Entanglement Studies in the Affleck–Kennedy–Lieb–Tasaki (AKLT) Spin 1 Biquadratic Model

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Overview

Why Spin Chain Systems?

Definition:

- Spin models are foundational elements in statistical mechanics, condensed matter physics and many-body physics.
- These provide a framework for understanding the behaviour of magnetic moments, commonly known as “spins”.

Motivation:

- In quantum physics, spins are interpreted as intrinsic angular momentum.
- These models provide critical insights into several phenomena, such as magnetic properties, phase transitions, superconductivity, and superfluidity etc.

Ising Model

Importance:

- Simplest mathematical model, defined by Ernst Ising.
- Defined to explain the phase transitions in ferromagnetic materials.
- The Hamiltonian consists of a single component of spin interaction.

Ising Model:

The Hamiltonian of the system can be given by,

$$\mathcal{H} = -J\sum_{i=1}^{N}\sigma_i^z\sigma_{i+1}^z - B\sum_{i=1}^{N}\sigma_i^z$$

Transverse Ising Model:

The Hamiltonian of the system can be given by,

$$\mathcal{H} = -J\sum_{i=1}^{N}\sigma_i^z\sigma_{i+1}^z - B\sum_{i=1}^{N}\sigma_i^x$$

Results for Ising Model

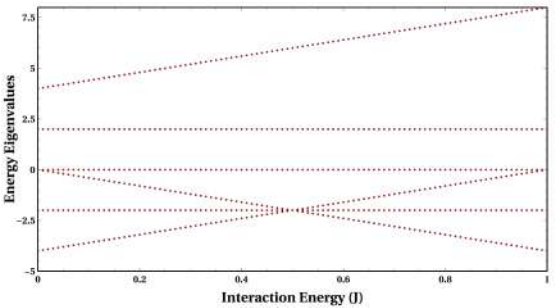


Figure: Energy Eigenvalue vs Interaction Energy (J) for 4 qubit Ising Model.

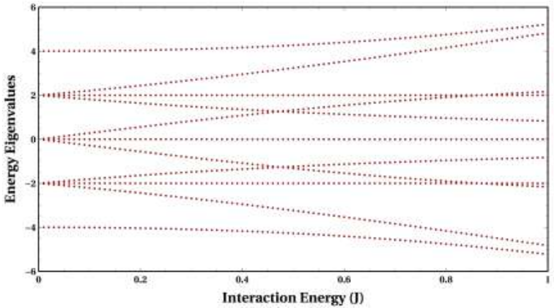
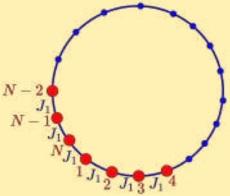


Figure: Energy Eigenvalue vs Interaction Energy (J) for 4 qubit Transverse Ising Model.

$$\langle\psi|\mathcal{H}|\psi\rangle = -J\underbrace{\sum_{i=1}^{N}\langle\psi|\sigma_i^z\sigma_{i+1}^z|\psi\rangle}_{\alpha} - B\underbrace{\sum_{i=1}^{N}\langle\psi|\sigma_i^z|\psi\rangle}_{\beta} \implies \mathcal{E} = -J\alpha - B\beta.$$

Multi Spin Interaction Models

Heisenberg Model:

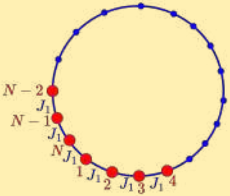


In this model, we consider nearest neighbour interactions for all three spin components. The Hamiltonian of the system can be given by,

$$\mathcal{H} = J \sum_{i=1}^{N} \vec{S}_i . \vec{S}_{i+1} .$$

Multi Spin Interaction Models

Heisenberg Model:



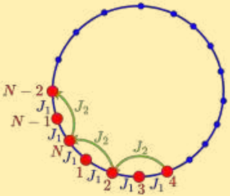
In this model, we consider nearest neighbour interactions for all three spin components. The Hamiltonian of the system can be given by,

$$\mathcal{H} = J\sum_{i=1}^{N} \vec{S}_i.\vec{S}_{i+1}.$$

- The Hamiltonian can be expanded as,
$$\mathcal{H} = \sum_{i=1}^{N} J_x(S_i^x.S_{i+1}^x) + J_y(S_i^y.S_{i+1}^y) + \sum_{i=1}^{N} J_z(S_i^z.S_{i+1}^z).$$
- This model can be solved analytically for the complete spectrum using the Bethe ansatz.
- $J_x \neq J_y \neq J_z \implies XYZ$ model.
- $J_x = J_y \neq J_z \implies XXZ$ model.
- $J_x = J_y = J_z \implies XXX$ model.

