New Physics from Tensor-Network Treatments of Potts and Heisenberg Models

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![Graphs showing thermodynamic properties and ground state energy per site](image.png)
Road Map

- tensor-network representations and RG techniques
- classical systems: the partition function
- **Potts models**, irregular lattices and partial order
- thermodynamics and phase transitions
- multiple transitions and types, subextensive entropic driving
- quantum systems: the wavefunction
- MPS, PEPS and SVD
- going beyond PEPS for frustrated systems: PESS
- Simplex Solid States, variational Ansätze, calculations
- the **$S = 1/2$ kagome Heisenberg antiferromagnet**
  - 3-, 5- and 9-PESS
  - energetic calculations
  - accuracy and symmetry
  - nature of the ground state
- summary
Tensor-Network Representations

Tensor-network states are expanding rapidly to many fields, including quantum information and quantum gravity. For lattice models a tensor network represents

- classical: partition function;
- quantum: wavefunction.

The degrees of freedom of a system with coordination number $z$ are represented by one or more rank-$z$ tensors. Each index has bond dimension $D$.

Tensor manipulation by
- contraction
- singular-value decomposition

gives rise to a tensor-based renormalisation group. Thus the method is infinite in space, with truncation achieved through $D$. 

\begin{align*}
\text{(a)} & \quad T_{ijkl} \\
\text{(b)} & \quad S_{jk} \\
\text{(c)} & \quad S_{jk}^2 \\
\text{(d)} & \quad T_{ijkl}^2
\end{align*}
Classical Systems: the Potts Model

The \( q \)-state Potts model is specified by

\[
\mathcal{H} = J \sum_{\langle i,j \rangle} \delta_{\sigma_i \sigma_j} - H \sum_i \delta_{\sigma_i,0},
\]

where \( \sigma_i = 0, 1, \ldots, q - 1 \) is a discrete variable taking one of \( q \) possible values. The Ising Model is \( q = 2 \).

We consider only the antiferromagnetic Potts model, \( J > 0 \).

\( H \) is a field coupling to one of the \( q \) components and can be used to deduce the effective magnetisation and the susceptibility.

The Potts model on any given lattice is characterised by \( q \), the number of degrees of freedom at each site, and \( z \), the coordination number number of the lattice.

### Crude generalisation:

- \( q > z \): entropy-dominated, no order.
- \( q \sim z \): multi-sublattice order, partial order, entropy-driven transitions ...
- \( q < z \): order, frustration, multiple transitions, ...

Any lattice has a value \( q_c \) where some form of order sets in, at a zero-temperature phase transition.
Two-Dimensional Lattices

The 8 Laves lattices: duals to the Archimedean lattices which are neither self-dual nor mutually dual.

The 11 Archimedean lattices.
Potts-Model Thermodynamics

The partition function is to be cast in the form of a tensor network,

\[ Z = \sum_{\alpha\beta\gamma\delta...} T_{\alpha\beta\gamma\delta...} \]

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Take the example of the Union Jack lattice

\[ \mathcal{H}_{UJ} = J(\delta_{\sigma_1\sigma_2} + \delta_{\sigma_2\sigma_3} + \delta_{\sigma_3\sigma_4} + \delta_{\sigma_4\sigma_1})/2 \]
\[ + J(\delta_{\sigma_1\sigma_5} + \delta_{\sigma_2\sigma_5} + \delta_{\sigma_3\sigma_5} + \delta_{\sigma_4\sigma_5}). \]

One may trace over \( \sigma_5 \) to obtain

\[ T_{\alpha\beta\gamma\eta} = e^{-\frac{\beta}{2}(\delta_{\alpha,0}+\delta_{\beta,0}+\delta_{\gamma,0}+\delta_{\eta,0})} \sum_{\theta} e^{-\beta(\delta_{\theta,0}+\delta_{\theta+\alpha,0}+\delta_{\theta+\alpha+\beta,0}+\delta_{\theta+\eta,0})} \]

The result is a tensor network defined and evaluated on the dual square lattice.

There are different techniques for the evaluation of a tensor network:

- renormalisation-group methods such as TRG and SRG;
- projective methods such as iTEBD, found to be most efficient here.

