A Dirac Spin Liquid May Fill the Gap in the Kagome Antiferromagnet

A. *Signatures of Dirac cones in a DMRG study of the Kagome Heisenberg model* , Yin-Chen He, Michael P. Zaletel, Masaki Oshikawa, and Frank Pollmann; arXiv:1611.06238

B. *Competing Spin Liquid Phases in the S=1/2 Heisenberg Model on the Kagome Lattice* Shenghan Jiang, Panjin Kim, Jung Hoon Han, Ying Ran, arXiv:1610.02024.

Recommended with a commentary by Ashvin Vishwanath, Harvard University

In 1930 Louis Neel made a radical proposal, that the ground state of a S=1/2 quantum antiferromagnet:

$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \tag{1}$$

has spins polarized in a fixed pattern, i..e magnetic order. The conventional thinking at that time was that quantum fluctuations would destroy order, an intuition reinforced by the exact solutions of Bethe and others to the one dimensional (1D) quantum spin chain. There, magnetic order is averted and gapless spin 1/2 excitations emerge, which may be thought of as electrically neutral fermions. In 1941 Pomeranchuk conjectured that a similar situation holds in higher dimensions[1]. The development of neutron scattering however, established that it was Neel's scenario that applied to a vast number of 2D and 3D magnetic materials. The state conjectured by Pomeranchuk (with the benefit of some significant hindsight) is now identified with a gapless quantum spin liquid, where gapless spin excitations are carried by emergent fermions coupled to gauge fields. Such an extraordinary state has yet to be unambiguously established in a 2D or 3D material, and is a long sought after goal in magnetism research.

Another key problem in magnetism is the question of the ground state of the Kagome quantum antiferromagnet (KQA) [2] which has vexed researchers for the last three decades. Various states have been proposed ranging from magnetic orders to valence bond crystals (which break crystal symmetries when spin form singlets or 'valence bonds' with specific neighboring sites) to quantum spin liquids of various kinds. A materials realization in the mineral Herbertsmithite [3] that is believed to be closely approximate by model (1) on the Kagome lattice has added an experimental dimension to this problem.

The featured references A, B provide a bridge between these two problems - by making an interesting theoretical case for a gapless quantum spin liquid with Dirac fermions as the ground state of the Kagome antiferromagnet.

The case for a quantum spin liquid proceeds in two steps. First, to show that conventional forms of order are absent, which on the Kagome lattice implies that a quantum spin liquid with fractionalized excitations must be realized. The second is to identify the specific type of spin liquid - eg. to distinguish between gapped and gapless states. Previous important work by Yan, Huse and White[4], who studied the problem numerically using the density matrix renormalization group (DMRG) technique, made a strong case for a spin liquid ground state by, for example, convincingly excluding various Valence Bond Crystals that had previously been the favorite candidates. However the precise nature of the spin liquid remained uncertain - the simplest possibility consistent with an energy gap to spin excitations was a gapped spin liquid with Z_2 topological order. For example the gap to spin excitations was estimated to be $\Delta_{S=1} = 0.125J$ although the gap to spin singlet excitations was much smaller $\Delta_{S=0} = 0.05J$. Subsequent calculations of other signatures of Z_2 gapped spin liquids seem to agree with this scenario and were covered in earlier Journal Club commentaries [5, 6]. The gapped and gapless spin liquids are in correspondence with Anderson's short and long ranged resonating valence bond states.

References A, B agree with previous work regarding the spin liquid nature of the ground state. They however disagree with reference [4] with regards to the energy gap. They conclude instead that this is a *gapless* spin liquid, most likely one that features emergent Dirac fermions coupled to an emergent electromagnetic field - a version of quantum electrodynamics, played out in a two dimensional world. Such a state was proposed in [7] using a fermionic 'parton' representation of spins, which was then treated within mean field theory. It was further studied using variational wavefunctions in [8, 9] where it was demonstrated to be very close in energy to the exact ground state. A puzzle then was to reconcile this with observation of a spin gap in the DMRG studies of [4].

Reference A went beyond earlier DMRG studies in two ways. First, they attempted to mitigate finite size effects (typical simulations are done on cylinders with circumferences of $L_y = 8$ unit cells) by considering different 'wrapping' geometries, and by tuning boundary conditions. Second, they compared the observations with the expectations for free Dirac fermions in the same geometries - a simple but illuminating comparison that quantifies the degree of finite size effects. DMRG simulations are performed on cylinders, which can be obtained from by rolling up the 2D lattice in different ways. This is reminiscent of obtaining