Multi Spin Interaction Models

Majumdar-Ghosh Model:

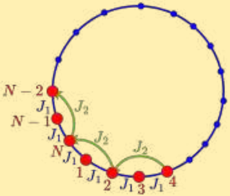


In this model, we consider nearest and second nearest neighbour interactions for all three spin components. So, the Hamiltonian can be given by,

$$\mathcal{H} = J_1 \sum_{i=1}^{N} \vec{S}_i \cdot \vec{S}_{i+1} + J_2 \sum_{i=1}^{N} \vec{S}_i \cdot \vec{S}_{i+2}$$

Multi Spin Interaction Models

Majumdar-Ghosh Model:



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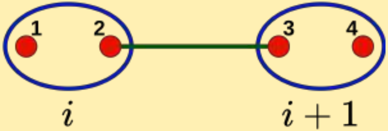
- Analytically this model is solvable only for the ground state of a specific case i.e., $J_2 = \frac{J_1}{2}$, this point is called Majumdar-Ghosh point.
- At this point the ground state of MG model are the tensor product of singlet states ($S = 0$), which are given as,

$$|R_N\rangle = [1\ 2][3\ 4][5\ 6]\cdots[N-1\ N],$$

$$|C_N\rangle = [2\ 3][4\ 5][5\ 6]\cdots[N\ 1].$$

Valence Bond States (VBS)

Singlet:



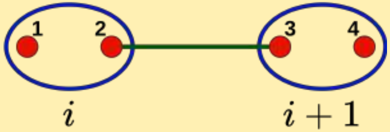
$$
\begin{aligned}
S_{tot}^2[2\ 3] &= (\vec{S_1} + \vec{S_2})^2[2\ 3] \\
&= S(S+1)[2\ 3] \\
&= 0(0+1)[2\ 3] = 0[2\ 3].
\end{aligned}
$$

$$S_{tot}^2[2\ 3] = 0[2\ 3].$$

$$[2\ 3] = \frac{|\uparrow\downarrow\rangle_{23} - |\downarrow\uparrow\rangle_{23}}{\sqrt{2}}.$$

Valence Bond States (VBS)

Singlet:



$$\begin{aligned} S_{tot}^2[2\ 3] &= (\vec{S_1}+\vec{S_2})^2[2\ 3] \\ &= S(S+1)[2\ 3] \\ &= 0(0+1)[2\ 3] = 0[2\ 3]. \end{aligned}$$

$$S_{tot}^2[2\ 3] = 0[2\ 3].$$

$$[2\ 3] = \frac{|\uparrow\downarrow\rangle_{23} - |\downarrow\uparrow\rangle_{23}}{\sqrt{2}}.$$

Projection Operator on $S = 2$:

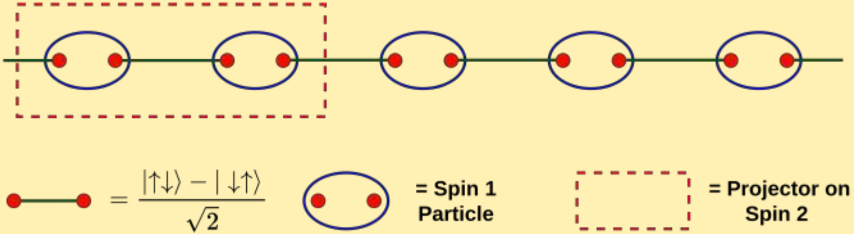
Net spin for particles 1 and 4 can be calculated as,

$$\begin{aligned} S &= |s_1 + s_4|, \cdots, |s_1 - s_4| \\ &= \left|\frac{1}{2}+\frac{1}{2}\right|, \cdots, \left|\frac{1}{2}-\frac{1}{2}\right| \\ S &= 1 \text{ and } 0. \end{aligned}$$

Since the maximum spin can be 1, we can take the Hamiltonian as projectors onto spin $S = 2$. The eigenvalues of the projection operator P_2 are 0 and 1.

AKLT Model

Hamiltonian:



The Hamiltonian can be defined as the projector on spin $S = 2$.

$$\mathcal{H} = \sum_{i=1}^{N} P_2(\vec{S}_i + \vec{S}_{i+1})$$

AKLT Model

Hamiltonian:

$$\mathcal{H} = \sum_{i=1}^{N} \left[\vec{S}_i.\vec{S}_{i+1} + \frac{1}{3}(\vec{S}_i.\vec{S}_{i+1})^2 \right].$$

where $\vec{S}_i$ is a spin half operator acting on i^{th} spin, where $\vec{S}_i$ is defined as,

$$\vec{S}_i = S_i^x \hat{x} + S_i^y \hat{y} + S_i^z \hat{z}.$$

where S_i^x, S_i^y and S_i^z are spin components.

$$\mathcal{H} = \frac{1}{4} \sum_{i=1}^{N} \vec{\sigma}_i \vec{\sigma}_{i+1} + \frac{1}{48} \sum_{i=1}^{N} (\vec{\sigma}_i \vec{\sigma}_{i+1})^2.$$

AKLT Model

Hamiltonian:

Now we have introduced the interaction energy J and an external magnetic field B to study the behaviour of the system. So, the Hamiltonian can be written as,