Once the partition function \( Z \) is obtained, one has access to all thermodynamic quantities. Of most interest in characterising Potts models are the free energy

\[ F = -k_B T \ln Z, \]

the entropy

\[ S(T) = -\frac{\partial F}{\partial T} \]

and the specific heat

\[ C(T) = -T \frac{\partial^2 F}{\partial T^2}. \]
Partial Order: the Diced Lattice

The diced lattice is dual to the kagome lattice. It has clearly inequivalent A and B sites with respective coordinations of 6 (1/3 of sites) and 3 (2/3). The Potts Model with \( q = 3 \) on the square lattice, which has the same average coordination, is critical at \( T = 0 \). The \( q = 3 \) Potts model on the diced lattice has

- a robust transition in \( C(T) \) at finite \( T_c = 0.508(1)J \),
- partial order only on the A-sublattice sites,
- obvious implications for the effects of an irregular lattice.

This partial order is driven by an extensive entropy: there exist very many states in the ground manifold with the same energy (all bonds satisfied), but many more with disorder on the B sites than on the A sites. These entropic contributions are calculated directly from \( Z \) and approach the expectation from \( q = 2 \) remaining degrees of freedom on 2/3 of the sites. Comparisons with exact solutions and QMC results validate the tensor-network method.
Partial Order: the Union Jack Lattice

The $q = 4$ Potts model on the Union-Jack lattice is far more subtle. The average coordination matches the triangular lattice, which is critical at $T = 0$. There are 2 competing sublattices on which partial order may occur. The result is an extremely subtle transition:

- difficult to detect
- previously unknown
- requires proof that the discontinuity in $C(T)$ is robust.

The entropy result $S_{\mu}(0) = 0.43097359$ allows very accurate characterisation of the ground state.

The existence of this transition is related to the 3-bond colouring problem on the dual $(4,8^2)$ lattice, the fully packed loop model on this lattice and the $q = 3$ Potts model on the square-kagome lattice.
Partial Order: Centred Diced Lattice

On the centred diced lattice there is no competition between sublattices. For the \( q = 4 \) Potts model, partial order on the highest-coordinated \( A \) sites sets in at a very robust transition.

The entropy \( S_{cd,q=4} = 0.510380 \) is almost exactly that of the \( q = 3 \) decorated honeycomb lattice, proving almost perfect \( A \)-sublattice order. This result is related to the 3-bond colouring and \( n = 2 \) FPL problems on the dual \((4,6,12)\) Archimedean lattice, and to \( n = 3 \) CPL and six-vertex models on the kagome lattice, all of which are non-critical.

*In fact the \( q = 5 \) Potts model is also ordered on this lattice, the highest value of \( q \) known in any 2D geometry.*
Partial Order: Magnetisation and Susceptibility

The field term in $\mathcal{H}$ can be used to define many different types of magnetisation and corresponding susceptibilities $\chi = \frac{\partial M}{\partial H}$.

- $M$ contains the most information to characterise the (partially) ordered state, including "defects" from perfect order.
- $\chi$ contains the clearest indication of a phase transition.
- Although $M$ can be calculated with larger $D$ than $C$, the $T$ grid specifies the accuracy in the determination of $T_c$.

$q = 3$ Potts model on the centred diced lattice (partially ordered phase at intermediate temperature).

$q = 4$ Potts model on the Union-Jack lattice.
Partial Order with Sub-Extensive Entropy

The entropy controls the onset of partial order. However, an extensive entropy is not a prerequisite. Certain models exhibit the same phenomenon with an entropy in 2D that scales only linearly in the system length:

- \( q = 3 \) Potts model on the generalised decorated square lattice (\( q = 4 \) is critical).
- \( q = 3 \) Potts model on the IIA dilute centred diced lattice.

\[
S_0 = \lim_{L \to \infty} \frac{\log(6 \times 2^L - 6)}{L^2} = 0
\]
Multiple Phase Transitions

Some Potts models, generally with $q < z$, have a complex phase diagram with intermediate-temperature partial order and more than one phase transition:

- Ising model on the Union-Jack lattice with $|J_C/J_{AB}| \sim 1$: complete loss of order between mutually incompatible competitors (one entropy-favoured).
- $q = 3$ Potts model on the Union-Jack lattice with $J_C > 2J_{AB}$: zero-entropy 3-sublattice-ordered ground state is overcome at finite temperatures.
Detecting Phase Transitions

Tensor-network techniques allow some physical properties to be detected directly from the properties of the tensor, rather than from thermodynamic indicators.

