



Gapless Spin-Liquid Ground State in the $S = 1/2$ Kagome Antiferromagnet

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The defining problem in frustrated quantum magnetism, the ground state of the nearest-neighbor $S = 1/2$ antiferromagnetic Heisenberg model on the kagome lattice, has defied all theoretical and numerical methods employed to date. We apply the formalism of tensor-network states, specifically the method of projected entangled simplex states, which combines infinite system size with a correct accounting for multipartite entanglement. By studying the ground-state energy, the finite magnetic order appearing at finite tensor bond dimensions, and the effects of a next-nearest-neighbor coupling, we demonstrate that the ground state is a gapless spin liquid. We discuss the comparison with other numerical studies and the physical interpretation of this result.

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In one spatial dimension (1D), quantum fluctuations dominate any physical system and semiclassical order is destroyed. In higher dimensions, frustrated quantum magnets offer perhaps the cleanest systems for seeking the same physics, including quantum spin-liquid states, fractionalized spin degrees of freedom, and exotic topological properties. This challenge has now become a central focus of efforts spanning theory, numerics, experiment, and materials synthesis [1–4]. While much has been understood about frustrated systems on the triangular, pyrochlore, Shastry-Sutherland, and other 2D and 3D lattices, it is fair to say that the ground-state properties of the $S = 1/2$ kagome Heisenberg antiferromagnet (KHAF) remain a complete enigma.

An analytical Schwinger-boson approach [5], coupled-cluster methods [6], and density-matrix renormalization-group (DMRG) calculations [7–9], including analysis of the topological entanglement entropy [10], all suggest a gapped spin liquid of Z_2 topology. The most sophisticated DMRG studies [9,11] estimate a triplet spin gap $\Delta \geq 0.05J$. Analytical large- N expansions [12] and numerical simulations by the variational Monte Carlo (VMC) technique [13,14] suggest a gapless spin liquid with $U(1)$ symmetry and a Dirac spectrum of spinons. Extensive exact-diagonalization calculations conclude that the accessible system sizes are simply too small to judge [15,16]. Debate continues between the gapped Z_2 and gapless $U(1)$ scenarios, with very recent arguments in support of both [17,18], while a study using symmetry-preserving tensor-network states (TNS) favors the gapped Z_2 ground state [19]. Experimental approaches to the kagome conundrum have made considerable progress in recent years, but for the purposes of the current theoretical analysis we defer a review to Sec. SI of the Supplemental Material (SM) [20].

In this Letter, we employ the projected entangled simplex states (PESS) description of the entangled many-body ground state to compute the properties of the KHAF. Because we consider an infinite system, our results provide hitherto unavailable insight. As functions of the finite tensor bond dimension, we find algebraic convergence of the ground-state energy and algebraic vanishing of a finite staggered magnetization, indicating a gapless spin liquid. We demonstrate that the phase diagram in the presence of next-nearest-neighbor coupling contains a finite region of this spin-liquid phase. Our results suggest that the physics of the KHAF is driven by maximizing the kinetic energy of gapless Dirac spinons.

The TNS formalism is based on expressing the wave function as a generalized matrix-product state (MPS) [52–54]. As we review in Sec. SII of the SM [20], this ansatz obeys the area law of entanglement and, crucially, allows the construction of a renormalization-group scheme to reach the limit of infinite lattice size. The truncation parameter is the tensor bond dimension, D . We introduced the PESS formulation [55] in order to capture the multipartite entanglement within each lattice unit, or simplex [55–57], which is the key element of frustrated systems and is missing in the conventional pairwise projected entangled pair states construction. Summarizing the numerical procedure (Sec. SII [20]), the optimized PESS approach is a projection technique, with tensor manipulation performed by higher-order singular-value decomposition, and freedom to choose the simplex, the unit cell, and a simple- or full-update treatment of the bond environment during tensor renormalization, the former allowing access to larger D but the latter achieving more rapid convergence.