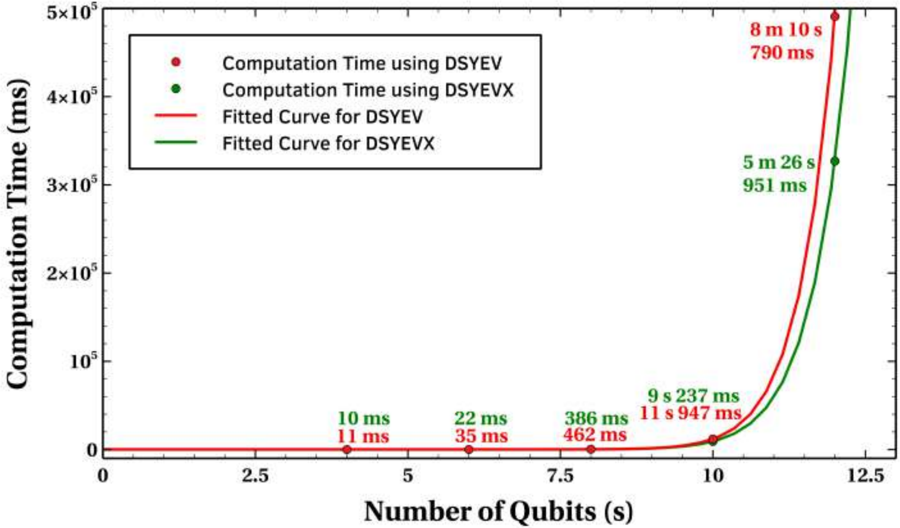
$$\mathcal{H} = \frac{J}{4}\sum_{i=1}^{N}\vec{\sigma}_i\vec{\sigma}_{i+1} + \frac{J}{48}\sum_{i=1}^{N}(\vec{\sigma}_i\vec{\sigma}_{i+1})^2 + B\sum_{i=1}^{N}\sigma_i^z\sigma_{i+1}^z.$$

This can be expanded as,

$$\mathcal{H} = \frac{J}{4}\sum_{i=1}^{N}(\sigma_i^x\sigma_{i+1}^x+\sigma_i^y\sigma_{i+1}^y+\sigma_i^z\sigma_{i+1}^z)+\frac{J}{48}\sum_{i=1}^{N}(\sigma_i^x\sigma_{i+1}^x+\sigma_i^y\sigma_{i+1}^y+\sigma_i^z\sigma_{i+1}^z)^2+B\sum_{i=1}^{N}\sigma_i^z\sigma_{i+1}^z,$$

where, σ^x, σ^y and σ^z are the Pauli Matrices.

DSYEV vs DSYEVX for Ground State Calculation



Sparsification

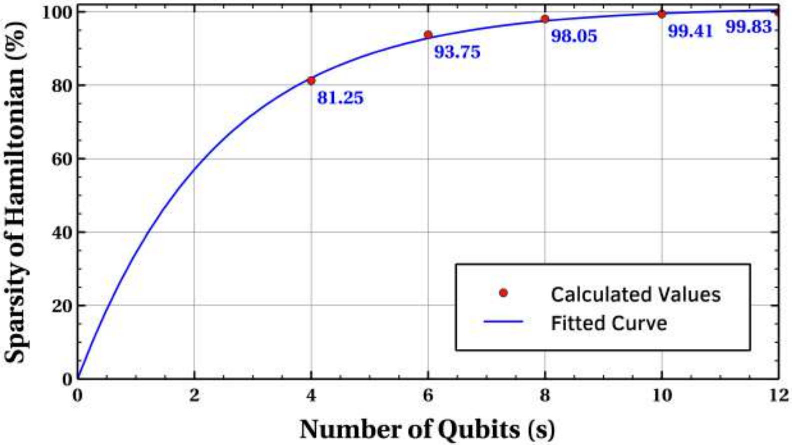
Definition:

- A matrix having **majority of elements** as **non-zero** is called a **Dense Matrix**.
- A matrix having **majority of elements** as **zero** is called a **Sparse Matrix**.
- **Sparsity** is defined as the **percentage of zero elements** in the matrix.

Motivation:

- Reduces computational time, complexity, and memory usage.
- Essential for large-scale quantum systems and simulations.
- Improves efficiency in matrix-based operations.
- Since most of the **Physical systems** are **Sparse** (also **our Hamiltonian**), it gives an upper hand.

Sparsity of AKLT Hamiltonian

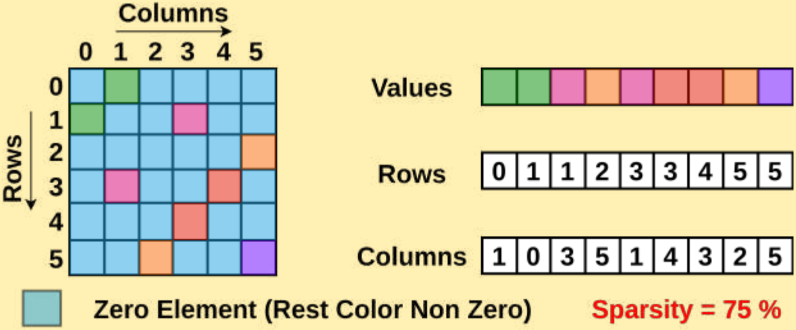


$$\text{Sparsity} = \frac{\text{Number of zero elements}}{\text{Number of total elements}} \times 100\%.$$