Define the quantity

\[ X = \frac{(\text{Tr} A)^2}{\text{Tr}(A^2)} \]

where \( A_{zz'} = \sum_{x,y} T_{xx'yy'zz'} \) is a \( D \times D \) matrix.

New physics becomes possible: consider the Potts model in 3D (simple cubic lattice).

- \( q = 2 \) (Ising): obtain 10 digits of accuracy in \( T_c \) with \( D = 23 \).
- \( q = 3 \) (first order): competitive accuracy with \( D = 21 \).

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<td>CTMRG (2001) [38]</td>
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<td>TPVA (2005) [39]</td>
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<td>HOTRG (D = 23, this work)</td>
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<td>Monte Carlo RG (1979) [14]</td>
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<td>Monte Carlo (1991, L = 36) [47]</td>
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<td>( (D = 14) )</td>
<td>( (D = 21) )</td>
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Quantum Mechanics: MPS and PEPS

A tensor-network state in 1D is a **matrix-product state** (MPS), the basis of DMRG. An MPS is a *trial wavefunction formed from virtual entangled pairs on neighbouring lattice sites* – a local description of many-body states based on their entanglement structure.

**Projected Entangled Pair States** (PEPS) are a generalisation of MPS:
- based on virtual maximally entangled pairs of neighbouring sites;
- satisfy the *area law of entanglement entropy* – thought to be the key factor differentiating quantum and classical systems (entanglement is the basis of *topological quantum order*);
- allow a system with exponentially many degrees of freedom to be represented/calculated in **polynomial time**.

**Singular Value Decomposition** (SVD)
The (entanglement) structure of any quantum wavefunction is revealed under Schmidt decomposition, which for DMRG is a SVD. PEPS are based on local entanglement, making wavefunction construction very simple.

**Problems with PEPS**
- bond dimension: only low-$z$ systems can be handled with accurate $D$.
- **frustration**: *fails completely for some systems, e.g. kagome ...* – need to generalise the entangled pair to a *simplex*. 
PESS Representation of Simplex Solid States

PESS: Projected Entangled Simplex States

- introduce one type of tensor, $A$, for the bond entanglement
- and a second type of tensor, $S$, for the local cluster, or simplex:
  - $S$ contains the multipartite entanglement of the $N$-site simplex unit.

$$|\Psi\rangle = Tr \left( \cdots S_{abc} A_{aa'} [\sigma_i] A_{bb'} [\sigma_j] A_{cc'} [\sigma_k] \cdots \right) |\cdots \sigma_i \sigma_j \sigma_k \cdots \rangle$$

Begin with Simplex Solid States of the SU(N) quantum antiferromagnet [1], a generalisation of the AKLT state. Each simplex contains a virtual singlet. Take the $S = 2$ kagome lattice as a system of $3 \times S = 1$ spins on each simplex – triangle: $1 \otimes 1 \otimes 1 = 0 \oplus (3 \times 1) \oplus (2 \times 2) \oplus 3$; bond: $2 \otimes 2 = 0 \oplus 1 \oplus 2 \oplus 3 \oplus 4$.

and the PESS for the simplex solid state is the exact ground state of the projection operator

$$H = \sum_{\langle ij \rangle} P_4 (ij)$$

Extending PESS for Simplex Solid States

Simplex solid states can be constructed for any higher spin and indeed any Lie algebra, including SU(N), as long as a unique singlet can be formed in each simplex.

