Computing Entanglement
In Quantum Matter

A new tool for the study of strongly-correlated systems

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Valence Bond and von Neumann Entanglement Entropy in Heisenberg Ladders

Measuring Renyi Entanglement Entropy with Quantum Monte Carlo

Finite-size scaling of mutual information in Monte Carlo simulations: Application to the spin-1/2 XXZ model

Finite temperature critical behavior of Mutual Information

Topological Entanglement Entropy of a Bose–Hubbard Spin Liquid
• Entanglement Entropy:
  - a resource in condensed matter physics
  - accessible in scalable simulation methods (QMC)

• Topological entanglement entropy in a quantum Spin Liquid
1) Identify models and materials with interesting, exotic or novel phenomena

**Strongly-correlated quantum systems:**

- superconductivity, supersolids, spin liquids, fractionalization, spin–charge separation, exotic quantum criticality

2) Develop tools to explore these systems

- Theoretical and numerical methods
- New measurements, observables, and estimators
- Lanczos exact diagonalization
  \[ 2^N \]

- Density Matrix Renormalization Group
  \[ d=1 \text{ only} \]

- Quantum Monte Carlo
  \[ O(N) \]
  \[ N \approx 10^7 \text{ – } 10^9 \]
  spin 1/2 particles
Traditional CMT tools

- Order Parameter (symmetry breaking)

- Correlation functions \( \langle S_i^z S_j^z \rangle \)

- Bulk properties \( C_v \), \( \chi \)

- Entanglement? \( |\Psi\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \)
\( \rho_A = \text{Tr}_B(\rho) \)

\( \rho = \sum_i \lambda_i |\Psi_i\rangle \langle \Psi_i| \)

\( S_1(\rho_A) = -\text{Tr}(\rho_A \ln \rho_A) \)

- Quantifies the entanglement between subregions A and B
- Does not depend on any choice of observable
- \( S_1(\rho_A) = S_1(\rho_B) \)
- \( S_1(\rho_A) = 0 \) if region A and B are unentangled
\[ |\Psi\rangle = \cos \alpha \left\uparrow\downarrow\right\downarrow\uparrow + \sin \alpha \left\downarrow\uparrow\uparrow\right\downarrow \]

\[ \rho_A = \begin{pmatrix} \cos^2 \alpha & 0 \\ 0 & \sin^2 \alpha \end{pmatrix} \]

\[ S_1 = -\cos^2 \alpha \ln \cos^2 \alpha - \sin^2 \alpha \ln \sin^2 \alpha \]

\[ \frac{1}{\sqrt{2}} \left( |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right) \]
\[ S_n(\rho_A) = \frac{1}{1-n} \ln \left[ \text{Tr}(\rho_A^n) \right] \]

\[ S_1(\rho_A) = -\text{Tr}(\rho_A \ln \rho_A) \]

\[ S_2(\rho_A) = -\ln \left[ \text{Tr}(\rho_A^2) \right] \]

- Gives a Lower bound

\[ S_n \geq S_m \quad \text{when} \quad n < m \]
For many interacting quantum spins, how does the entanglement entropy depend on the size of the region A?

1) $S$ depends on the “volume” of region A

2) $S$ depends on the boundary size
Example: singlet crystal (valence bond solid)

\[ S_1 \sim l \] “area” or boundary law

Most “well behaved” quantum condensed matter groundstate wavefunctions are expected to obey an area law.

- Gapped wavefunctions
- Hamiltonians with local interactions

Implied heuristically by the existence of a characteristic length scale and/or localized correlations.

\[ S_1 \sim \ell \]

**Universal corrections**

- **Subleading corrections** are believed to harbour new universal physics. These can be used as a resource to diagnose new phases and phase transitions in condensed matter systems.

\[
S_1 = a \ell + \cdots \\
S_1 = a \ell - \gamma + \cdots \\
S_1 = a \ell + c_1 \ln(\ell) + \cdots \\
S_1 = c \ell \ln(\ell) + \cdots \\
\]

- We have no proof and no exact calculations in \(d>1\), apart from a few non-interacting systems.
1D example

Conformal Field Theory:

\[ S_n(x) = \frac{c}{6} \left( 1 + \frac{1}{n} \right) \cdot \ln [x'] + \cdots \]

\[ x' = \frac{L}{\pi} \sin \left( \frac{\pi x}{L} \right) \]

\( c = 1 \): central charge of CFT

\[ H = J \sum_{\langle ij \rangle} S_i \cdot S_j \]

\( x = 4 \)

\( L = 200 \)

\( c = 1.011 \)

\( c = 1.013 \)

Holzhey, Larsen, Wilczek

Calabrese and Cardy,

Capponi, Alet, Mambrini,
arXiv:1011.6530
A scalable simulation method applicable to any dimension

Finite and zero-temperature methods available

\[ Z = \sum_{\alpha} \langle \alpha | e^{-\beta \hat{H}} | \alpha \rangle = \sum_{\alpha} \sum_{n} \frac{(-\beta)^n}{n!} \langle \alpha | H^n | \alpha \rangle \]

\[ = \sum_{\alpha} \sum_{n} \sum_{S_n} \frac{(-\beta)^n}{n!} \langle \alpha | \prod_{i=1}^{n} H_{b_i} | \alpha \rangle \]