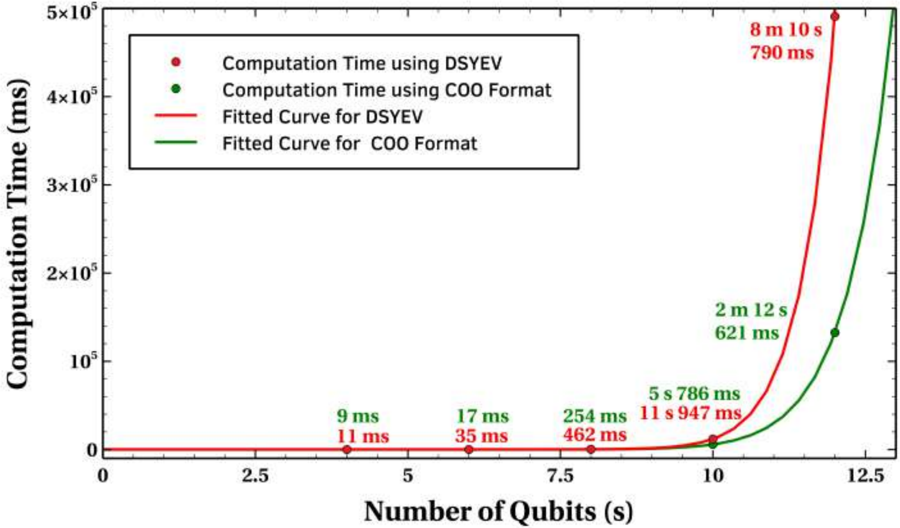
COO Format

Coordinate Format (COO):

In **COO format** we **store every non-zero element** along with its **row index** and **column index**.



DSYEV vs Sparsification (COO Format)



Parallel Programming (CPU & GPU)

Motivation:

- The AKLT model involves biquadratic systems, leading to exponential growth of the Hilbert space with system size.
- Simultaneous computation for varying magnetic field, entanglement entropy, and concurrence can be parallelized.

CPU vs GPU

Feature	CPU	GPU
Cores	Typically 4–16 cores.	Thousands of cores.
Focus	Optimized in sequential tasks.	Optimized for parallel tasks.
Memory Bandwidth	Lower Bandwidth.	Higher Bandwidth.
Performance	Control-heavy operations.	Best for data-parallel operations.

Concurrence for Pure State

Concurrence for 2-qubit Pure State:

Concurrence for a 2 qubit pure state $|\psi\rangle$ is defined as,

$$\mathcal{C} = |\langle\psi|\tilde{\psi}\rangle|, \tag{1}$$

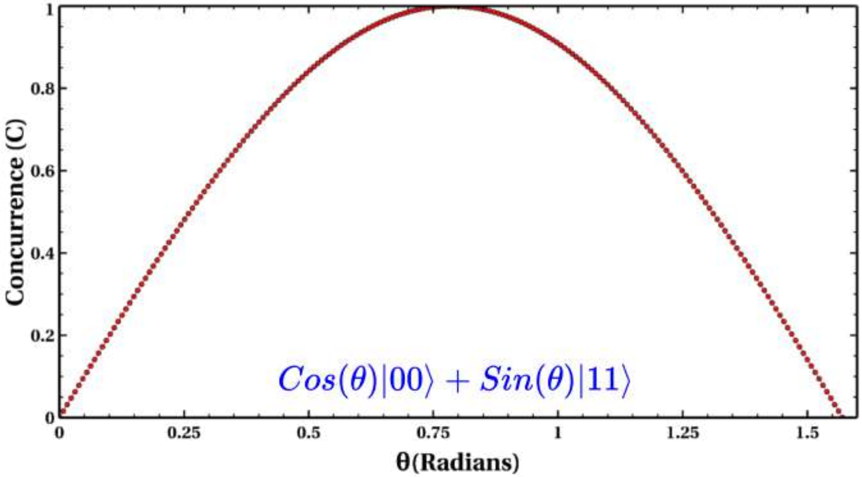
where,

$$|\tilde{\psi}\rangle = (\sigma_y \otimes \sigma_y)|\psi^*\rangle, \tag{2}$$

where $|\tilde{\psi}\rangle$ is the "**spin flip**" transformation for 2 qubit pure state.

- For a **separable state**, **concurrence** comes to be **zero** (i.e. $\mathcal{C} = 0$).
- For a **maximally entangled state**, **concurrence** comes to be **one** (i.e. $\mathcal{C} = 1$).

Concurrence for 2-qubit Pure State



Concurrence for Mixed State

Concurrence for 2-qubit Mixed State:

Concurrence for a 2-qubit mixed state ρ is defined as,

$$\mathcal{C}(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}, \tag{3}$$

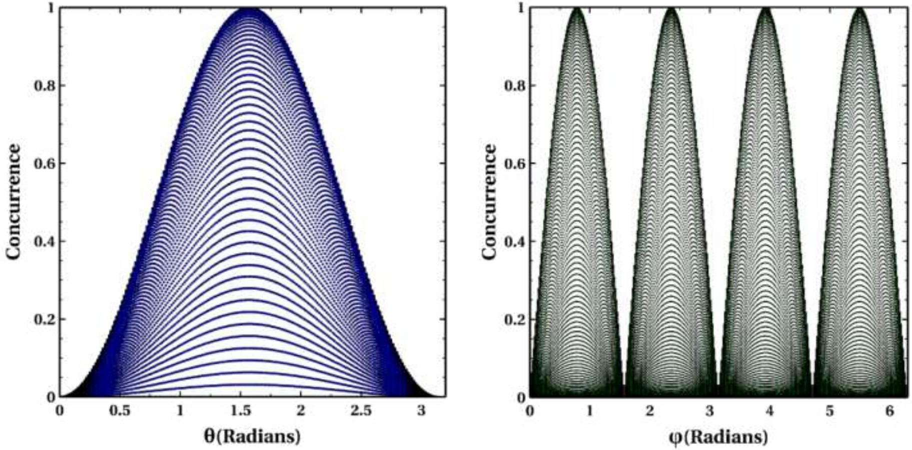
where $\lambda_1, \lambda_2, \lambda_3, \lambda_4$ are square root of the eigenvalues of $\rho\tilde{\rho}$ in non increasing order and $\tilde{\rho}$ is defined as,

$$\tilde{\rho} = (\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y), \tag{4}$$