**Triangular lattice:** SSS defined on a honeycomb lattice, projection tensor $A$ has dimension $dD^3$ ($d$ = number of physical indices), much less than $dD^6$ for PEPS treatment. With virtual $S = 1$ states, each triangle is $S = 3$ and $J_1 - J_2$ square lattice: no unique choice of PESS decomposition – can be edge-sharing simplices with tensor dimension $dD^4$ or corner-sharing simplices with tensor dimension $dD^2$ – strong simplification of numerics.

$$S_{ijk} = \varepsilon_{ijk}$$

$$H = \sum_{\langle ij \rangle} P_6 (ij)$$
PESS as a Variational Ansatz I

PESS provide a good approximation – which obeys the entanglement area law – for the ground state of any quantum lattice model, and therefore can be used as a variational wavefunction. If

\[ H = H_x + H_y + H_z = J \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z) \]

the partition function may be approximated by

\[
Z = \text{Tr} e^{-\beta H} \approx \text{Tr} \left( e^{-\tau H} \right)^M \approx \text{Tr} \left( e^{-\tau H_x} e^{-\tau H_y} e^{-\tau H_z} \right)^M \\
\approx \sum_{\{\sigma^x, \sigma^y, \sigma^z\}} \prod_{n=1}^{M} \langle \sigma^{x,n} | e^{-\tau H_x} | \sigma^{x,n} \rangle \langle \sigma^{x,n} | \sigma^{y,n} \rangle \\
\times \langle \sigma^{y,n} | e^{-\tau H_y} | \sigma^{y,n} \rangle \langle \sigma^{y,n} | \sigma^{z,n} \rangle \\
\times \langle \sigma^{z,n} | e^{-\tau H_z} | \sigma^{z,n} \rangle \langle \sigma^{z,n} | \sigma^{x,n-1} \rangle.
\]

where the (local, Ising, i.e. classical) basis sets are connected by the local transformation matrices

\[
A_{\sigma^{x,n}, \sigma^{y,n}}^{x} = \langle \sigma^{x,n} | \sigma^{y,n} \rangle = \prod_{j} A_{j, \sigma^{x,n}, \sigma^{y,n}}^{x}
\]

and \( \langle \sigma^{\alpha,n} | e^{-\tau H_\alpha} | \sigma^{\alpha,n} \rangle = \prod_{\nabla_{ijk}} S_{\sigma_i^{\alpha,n}, \sigma_j^{\alpha,n}, \sigma_k^{\alpha,n}}^{\alpha} \)

is the Boltzmann weight of \( H_\alpha \) in the same basis, with

\[
S_{\sigma_i, \sigma_j, \sigma_k}^{\alpha} = \exp \left[ -\tau J \left( \sigma_i \sigma_j + \sigma_k \sigma_i + \sigma_j \sigma_k \right) \right]
\]

Now:

\[ Z \approx \text{Tr} T^M \]

with \( T = T_x T_y T_z \)

and

\[ \langle \sigma' | T^\alpha | \sigma \rangle = \prod_{\nabla_{ijk}} S_{\sigma_i', \sigma_j', \sigma_k'}^{\alpha} \prod_{j} A_{\sigma_j', \sigma_j}^{j}. \]

\( T^\alpha \) is a simplex tensor network operator on the honeycomb lattice whose matrix elements contain both the entangled simplex (\( \nabla \)) and projection tensors.
PESS Calculations: Projection, Simplex Choice and Update Scheme

The wavefunction is a product of simplex tensor network operators. With an arbitrary initial PESS wavefunction, application of $T^\alpha$ retains the PESS structure. Systematic projection (a type of iTEBD) yields an increasingly accurate ground state.

- as $\tau \to 0$, non-commutativity errors vanish.
- the PESS bond dimension is doubled at each projection: systematic truncation is required.

Larger simplices yield increasingly accurate results.