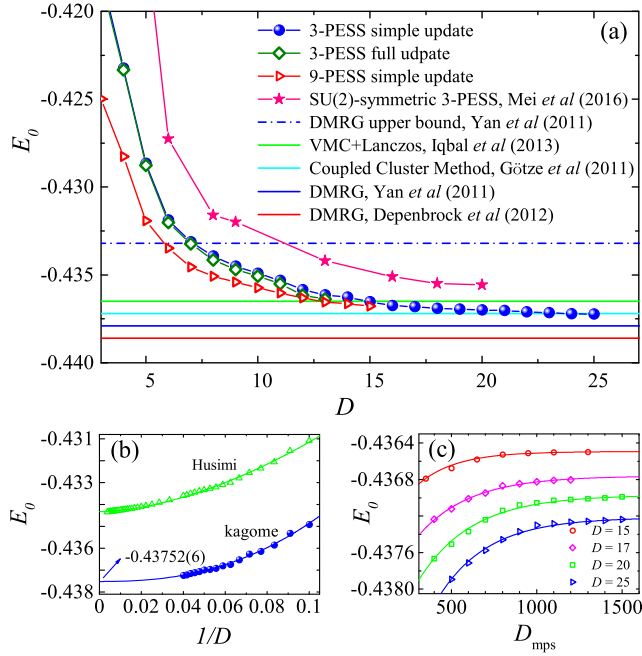


FIG. 1. Ground-state energy of the KHAF. (a) E_0 as a function of D , shown for the 3-PESS and simple-update method up to $D = 25$, 3-PESS by full update to $D = 13$, and 9-PESS with simple update to $D = 15$. Shown for comparison are results from other numerical studies. (b) $E_0(D)$ for the 3-PESS ansatz, shown as a function of $1/D$ and compared with results obtained for the Husimi lattice [57]. (c) Convergence of $E_0(D)$ as a function of D_{mps} , shown for several values of D .

However, TNS calculations are a two-step process, where the wave function is obtained first and then used to calculate physical expectation values. This latter step requires projection onto a 1D MPS basis, whose dimension for convergence is found to scale approximately as $D_{\text{mps}} \approx 4D^2$. Once $D \gtrsim 15$, the evaluation step becomes the more computationally intensive problem, and here we implement new methodology (outlined in Sec. SII [20]) by which we extend the accessible D range.

We begin by presenting results from the 3-site-simplex (3-PESS) ansatz for all accessible D values. The ground-state energy, $E_0(D)$, of the nearest-neighbor KHAF is shown in Fig. 1(a). At large D , our estimate lies below those obtained from all known techniques other than DMRG studies of specific clusters, which are not an upper bound. We remark that our $E_0(D)$ values are significantly lower than those of an SU(2)-invariant TNS analysis [19]. We find that $E_0(D)$ converges algebraically with D , as on the Husimi lattice [57], indicating a gapless ground state [58]. The power-law form $E_0(D) = e_0 + aD^{-\alpha}$, shown in Fig. 1(b), delivers our best estimate of the ground-state energy, $e_0 = -0.43752(6)J$. Figure 1(c) illustrates the convergence of $E_0(D_{\text{mps}})$ for selected values of D ; we note that this part of the process is not variational and comment in detail in Sec. SII of the SM [20]. Optimized fits