Simulations don’t have access to the wavefunction

The “sign problem” inhibits the simulation of frustrated spins or fermions
Replica Trick

\begin{equation}
S_n(\rho_A) = \frac{1}{1 - n} \ln \left[ \text{Tr}(\rho_A^n) \right] = \frac{1}{1 - n} \ln \frac{Z[A, n, T]}{Z(T)^n}
\end{equation}

where \( Z[A, n, T] \) is the partition function of the system with special topology – the \( n \)-sheeted Riemann surface.
\[ Z[A, 2, T] \]
Thermodynamic Integration

\[ S_2 = -\ln \text{Tr}(\rho_A^2) = -\ln \left\{ \frac{Z[A, 2, \beta]}{Z(\beta)^2} \right\} = -\ln Z[A, 2, \beta] + 2 \ln Z(\beta) \]

\[ = -S_A(\beta = 0) + \int_0^\beta \langle E \rangle_A d\beta + 2S_0(\beta = 0) - 2 \int_0^\beta \langle E \rangle_0 d\beta \]

XXZ model \hspace{1cm} H = \sum_{\langle ij \rangle} (\Delta S_i^z S_j^z + S_i^x S_j^x + S_i^y S_j^y)

\[ S_A = S_B \]
Entanglement Entropy:
- a resource in condensed matter physics
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Topological entanglement entropy in a quantum Spin Liquid
T=0 paramagnetic states ("spin liquids") have no local order parameters: it makes them notoriously difficult to find


### Table 1 | Some experimental materials studied in the search for QSLs

<table>
<thead>
<tr>
<th>Material</th>
<th>Lattice</th>
<th>S</th>
<th>Status or explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\kappa$-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$</td>
<td>Triangular†</td>
<td>$\frac{1}{2}$</td>
<td>Possible QSL</td>
</tr>
<tr>
<td>EtMe$_3$Sb[Pd(dmit)$_2$]$_2$</td>
<td>Triangular†</td>
<td>$\frac{1}{2}$</td>
<td>Possible QSL</td>
</tr>
<tr>
<td>Cu$_3$V$_2$O$_7$(OH)$_2$•2H$_2$O (volborthite)</td>
<td>Kagomé†</td>
<td>$\frac{1}{2}$</td>
<td>Magnetic</td>
</tr>
<tr>
<td>ZnCu$_3$(OH)$_6$Cl$_2$ (herbertsmithite)</td>
<td>Kagomé</td>
<td>$\frac{1}{2}$</td>
<td>Possible QSL</td>
</tr>
<tr>
<td>BaCu$_3$V$_2$O$_8$(OH)$_2$ (vesignieite)</td>
<td>Kagomé†</td>
<td>$\frac{1}{2}$</td>
<td>Possible QSL</td>
</tr>
<tr>
<td>Na$_4$Ir$_3$O$_8$</td>
<td>Hyperkagomé</td>
<td>$\frac{1}{2}$</td>
<td>Possible QSL</td>
</tr>
<tr>
<td>Cs$_2$CuCl$_4$</td>
<td>Triangular†</td>
<td>$\frac{1}{2}$</td>
<td>Dimensional reduction</td>
</tr>
<tr>
<td>FeSc$_2$S$_4$</td>
<td>Diamond</td>
<td>2</td>
<td>Quantum criticality</td>
</tr>
</tbody>
</table>
Spin Liquids: models

- The precise ingredients that are needed to make spin liquid states in microscopic models are unknown

- Frustration is a major player
  Yan, Huse, White, Science, 332 1173 (2011)

\[ H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \]


\[ H = -t \sum_{\langle i,j \rangle, \alpha} (c_{i\alpha}^{\dagger} c_{j\alpha} + c_{j\alpha}^{\dagger} c_{i\alpha}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \]
\[ H = H_0 + H_1 \]

\[ H_0 = V \sum_{\Omega} (S^z_\Omega)^2 \]

\[ H_1 = -t \sum_{\langle i,j \rangle} (S^+_i S^-_j + S^+_j S^-_i) \]

• QCP is in the 2D XY universality class

\[ \nu = 0.6717 \]
The standard method of “detecting” spin liquids is negative signatures of ordering in two-point correlations functions.

\[
S_s(q_x, q_y) = \frac{1}{N} \sum_{k,l} e^{i(r_k - r_l) \cdot \mathbf{q}} \langle S^z_k S^z_l \rangle
\]

\[
S_p(q_x, q_y) = \frac{1}{N} \sum_{a,b} e^{i(r_a - r_b) \cdot \mathbf{q}} \langle P_a P_b \rangle
\]

\[
P_a = (S^+_i S^-_j S^+_k S^-_l + \text{h.c.})
\]
Gapped spin liquids have a topological order (or degeneracy) in the ground state wavefunction.

• Topological order is manifest as a universal correction in the entanglement entropy

\[ S_1 = a \ell - \gamma + \cdots \]

for a Z2 spin liquid \( \gamma = \ln(2) \)

from the description of the groundstate as a “loop gas”

exhaustively studied as the groundstate wavefunction of Kitaev’s Toric Code

\[ H = -\lambda_B \sum_p B_p - \lambda_A \sum_v A_v \]

\[ B_p = \prod_{i \in p} \sigma_i^z \quad A_v = \prod_{j \in v} \sigma_j^x \]
This $\gamma$ can serve as an “order parameter” for a spin liquid (it identifies the underlying emergent gauge symmetry).

\[ 2\gamma = \lim_{r,R \to \infty} [-S_{VN}^{1_A} + S_{VN}^{2_A} + S_{VN}^{3_A} - S_{VN}^{4_A}] \]

finite-size systems retain a statistical contribution to the topological EE.

Entanglement and topological entropy of the toric code at finite temperature
Claudio Castelnovo and Claudio Chamon, PRB 76, 184442 2007
Conclusions

- Entanglement entropy can be used as a resource to detect and classify phases and phase transitions

- Renyi entropies can be measured in large-scale numerical simulations with QMC methods

- Subleading corrections to the area law are a practical tool to detect topologically ordered spin liquid phases

- This effort is only about two years old – there are many more exciting applications to study