PESS calculations still face problems in accessing sufficiently large $D$. One way to reduce their cost is the simple update scheme where the bond environment is not computed simultaneously, yielding a rapid algorithm reaching larger $D$. 
PESS Calculations: HOSVD

The Hamiltonian for alternating simplices, \( H = H_\Delta + H_\nabla \), has non-commuting terms and is evaluated in a two-step process with
\[
e^{-\tau H} = e^{-\tau H_\Delta} e^{-\tau H_\nabla} + \mathcal{O}(\tau^2),
\]

In the PESS formalism,
\[
e^{-\tau H_\nabla} |\Psi_0\rangle = Tr\left(\ldots T_{\alpha\sigma_i,\sigma_j,\sigma_k}^{\alpha\nabla} S_{\sigma_{i\sigma_j\sigma_k}}^{\beta\Delta} \ldots \right)|\sigma_i\sigma_j\sigma_k\ldots\rangle
\]
with
\[
T_{\alpha\sigma_i,\sigma_j,\sigma_k}^{\alpha\nabla} = \sum_{\sigma_{i\sigma_j\sigma_k}} \langle\sigma_i\sigma_j\sigma_k|e^{-\tau H_\nabla\alpha}\sigma_i'^{\sigma_i'}\sigma_j'^{\sigma_j'}\sigma_k'^{\sigma_k'} S_{\sigma_{i\sigma_j\sigma_k}}^{\alpha\nabla} A_a^{\alpha'} A_b^{\beta} A_c^{\gamma} [\sigma_i'] [\sigma_j'] [\sigma_k'] \rangle.
\]

Now HOSVD is used to decompose \( T \) into renormalised projection and simplex tensors and to include the environment tensors surrounding \( T \), which appear as a singular bond vector \( \lambda \):
\[
\overline{T}_{\alpha\sigma_i,\sigma_j,\sigma_k}^{\alpha\nabla} = \lambda_{\alpha\beta,a}\lambda_{\alpha\beta,b}\lambda_{\alpha\beta,c} T_{\alpha\sigma_i,\sigma_j,\sigma_k}^{\alpha\nabla}
\]
From the HOSVD,
\[
\overline{T}_{\alpha\sigma_i,\sigma_j,\sigma_k}^{\alpha\nabla} = \sum_{a'b'c'} \overline{S}_{\alpha\sigma_i,\sigma_j,\sigma_k}^{\alpha\nabla} U_{\beta,a}^{\alpha'} U_{\beta,b}^{\beta} U_{\beta,c}^{\gamma}
\]
where \( \overline{S}_{\alpha\sigma_i,\sigma_j,\sigma_k}^{\alpha\nabla} \) is the core tensor and \( U \) is a unitary matrix determined by diagonalising the density matrix. The renormalised \( A \) tensor is given by
\[
A_{\alpha\beta}^{\alpha'} [\sigma] = U_{\alpha',\alpha\sigma} \lambda_{\beta,a}^{-1}
\]
By keeping the first \( D \) states for each index, one truncates to a \( DxDxD \) matrix \( S_{\alpha\sigma_i,\sigma_j,\sigma_k}^{\alpha\nabla} \).
The kagome lattice is one of the most frustrated geometries known in real materials. The $S = \frac{1}{2}$ nearest-neighbour kagome Heisenberg antiferromagnet is a candidate quantum spin liquid – a state with:

- no magnetic order,
- breaking no lattice symmetries and
- with a specific topological quantum order.

Understanding the kagome system is currently one of the defining challenges in condensed matter:

- theory: entanglement, fractionalisation, topological order.
- numerics: frustration, high-dimensions, entanglement.
- experiment: unambiguous probes of spin-liquid nature.
- materials growth: realisation, as large single crystals.
Materials with Kagome Geometry

- jarosites, volborthites, langasites, …, organometallics.
- herbertsmithite: \( \text{Cu}^{2+} \) system, \( S = \frac{1}{2} (\text{ZnCu}_3(\text{OH})_6\text{Cl}_2) \);
- pyrochlore geometry, with Zn ions on triangular planes and Cu ions and Zn impurities on kagome planes.
- many experiments supporting spin-liquid nature …
- triangular geometry with Cu ions leads to DM interactions.