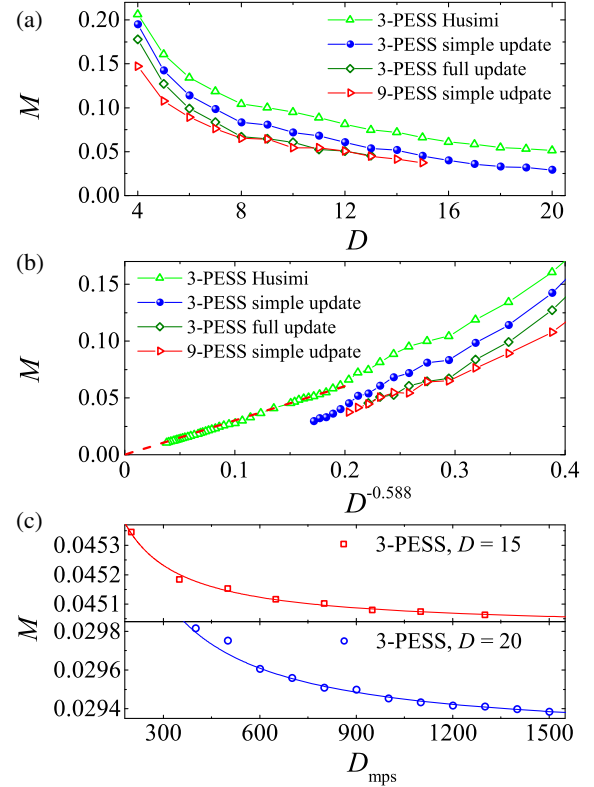


FIG. 2. Staggered magnetization of the KHAF at finite D . (a) M as a function of D , shown for the 3-PESS and simple-update method up to $D = 20$, 3-PESS by full update to $D = 13$, and 9-PESS with simple update to $D = 15$. Shown for comparison are results obtained for the Husimi lattice [57]. (b) M as a function of $1/D^{0.588}$, the power-law form obtained for the Husimi lattice. (c) Convergence of $M(D)$ as a function of D_{mps} , shown for $D = 15$ and $D = 20$.

to a regime of exponential convergence in D_{mps} were used to extrapolate towards the values of $E_0(D)$ shown in Figs. 1(a) and 1(b), and to determine the associated error bars, on the basis of which we limit our claims of reliability to $D \leq 25$.

One key qualitative property of our PESS wave function is a finite 120° magnetic order at all finite D values, as shown in Figs. 2(a) and 2(b). The order parameter, $M(D)$, varies algebraically with $1/D$ over the available D range, tending to zero as $D \rightarrow \infty$, as required of a spin liquid. Figure 2(c) illustrates the convergence of $M(D_{\text{mps}})$ for $D = 15$ and 20 , where an algebraic form was deduced from the truncation error, and reliable extrapolations to large D_{mps} were obtained only for $D \leq 20$.

The Husimi lattice provides essential confirmation of our results. It possesses the same local physics as the kagome lattice, but less frustration from longer paths, and it allows PESS calculations up to $D = 260$, yielding accurate extrapolations to the large- D limit [57]. It confirms the crucial qualitative statement that magnetically ordered states have the lowest energies for spatially infinite systems