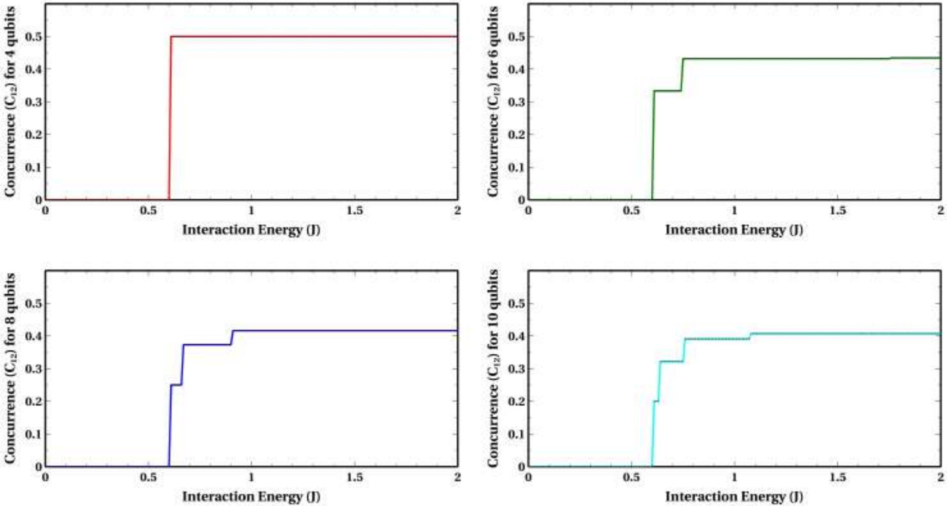
where $\tilde{\rho}$ is the "**spin flip**" transformation for 2 qubit density matrix.

Concurrence for 2-qubit Mixed State

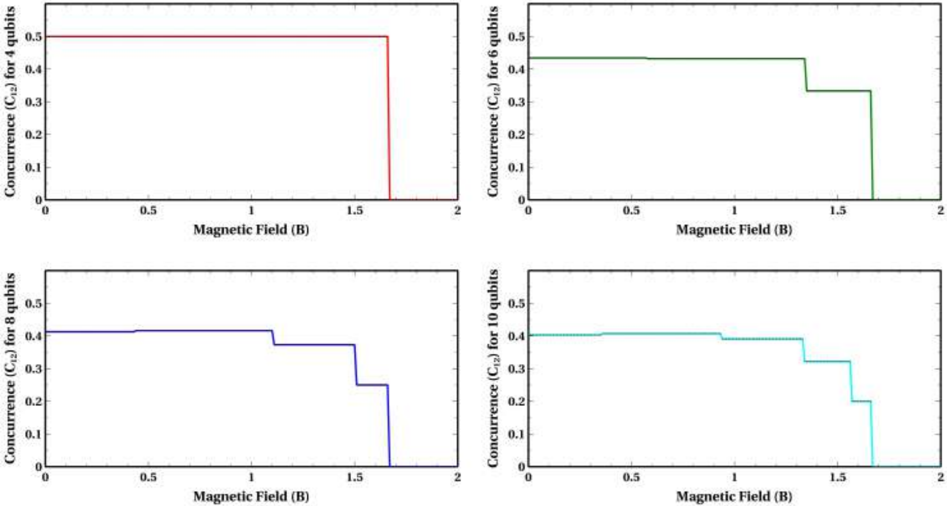
$$Cos(\theta)|001\rangle + Sin(\theta)Cos(\phi)|010\rangle + Sin(\theta)Sin(\phi)|100\rangle$$



Concurrence (C_{12}) vs Interaction Energy (J) for AKLT Model



Concurrence (C_{12}) vs Magnetic Field (B) for AKLT Model



Entropy

von Neumann Entropy:

- Suppose we have two subsystems in the Hilbert space $\mathbf{H} = \mathbf{H_A} \otimes \mathbf{H_B}$ where **A** stands for the first subsystem and **B** stands for the second subsystem, and the state of the composite system of two subsystems is given by ρ_{AB}.
- We use an entanglement measure called von Neumann entropy, also known as entanglement entropy, defined as,

$$S(\rho_A) = S(\rho_B) = -\sum_{i}^{dim(\rho_A)} \lambda_i log_2 \lambda_i = -\sum_{j}^{dim(\rho_B)} \lambda_j log_2 \lambda_j, \tag{5}$$

where ρ_A and ρ_B are reduced density matrices and λ_i's and λ_j's are the nonzero eigenvalues corresponding to respective subsystems **A** and **B**.

