \)
Phase diagram

Case 1

Case 1A

Case 1B

Case 2
Barouch-McCoy circle $h = 2\sqrt{1 - \gamma^2}$

$$|GS\rangle = |GS_1\rangle + |GS_2\rangle$$

$$|GS_1\rangle = \prod_{n \in \text{lattice}} \left[ \cos(\theta)|\uparrow_n\rangle + \sin(\theta)|\downarrow_n\rangle \right],$$

$$|GS_2\rangle = \prod_{n \in \text{lattice}} \left[ \cos(\theta)|\uparrow_n\rangle - \sin(\theta)|\downarrow_n\rangle \right]$$

$$\cos^2(2\theta) = (1 - \gamma)/(1 + \gamma)$$

Partially ordered state.
Von Neumann Entropy

Entropy of a large block has a limit:

\[ S(\rho_B) = \frac{1}{2} \int_1^\infty \ln \left( \frac{\theta_3(\beta(\lambda) + \frac{\tau}{2}) \theta_3(\beta(\lambda) - \frac{\tau}{2})}{\theta_3^2\left(\frac{\sigma\tau}{2}\right)} \right) d\lambda \]

\[ \beta(\lambda) = \frac{1}{2\pi i} \ln \frac{\lambda + 1}{\lambda - 1}, \quad \tau = i \frac{l(k')}{l(k)}, \quad k = \sqrt{\frac{1 - (h/2)^2 - \gamma^2}{1 - (h/2)^2}} \]

\[ (k')^2 + k^2 = 1 \]

\[ \theta_3 \text{ the Jacobi theta-function;} \]

Entropy is constant on the ellipsis: \( k = \text{const} \)

Complete elliptic integral of the first kind \( l(k) = \int_0^1 \frac{dx}{\sqrt{(1-x^2)(1-x^2k^2)}} \)
First analytical expression for limiting entropy of the large block of spin in the ground state of XY spin chain on infinite lattice. Its, Jin, Korepin: September 3 of 2004, see http://arxiv.org/abs/quant-ph/0409027

Shortly after on 16 Oct 2004 Ingo Peschel simplified our expression, see http://arxiv.org/abs/cond-mat/0410416
Limiting entropy in the region $0 < h < 2$ is:

$$S(\rho_B, \alpha) = \frac{1}{6} \frac{\alpha}{1-\alpha} \ln \left( \frac{k'}{k^2} \right) + \frac{1}{3} \frac{1}{1-\alpha} \ln \left( \frac{\theta_2(0,q^\alpha)\theta_4(0,q^\alpha)}{\theta_3^2(0,q^\alpha)} \right) + \frac{1}{3} \ln 2$$

$$\tau = i \frac{l(k')}{l(k)} \equiv i\tau_0, \quad q = e^{\pi i \tau}$$

$p_m$ are eigenvalues of the limiting density matrix. They form exact geometric sequence:

$$p_m = p_0 e^{-\pi \tau_0 m}, \quad m = 0, 1, 2, \ldots \infty, \quad \tau_0 = \frac{l(k')}{l(k)} > 0$$

Here $m$ is a label of eigenvalue. The maximum eigenvalue

$$p_0 = \left(\frac{kk'}{4}\right)^{1/6} \exp \left[\frac{\pi}{12} \tau_0\right]$$

is unique

Degeneracy increases as eigenvalue diminishes:

$$\text{Degeneracy} \rightarrow (192)^{-1/4} (m)^{-3/4} e^{\pi \sqrt{m/3}}, \quad m \rightarrow \infty$$

Spin chain consists of $N$ spin-1’s in the bulk and two spin-1/2 on the boundary: $\vec{S}_k$ is spin-1 and $\vec{\mathbf{s}}_b$ is spin-1/2.

$$H = \sum_{k=1}^{N-1} \left( \vec{S}_k \vec{S}_{k+1} + \frac{1}{3} (\vec{S}_k \vec{S}_{k+1})^2 + \frac{2}{3} \right) + \pi_{0,1} + \pi_{N,N+1}.$$ 