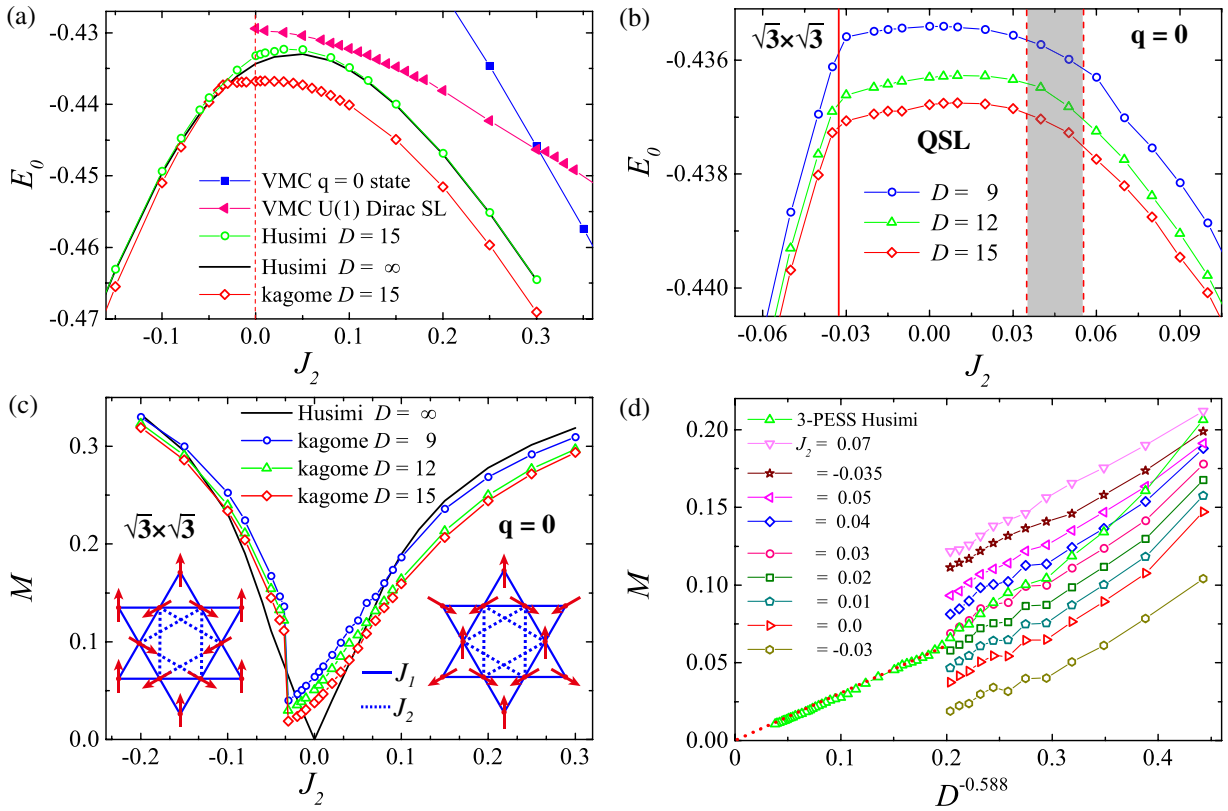


FIG. 3. Energy and staggered magnetization of the KHAF with next-nearest-neighbor coupling. (a) $E_0(J_2)$ calculated with a 9-PESS using $D = 15$. Shown for comparison are results for the Husimi lattice with $D = 15$ and $D = \infty$, as well as the VMC results of Ref. [14]. (b) Detail of $E_0(J_2)$ near $J_2 = 0$; with increasing D , a cusp-type discontinuity emerges near $J_2 = -0.03$ (red solid line). The shaded region denotes the location of the continuous transition at small positive J_2 , deduced from the magnetization of panel (d). (c) $M(J_2)$ calculated using $D = 9, 12$, and 15 , compared with results for the Husimi lattice at $D = \infty$. Insets represent the $\sqrt{3} \times \sqrt{3}$ (left) and $q = 0$ ordered phases (right). (d) M as a function of $1/D^{0.588}$, with the Husimi result indicating J_2 values for which M may extrapolate to zero within the error bars.

at finite D . It benchmarks the algebraic nature of $E_0(D)$ [Fig. 1(b)] and $M(D)$ [Fig. 2(b)], the latter vanishing exactly at large D . The Husimi $M(D)$ sets an upper bound on the kagome $M(D)$ (Sec. SIII of the SM [20]). Our kagome results lie well below this bound, but with no evidence for deviation from a similar algebraic form, reinforcing the conclusion that the ground state of the KHAF is a gapless spin liquid.