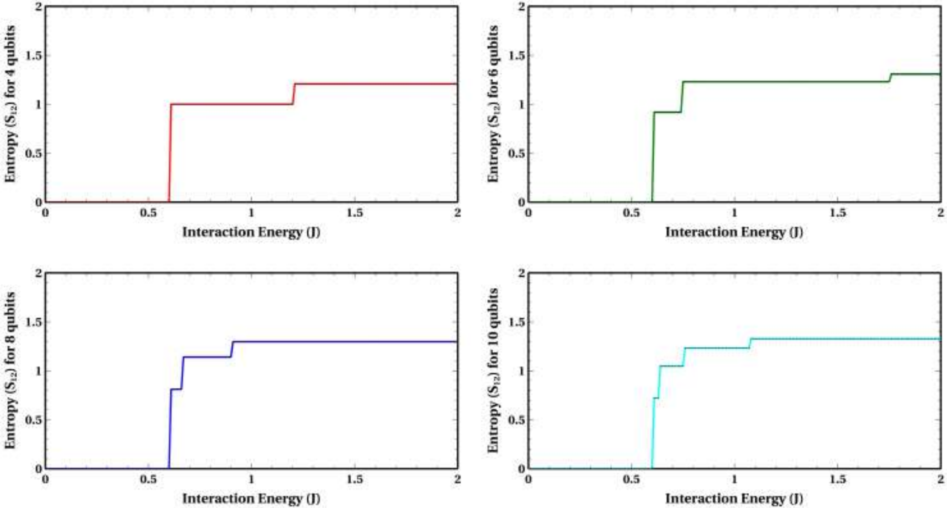
Entropy

Block Entropy:

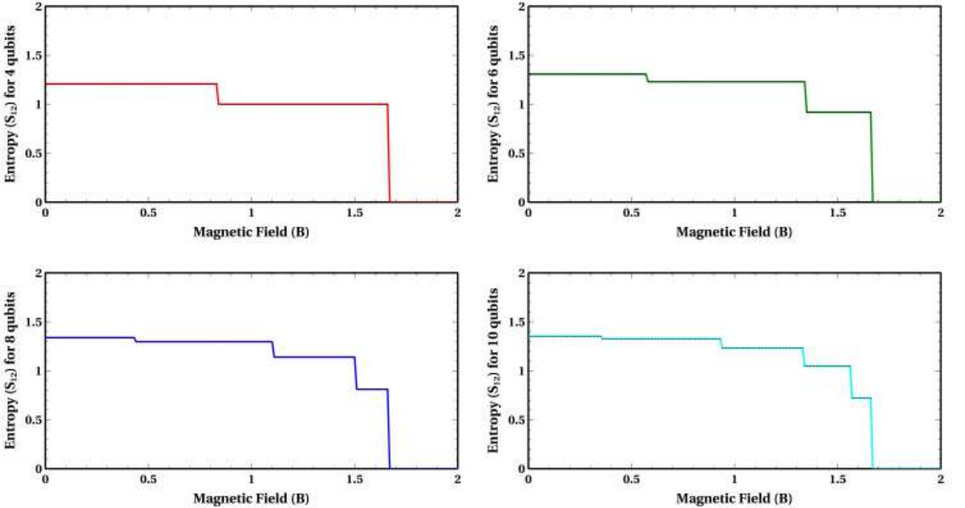
- For multi-qubit entanglement, the concept of Block entropy comes into the picture, which is nothing but the extension of von Neumann entropy only.
- We split the system into two subsystems, and the block entropy corresponding to these two blocks is as follows,

$$\begin{aligned} S(\rho_L) &= -\mathrm{Tr}(\rho_L \log_2 \rho_L) \\ &= -\sum_{i=1}^{\dim(\rho_L)} \lambda_i' \log_2 \lambda_i' \end{aligned} \tag{6}$$

Entropy (S_{12}) vs Interaction Energy (J) for AKLT Model



Entropy (S_{12}) vs Magnetic Field (B) for AKLT Model



Analytical Study of 4-qubit AKLT Model Ground State

For $0 \leq J \leq 0.6$

$$|\psi\rangle_{gs} = |1111\rangle$$

For $0.61 \leq J \leq 1.20$

$$\begin{aligned}
|\psi\rangle_{gs} &= \frac{|1110\rangle - |1101\rangle + |1011\rangle - |0111\rangle}{2} \\
&= \frac{|11\rangle_{12}}{\sqrt{2}} \otimes \frac{(|10\rangle - |01\rangle)_{34}}{\sqrt{2}} + \frac{(|10\rangle - |01\rangle)_{12}}{\sqrt{2}} \otimes \frac{|11\rangle_{34}}{\sqrt{2}} \\
&= -\frac{|11\rangle_{12}}{\sqrt{2}} \otimes S_{34} - S_{12} \otimes \frac{|11\rangle_{34}}{\sqrt{2}}
\end{aligned}$$

Analytical Study of 4-qubit AKLT Model Ground State

For $1.21 \leq J \leq 2$

$$
\begin{aligned}
|\psi\rangle_{gs} &= \frac{|1010\rangle + |0101\rangle}{\sqrt{3}} - \frac{|0011\rangle + |0110\rangle + |1001\rangle + |1100\rangle}{2\sqrt{3}} \\
&= \frac{|1010\rangle + |0101\rangle - |0011\rangle - |0110\rangle - |1001\rangle - |1100\rangle + |1010\rangle + |0101\rangle}{2\sqrt{3}} \\
&= \frac{(|01\rangle - |10\rangle)_{12} \otimes (|01\rangle - |10\rangle)_{34} + (I + \sigma_x^{\otimes 4})|1\rangle_1 \otimes (|01\rangle - |10\rangle)_{23} \otimes |0\rangle_4}{\sqrt{2}\sqrt{2}\sqrt{3}} \\
&= \frac{S_{12} \otimes S_{34}}{\sqrt{3}} + \frac{(I + \sigma_x^{\otimes 4})|1\rangle_1 \otimes S_{23} \otimes |0\rangle_4}{\sqrt{6}}
\end{aligned}
$$

Concurrence for Qudits

We are proposing to extend Wootters Concurrence for d-dimensional qudits.