$S = \frac{1}{2}$ kagome antiferromagnet: old news

- ground state: no magnetic order
- ultra-short spin correlation length ($\sim 1.3a$)
- ... but dimer-dimer correlations of longer range
- continuum of low-lying singlets, extensive density $N_{\text{sing}} \sim 1.15^N$
- excellent description in terms of nearest-neighbour dimers – “short-range RVB”

**Numerics:**

- ground-state energy: $e_0 = -0.438J$ per site
- gap (singlet-triplet): not so small, $\Delta \sim 0.18J$
- gap (singlet-singlet): small or zero ...
- $1/3$ magnetisation plateau (a gapped state)

**Spin correlations:** exponential decay.

**Dimer correlations:** long-ranged decay ... ?

Various pieces of numerical and analytical evidence in support of spinons, fractionalisation, spin and/or charge deconfinement, ...
Types of spin-liquid ground state

(a) Manifold of degenerate basis states
(b) Type-I gapped spin liquid
(c) Type-II gapped spin liquid
(d) Algebraic spin liquid
All options are still on the table …

SRRVB probably means a type-II gapped spin liquid:
- finite gap,
- no discernible order,
- favoured by some DMRG studies [2],
- \( E = -0.43552J \).

Projected wave-function study (“flux phase”, large-\( N \)) [3] favours
- U(1) Dirac fermions,
- gapless,
- algebraic spin liquid,
- \( E = -0.42866J \).

Large-unit-cell VBC:
- 36- or 72-site unit cell,
- very small gap,
- support from series expansions [1],
- \( E = -0.433J \).

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PESS: computing physical properties

**Evaluation of PESS expectation values:** the wavefunction is projected onto an MPS basis (boundary construction). This process is not variational, but for an MPS basis bond dimension $D_{mps} > 60$, the truncation error $\varepsilon < 10^{-4}$ for the 3- and 9-PESS (more for the 5-PESS, even with $D_{mps} = 140$).

**Benchmarking PESS results:**
- the 3- and 9-PESS formulations break up/down triangle symmetry;
- the 5-PESS geometry breaks threefold rotation symmetry.

Verify that all associated energies become equal in the limits of small $\tau$ and large $D$ and $D_{mps}$ (which are interdependent):
- all symmetries restored in the asymptotic limits,
- expect this to be true also for all other expectation values.
The PESS energy is highly competitive. It will clearly become lower as $D$ is increased. This value is an upper bound (variational); all improvements will deliver lower energies.

The current optimal value is $e_0 = -0.4364(1) \text{J}$ for the 9-PESS with $D = 13$. Values should converge exponentially, but none of the data have reached this regime.

**Work in progress …**
Nature of the Kagome Ground State

PESS, like MPS, is based on gapped phases. Thus it is highly likely that a maximally refined PESS wavefunction will describe a gapped spin liquid [1,2]:

- large singlet-triplet gap,
- very short spin correlation length,
- $\mathbb{Z}_2$ topological order,
- RVB phase; dominant dimer resonance processes debated [1].

1) One competing scenario is the **algebraic spin liquid** based on $U(1)$ Dirac fermions. An optimised variational calculation [3] gives $e_0 = -0.4365J$.

**Could PESS find this phase? Can the correlation length $\xi$ diverge with $D$?**

2) Another is a **chiral spin liquid** ($S_i S_j x S_k$ finite, spontaneous breaking of TRS), which appears in models with Ising-type next-neighbour couplings [4]…

3) … or perhaps this is some kind of **double-semion state** (TRS-preserving), appearing even in systems with isotropic next-neighbour couplings [5].

Calculations are of necessity moving towards more sophisticated indicators of the ground-state nature, e.g. **entanglement spectrum, modular matrices**.

Summary

- tensor-network methods for lattice models: huge progress.
- classical systems: application to any lattice; infinite system size.
- all thermodynamic quantities, identify phase transitions and exponents.
- irregular lattices: new phase transitions, partial order, very high $q_c$.
- frustrated quantum systems: PESS is a qualitative breakthrough.
- PESS reduces required tensor sizes and enlarges the accessible $D$ range.
- HOSVD + iTEBD + simple update scheme = powerful calculational method.
- application to kagome lattice: $e_o/J = -0.4364(1)$ … so far – very competitive energy with clear scope for improvement.
- immediate future: i) larger $D$ – calculations in progress to reach $D = 30$.
  ii) correlation functions, entanglements, modular matrices ...
  iii) better treatment of bond environment,
  iv) further frustrated quantum lattice models.

- physics: new insight into a) phase transitions in Potts models and b) the kagome wavefunction and its entanglement structure.