For full rigor we consider every aspect of the PESS procedure. Full-update calculations confirm the accuracy of the simple-update approximation for all accessible D values. $E_0(D)$ lies only slightly lower [Fig. 1(a)], with no change in functional form; similarly, $M(D)$ is suppressed by several percent [Figs. 2(a) and 2(b)], reinforcing the argument for convergence to $M = 0$ at large D , but still shows algebraic behavior. To investigate whether magnetic order might be artificially enhanced by the 3-PESS ansatz, in Figs. 1(a), 2(a), and 2(b) we also present results obtained using a 9-site simplex (9-PESS) [55], which again confirm the algebraic form of $E_0(D)$ and $M(D)$, with no evidence either of a crossover to exponential behavior of $E_0(D)$ or of

a collapse of $M(D)$ to zero at finite D . 3-PESS calculations may be performed with a unit cell containing any number of simplices (Sec. SII [20]); our results for 3-, 9-, and 12-site unit cells are identical, again confirming no inherent bias of this type.

Further essential confirmation is obtained by adding a next-nearest-neighbor coupling, J_2 . These calculations are performed most efficiently with a 9-PESS ansatz and we reach $D = 15$ with simple updates. As shown in Fig. 3(a), $E_0(J_2)$ is maximal (the system is most frustrated) close to $J_2 = 0$ and is not symmetrical about this point. For the Husimi lattice, $E_0(J_2)$ is continuous, with maximal frustration at $J_2 \approx 0.04$. By contrast, the kagome case shows a regime of almost constant energy when $-0.03 \lesssim J_2 \lesssim 0.04$ [Fig. 3(b)]. To understand the nature of these states, we consider in Fig. 3(c) the finite- D magnetization and in Fig. 3(d) $M(D)$ for selected values of J_2 . For the Husimi lattice, $M(J_2)$ is zero only at $J_2 = 0$, where it has a discontinuity, and [despite the form of $E_0(J_2)$] is almost symmetrical. For kagome, the expected ordered phases are the $q = 0$ structure at $J_2 > 0$ and the $\sqrt{3} \times \sqrt{3}$ structure at

$J_2 < 0$ [Fig. 3(c)]. However, $M(J_2)$ at finite D continues to fall through $J_2 = 0$ from above, indicating a region of $q = 0$ order at $J_2 < 0$, which is terminated at $J_2 \simeq -0.03$ by a discontinuous jump to $\sqrt{3} \times \sqrt{3}$ order. From Fig. 3(d), $M(D)$ appears to extrapolate to zero over a range of J_2 values, which we estimate from the Husimi magnetization to be fully consistent with the “plateau” in $E(J_2)$ [Fig. 3(b)].

The gapless spin liquid should exist over a finite range of J_2 if it is a robust quantum ground state. The Husimi case, with magnetic order at all finite values of $|J_2|$ and a spin liquid only at the single point $J_2 = 0$, is a type of “phase diagram” allowed only because of the pathological Husimi geometry. In the kagome case, indeed we find a finite disordered regime, bounded by a first-order transition at $J_2 \simeq -0.03$ and an apparent second-order transition at $J_2 = 0.045 \pm 0.01$. Evidently the additional quantum fluctuations due to the presence of loops in the kagome geometry act to create the same gapless spin-liquid ground state as the nearest-neighbor model ($J_2 = 0$, Figs. 1 and 2). Our results are in qualitative accord with those proposed in Ref. [14] on the basis of VMC studies of a finite system, although quantitatively the range of stability we deduce is much narrower.

PESS can be used to calculate further ground-state expectation values. However, the finite $M(D)$ means that the field-induced magnetization contains no information useful at zero field. Similarly, finite- D correlation functions have a constant part, which masks the nontrivial power-law behavior expected of a gapless spin liquid. We have nevertheless obtained definitive numerical results, in the thermodynamic limit, for the two key characteristic quantities, $E_0(D, J_2)$ and $M(D, J_2)$. Although our method is based on gapped states, it is able to indicate its own “breakdown” in the event of continuing algebraic convergence [58], and thus the conclusion of a gapless spin-liquid ground state is robust.