$\frac{1}{2} \vec{S}_k \vec{S}_{k+1} + \frac{1}{6} (\vec{S}_k \vec{S}_{k+1})^2 + \frac{1}{3}$ is a projector on a state of spin 2. The $\pi$ is a projector on a state with spin 3/2:

$$\pi_{0,1} = \frac{2}{3} \left( 1 + \vec{\mathbf{s}}_0 \vec{\mathbf{S}}_1 \right), \quad \pi_{N,N+1} = \frac{2}{3} \left( 1 + \vec{\mathbf{s}}_{N+1} \vec{\mathbf{S}}_N \right).$$
Kirillov-Korepin set up 1989. Ground state is unique:

A dot is spin-$\frac{1}{2}$; circle means symmetrisation [makes spin 1]. A line is a anti-symmetrisation ($|↑↓⟩ - |↓↑⟩$). Each projector annihilates the ground state (no frustration). The ground state is called VBS. Exact formula for correlation function at any distance is:

$$\frac{3}{4} < \hat{S}_x \hat{S}_1 > = \left(-\frac{1}{3}\right)^x = p(x)$$
AKLT again. Fan, Korepin and Roychowdhury 2004 calculated exactly the entropy of the block of the size $x$ on a finite lattice:

$$ S(x) = -3 \frac{(1-p(x))}{4} \log \left( \frac{1-p(x)}{4} \right) - $$

$$ - \frac{1+3p(x)}{4} \log \left( \frac{1+3p(x)}{4} \right) $$

It does not depend on the size of the lattice. For large block

$$ S(x) \rightarrow \ln 4 \quad \text{as} \quad x \rightarrow \infty $$
Fan, Korepin and Roychowdhury 2004 PRL: the density matrix of finite block of $x$ spins on the finite lattice has only **4 non-zero eigenvalues**. One

$$p_0 = \frac{1 + 3\rho(x)}{4}$$

and three

$$p_{1,2,3} = \frac{1 - \rho(x)}{4}$$

Does not depend on the length of the lattice.
Consider 'block' Hamiltonian

\[
H_B = \sum_{k \in \text{block}}^{(k+1) \in \text{block}} \left( \vec{S}_k \vec{S}_{k+1} + \frac{1}{3}(\vec{S}_k \vec{S}_{k+1})^2 + \frac{2}{3} \right).
\]

It describes interaction of spins 1 inside of the block. The ground state is quadruple degenerated: these are eigenvectors of the density matrix corresponding non-zero eigenvalues.

\[
\rho_B = \lim_{\beta \to \infty} \left( \frac{e^{-\beta H_B}}{\text{Tr}e^{-\beta H_B}} \right)
\]
Together with Hosho Katsura and Ying Xu these results for VBS we generalized to:

- For higher spins $s$ the entropy $S = 2 \ln(s + 1)$
- Other Lie algebras: for $SU(n)$ for smallest non-trivial representation the entropy $S = 2 \ln n$
- For AKLT on a connected graph we established rank of the density matrix.
Spin 3/2 is present in each site. Only nearest neighbors interact. Density of the Hamiltonian is projector on spin 3

\[ H_{AKLT} = \sum_{<kl>} P_3(S_K, S_l) \]

The ● will represent spin 1/2. Symmetrization of product of three spins 1/2 will give spin 3/2. Solid circle will represent symmetrization.
Figure: • is spin 1/2, solid circle is symmetrization. Part of straight line is antisymmetrization. Doted circle is the block.
Collaboration with Anatol Kirillov and Hosho Katsura. Only $2^L$ eigenvalues of the block density matrix not vanish. Here $L$ is the length of the boundary.

The entropy of the block is

$$S_B \rightarrow (\text{coeff}) \ L + o(L^{-1}), \quad \text{as} \quad L \rightarrow \infty$$

In agreement with area law.

$$0 < \text{coeff} \leq \ln 2$$
For Further Reading I

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