Four-coloring model and frustrated superfluidity in the diamond lattice: Supplementary material

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ANTIFERROMAGNETIC POTTS MODEL ON PYROCHLORE LATTICE.

Here we present a numerical estimate of the residual entropy of the 4-coloring model on the diamond lattice. Since the color variables are defined on bonds of the diamond lattice, it is more convenient to consider an equivalent Potts model on the pyrochlore lattice whose sites correspond to the bond midpoints in the diamond lattice; see Fig. 1 in the main text. For convenience, we shall use i, $j, \cdots$ to denote the diamond sites, and use m, $n, \cdots$ for the sites on pyrochlore lattice. A Potts variable $\sigma_m = \sigma_{ij} = 0, 1, 2, 3$ is assigned to each pyrochlore site such that the corresponding phase is given by $\phi_m = \theta + \sigma_m \frac{\pi}{2}$, where θ is the global U(1) phase. The constraint that bonds attached to the same vertex have different colors translates to an antiferromagnetic interaction between nearest-neighbor Potts variables on the pyrochlore lattice:

$$H = J \sum_{\langle ml \rangle} \delta(\sigma_m, \sigma_l), \tag{1}$$

Here the coupling constant $J \sim n\, t_{\parallel}$. To avoid confusion, we use m, l to label the pyrochlore sites. The hard constraint of the 4-coloring model is recovered in the $J \to \infty$ limit. Consider first a single tetrahedron, there are $4\,! = 24$ ground states in which the four sites are in different Potts states. These correspond to the 24 coloring schemes on a diamond site.

The pyrochlore Potts model (1) represents an under-constrained system with an extensively degenerate ground state, similar to their two-dimensional counterparts [1, 2]. The residual entropy of the 4-coloring model can be computed by performing finite temperature Monte Carlo simulations of the pyrochlore Potts model (1). As shown in Fig. 1(a), by integrating the numerical specific-heat curve and fixing the high-T entropy density to $k_B \ln 4$ (a Potts paramagnet), we obtain a zero-temperature entropy density $S_0 \approx 0.2112\, k_B$. The degeneracy can also be computed using a method similar to the Pauling estimation for the degeneracy of water ice [3]. Consider a single tetrahedron, $4\,!$ out of 4^4 Potts configurations satisfy the color constraint. Treating the constraints imposed by different tetrahedra as independent, the number of degenerate ground states is $W \sim 4^N (4!/4^4)^{N/2}$, where N is the number of Potts variables and $N/2$ is the number of tetrahedra (or diamond sites). This estimation gives an entropy density: $S_0/k_B = (1/2)\ln(3/2) \approx 0.2027$, which is very close to the numerical value $S_0 \approx 0.2112\, k_B$.

MAPPING TO EMERGENT FLUX FIELDS.

To map the highly constrained 4-coloring manifold to the emergent flux fields, and to make manifest the analogy with the frustrated spin systems, we consider a Heisenberg antiferromagnet on the pyrochlore lattice:

$$H = \mathcal{J} \sum_{\langle ml \rangle} \mathbf{S}_m \cdot \mathbf{S}_l + D \sum_m f(\mathbf{S}_m; \{\boldsymbol{\tau}_s\}). \tag{2}$$

Here $\mathcal{J} > 0$ and $\mathbf{S}_m$ denotes a classical $O(3)$ vector of unit length. The second term represents a special 'tetrahedral' anisotropy: the function $f(\mathbf{S})$ has four degenerate minimum at directions $\boldsymbol{\tau}_s$ pointing toward different coners of a regular tetrahedron; see the inset of Fig. 3(a) in the main text. In the $D \to \infty$ limit, Hamiltonian (2) reduces to the Potts model as the spins are aligned to the tetrahedral vectors according to $\mathbf{S}_m = \boldsymbol{\tau}_{\sigma_m}$, where σ_m is the corresponding Potts variable at site m. The exchange term in (2) can be rewritten as $(\mathcal{J}/2) \sum_{\boxtimes} |\mathbf{S}_{\boxtimes}|^2$ up to an irrelevant constant, where $\mathbf{S}_{\boxtimes} = \sum_{m \in \boxtimes} \mathbf{S}_m$ denotes the total spin of a tetrahedron. The ground state of the above spin model is reached when the total spin $\mathbf{S}_{\boxtimes} = 0$ for all tetrahedra.