Wootters Paper:

VOLUME 80, NUMBER 10 PHYSICAL REVIEW LETTERS 9 MARCH 1998

Entanglement of Formation of an Arbitrary State of Two Qubits

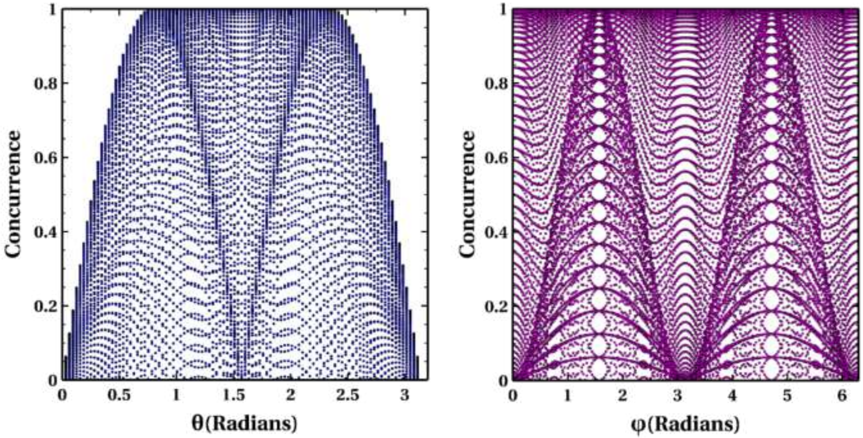
William K. Wootters
Department of Physics, Williams College, Williamstown, Massachusetts 01267
(Received 12 September 1997)

The entanglement of a pure state of a pair of quantum systems is defined as the entropy of either member of the pair. The entanglement of formation of a mixed state ρ is the minimum average entanglement of an ensemble of pure states that represents ρ. An earlier paper conjectured an explicit formula for the entanglement of formation of a pair of *binary* quantum objects (qubits) as a function of their density matrix, and proved the formula for special states. The present paper extends the proof to arbitrary states of this system and shows how to construct entanglement-minimizing decompositions. [S0031-9007(98)05470-2]

PACS numbers: 03.67.–a, 03.65.Bz, 89.70.+c

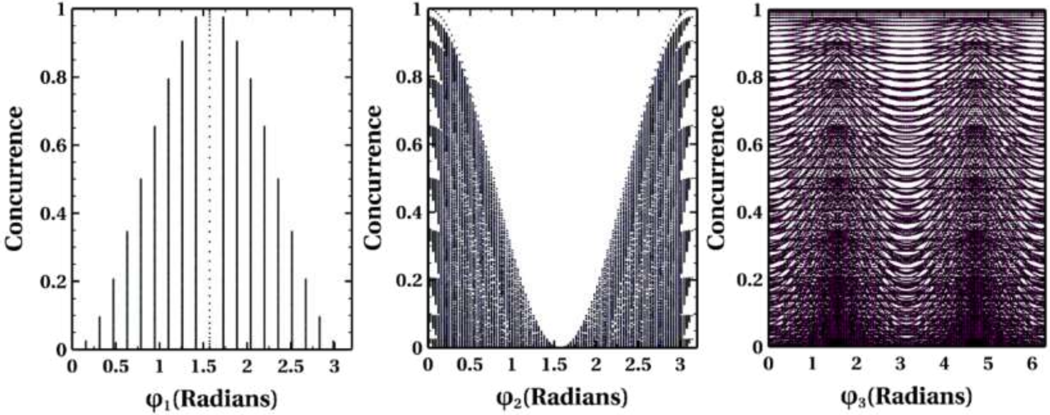
Extension of Wootters Concurrence for 3-Dimensional Qudits

$$Cos(\theta)|00\rangle + Sin(\theta)Cos(\phi)|11\rangle + Sin(\theta)Sin(\phi)|22\rangle$$



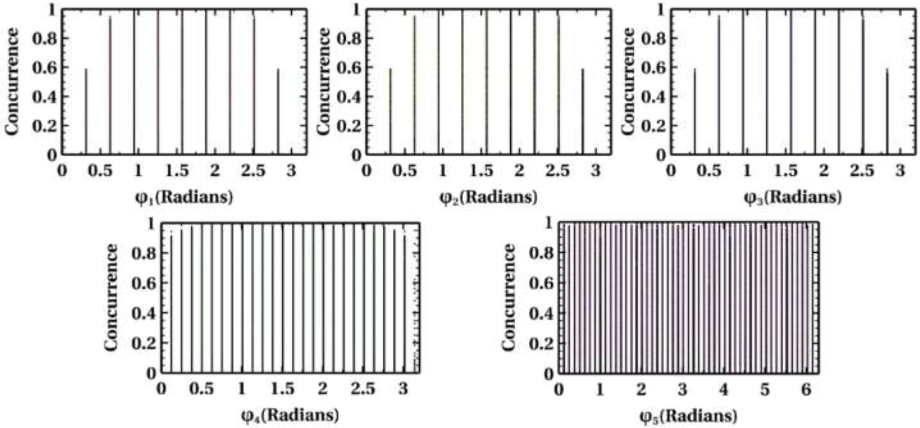
Extension of Wootters Concurrence for 3-Dimensional Qudits

$$Cos(\phi_1)|000\rangle + Sin(\phi_1)Cos(\phi_2)|111\rangle + Sin(\phi_1)Sin(\phi_2)Cos(\phi_3)|222\rangle + Sin(\phi_1)Sin(\phi_2)Sin(\phi_3)|120\rangle$$