To interpret the physical implications of this result, the leading candidate gapless wave function is the U(1) Dirac-fermion state proposed in Ref. [12]. Although there exist gapless Z_2 spin-liquid states of the KHAF [59], there is currently neither numerical evidence [14] nor a physical argument in support of these. Heuristically, gapped spin liquids are favored by the formation of low-energy local states, such as dimer or plaquette singlets, whereas systems with a net odd-half-integer spin per simplex do not offer this option. Our results imply that there is no local unit (such as the hexagon) on the kagome lattice, and instead the optimal energy is gained by maximizing the kinetic energy of mobile spinons, leading to the U(1) Dirac-fermion state [12], or by maximizing the contributions from gauge fluctuations [60]. The gapless spin liquid is expected to have long-ranged entanglement and correlation functions [61], and the U(1) state has no well-characterized topological order.

Turning to the general question of numerical KHAF studies, our results constitute a major breakthrough because of the infinite system size. The fact that all ED and DMRG studies consistently favor gapped states suggests that systems finite even in only one dimension are not able to account appropriately for spinon kinetic-energy contributions. Regarding the question of enforced or emerging spin symmetries, PESS studies enforcing U(1) [62] or SU(2) [19] symmetry find gapped states with energies higher than ours (Fig. 1). In our calculations, it is straightforward to start with a gapped trial PESS wave function and show that an ordered state of lower energy emerges on projection. In fact all starting wave functions (symmetric, ordered, arbitrary) lead to the same final state for a given simplex and update type, with $E_0(D)$ and $M(D)$ as shown in Figs. 1 and 2. Thus it appears that symmetry-enforcing studies are finding excited states, and it is likely that the same applies on finite systems. Indeed it is argued in Ref. [18] that a gapped Z_2 ground state can lie at lower energy than the gapless U(1) state on a finite system, but not in the thermodynamic limit. A very recent study using VMC evaluation of TNS wave functions on finite systems also supports a U(1) rather than any competing Z_2 state [63].

Clearly the KHAF is a problem where competing states of very different character lie very close in energy. We deduce that the large- N approach offers the best available account of quantum fluctuation effects, specifically by capturing the kinetic-energy gain of mobile spinons. Our results also demonstrate the qualitative value of the VMC calculations [14], which arrive at the gapless spin-liquid ground state by a different route from PESS, without allowing states of finite M . It is also essential to benchmark whether the PESS ansatz is “neutral” in its energy accounting, and does not overemphasize gapless or ordered states, a question we addressed by comparing the 3- and 9-PESS results in Figs. 1(a) and 2(a).

A further question is whether the algebraic convergence we observe could cross over to exponential beyond the range of our PESS calculations. If such a crossover were to begin at $D = 26$, it is hard to argue [consider Fig. 1(b)] that the difference in extrapolated ground-state energies could exceed $\Delta E = 0.0001J$. One is then faced with the emergence of an extremely small energy scale for no apparent reason. This minuscule energy would have to be the spin gap of the corresponding Z_2 state, but clearly lies far below the DMRG gap. ΔE lies well below the “stabilization energy” of any of the competing states, whether they arise due to local resonances, spinon kinetic energy, gauge fluctuations, or any other mechanism.

Turning briefly to experiment, some studies of the material herbertsmithite, which offers Cu^{2+} ions in an ideal kagome geometry, have indeed suggested a continuum of fractional spin excitations (Sec. SI of the SM [20]). However, the most recent measurements face competing gapped

[64,65] and gapless [66,67] interpretations. In addition, it remains unclear whether, due to interplane disorder and Dzyaloshinskii-Moriya interactions, this material is providing a true reflection of kagome physics.

In summary, we have used the method of projected entangled simplex states to demonstrate that the ground state of the Heisenberg antiferromagnet for $S = 1/2$ spins on the kagome lattice with only next-nearest-neighbor interactions is a gapless quantum spin liquid. A finite next-neighbor interaction reveals the presence of a narrow regime of gapless spin liquid between states of finite 120° staggered magnetic order. This spin liquid is thought to be the U(1) Dirac-fermion state, in which the primary driving force for spin-liquid behavior is the maximization of spinon kinetic energy.

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