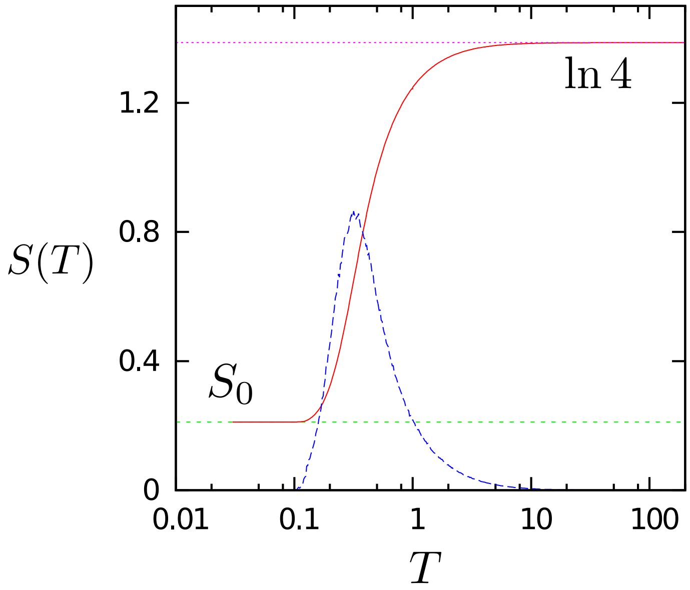

FIG. 1: (Color online) Monte Carlo simulations of the antiferromagnetic 4-state Potts model Eq. (1) on pyrochlore lattice: entropy S and specific heat C as a function of temperature T; the energy is measured in units of J. Fixing the high-T entropy density to $k_B \ln 4$ gives a residual $S_0 \approx 0.2112 k_B$.

Since the Potts variables σ_m in any individual tetrahedra assume four different values for a valid 4-coloring configuration on the diamond lattice, and noting that the four $\boldsymbol{\tau}_s$ vectors sum to zero, we have:

$$\mathbf{S}_{\boxtimes} = \sum_{m \in \boxtimes} \mathbf{S}_m = \sum_{m \in \boxtimes} \boldsymbol{\tau}_{\sigma_m} = 0, \tag{3}$$

for all tetrahedra, indicating the corresponding magnetic state $\{\mathbf{S}_m\}$ is a ground state of the spin model. We thus establish an one-to-one correspondence between the 4-coloring configuration and the ground states of the spin model.

The mapping to the spin model (2) also allows us to recast the color constraint into a conservation law of effective magnetic flux similar to the case of pyrochlore spin model discussed in Refs. [4–6]. We first define three 'magnetic' fields, each corresponds to a component of the Heisenberg spin, on the diamond site

$$\mathbf{B}^{\alpha}(\mathbf{r}_i) = \sum_{\nu=0}^{3} S^{\alpha}_{\langle ij \rangle}\, \hat{\mathbf{n}}_{\nu} = \sum_{\nu=0}^{3} \tau^{\alpha}_{\sigma_m}\, \hat{\mathbf{n}}_{\nu}. \tag{4}$$

Here $\alpha = x, y, z$, the summation is over the four nearest-neighbor bond directions $\hat{\mathbf{n}}_\nu$, and the pyrochlore site m corresponds to the bond $\langle ij \rangle \parallel \hat{\mathbf{n}}_\nu$ in the diamond lattice. Since for every tetrahedra in the ground state, there are two $+$ and two $-$ signs for each component α of the four $\boldsymbol{\tau}_{\sigma_m}$ vectors. Thus the $\mathbf{B}$ field for *each* spin component α corresponds to a two-in-two-out configuration, i.e. the flux fields are conserved in each tetrahedra (no source or sink). In the coarse-grained approximation, the color constraints $\mathbf{S}_{\boxtimes} = 0$ translate to a divergence constraint $\nabla \cdot \mathbf{B}^{\alpha}(\mathbf{r}) = 0$ for the magnetic fields [7].

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