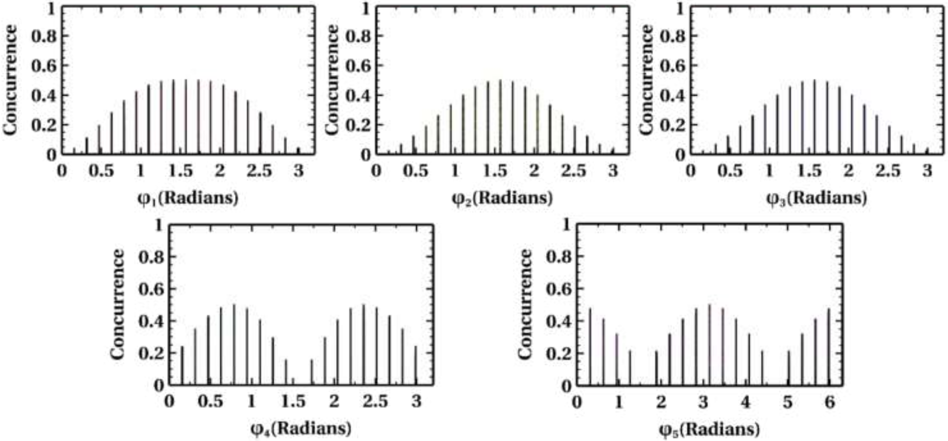
Extension of Wootters Concurrence for 6-Dimensional Qudits

$$Cos(\phi_1)|00\rangle + Sin(\phi_1)Cos(\phi_2)|11\rangle + Sin(\phi_1)Sin(\phi_2)Cos(\phi_3)|22\rangle + Sin(\phi_1)Sin(\phi_2)Sin(\phi_3)Cos(\phi_4)|33\rangle +$$
$$Sin(\phi_1)Sin(\phi_2)Sin(\phi_3)Sin(\phi_4)Cos(\phi_5)|44\rangle + Sin(\phi_1)Sin(\phi_2)Sin(\phi_3)Sin(\phi_4)Sin(\phi_5)|55\rangle$$



Extension of Wootters Concurrence for 6-Dimensional Qudits

$$Cos(\phi_1)|000\rangle + Sin(\phi_1)Cos(\phi_2)|112\rangle + Sin(\phi_1)Sin(\phi_2)Cos(\phi_3)|224\rangle + n(\phi_1)Sin(\phi_2)Sin(\phi_3)Cos(\phi_4)|330\rangle +$$
$$Sin(\phi_1)Sin(\phi_2)Sin(\phi_3)Sin(\phi_4)Cos(\phi_5)|441\rangle + Sin(\phi_1)Sin(\phi_2)Sin(\phi_3)Sin(\phi_4)Sin(\phi_5)|552\rangle$$



General Partial Trace (d-dimensional, n-parties)

Motivation:

- It is important when we want to study a subsystem of a complete system.
- No subroutine on Fortran does d-dimensional, n-parties partial trace.

Importance:

- n parties partial trace is important as it gives me the upper hand to trace out any number of parties.
- d-dimensional partial trace is important as it allows us to perform partial trace for any level system (i.e., qubits, qutrits, ququrt, etc.).

Future Work

Future Directions:

- It will be interesting to solve the model analytically and find the general relations for concurrence and entropy.
- We are currently working on the Concurrence for d-dimensional qudits, which will be of great importance.
- It will be very interesting to study the properties of the AKLT Model for different types of interaction energies.

Acknowledgement

First and foremost, I would like to express my heartfelt gratitude to my professor and guide, ***Dr. M. S. Ramkarthik****, for his invaluable guidance throughout this project. His deep understanding across diverse areas of Physics has been a constant source of inspiration, reinforcing the importance of persistent reading and exploration in scientific inquiry.*

I am deeply grateful to my parents, ***Mrs. Mamta Joshi*** *and* ***Mr. Naveen Chandra Joshi****, and to my guardians,* ***Mrs. Vimla Pant****,* ***Mr. Kamlesh Pant****, and* ***Mrs. Rekha Pant****, for their unwavering support and belief in my decisions. Their encouragement formed the backbone of this journey.*

I would also like to sincerely thank my friend ***Ankan Bhattacharyya****, whose insights and suggestions helped me navigate several challenges. Your guidance in the initial phases and throughout the project gave me clarity and direction whenever I felt lost.*

My gratitude extends to my group members — ***Gargee Arun Tammadwar****,* ***Divyani Vilas Bhagat****,* ***Durgesh Thail Vasant****,* ***Om Sanjay Shah****, and* ***Atul****. Without you, the journey would have lacked its flavor and color.*

Lastly, I want to thank all my friends who were part of this short but meaningful journey.

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Thank you!!

Questions?