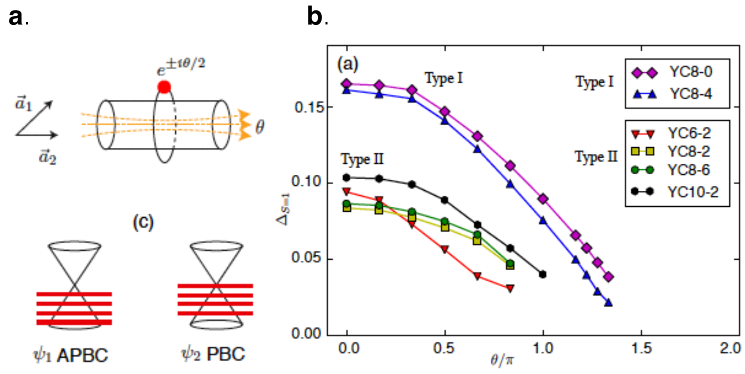

FIG. 1: (a) The Kagome antiferromagnet simulated on the cylinder geometry. The flux through the cylinder is determined by energetics, and the gap in the cylinder geometry is determined by both the wrapping geometry and the flux within the cylinder. (b) The spin gap as a function of boundary conditions. The reduction of the spin gap is consistent with the reduction of the finite size gap for the 2D Dirac nodes. From reference A.

carbon nanotubes from 1D graphene sheets, whose conducting/insulating properties depend on the choice of wrapping. For certain choices the Dirac node of the 2D band structure is preserved in the 1D geometry. For the Dirac spin liquids, an additional feature is that the gauge field is internally generated, and hence the gaplessness on the cylinder is not determined by geometry alone. In fact, since a suitable choice of flux will allow the system to remain gapped, this could be energetically favored. This finite size effect is proposed to be the origin of the energy gap seen in previous numerics, and is demonstrated by showing that the gap is significantly reduced on twisting the boundary conditions around the cylinder by suitably modifying the spin Hamiltonian (Figure 1 b). The gapless state itself is not reached due to a new ordered phase appearing at the critical flux.

The second piece of evidence presented in reference A is to utilize correlation functions as a proxy for the excitation spectrum. After benchmarking this connection, the 'spectrum' for the KQA and free Dirac fermions on the same lattice geometries are compared in Figure 2a. The 'particle-hole' excitations of the free Dirac fermions look rather similar to the nontrivial spin carrying excitations of the KQA.

Reference B takes a rather different approach by constructing a classes of wavefunctions representing the distinct *gapped* spin liquids on the Kagome lattice. Similar to earlier variational studies, in this approach the quantum state represented by these wavefunctions is

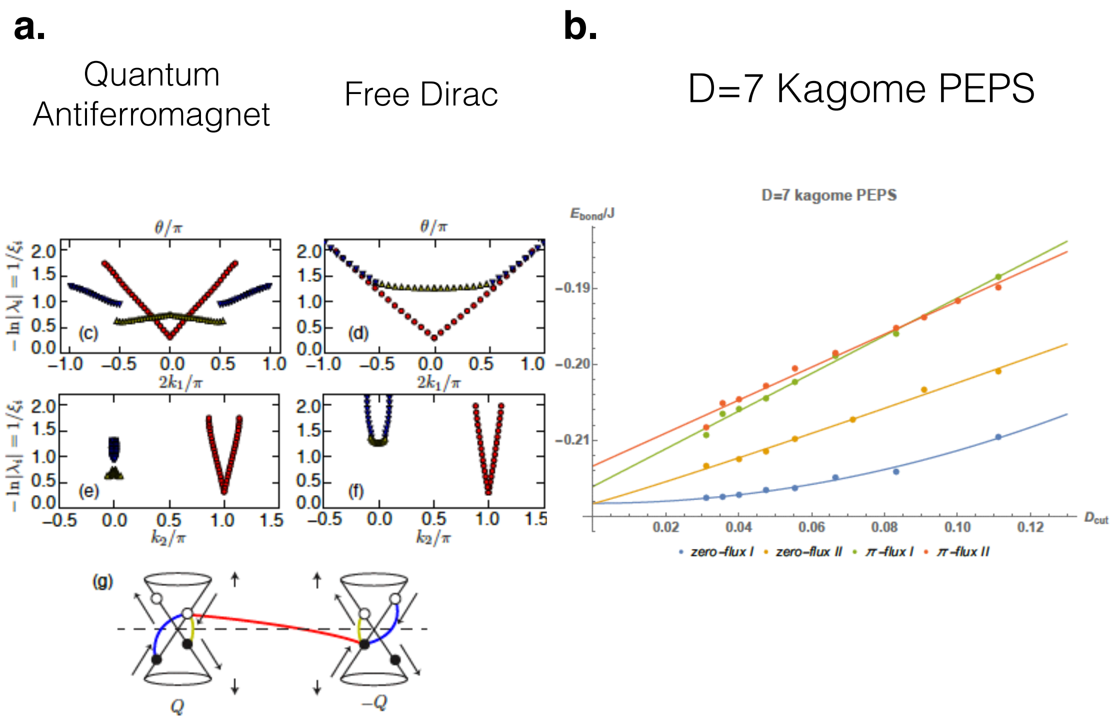

FIG. 2: (a) Similarity between the spectrum of the KQA and free Dirac fermions on lattices with the same geometry. (the vertical axis is actually related to decay of correlations which serves as a proxy for the lowest excitation energy in that sector). Taken from reference A. (b) Energy of 4 different gapped spin liquids, two of which are found to converge to the same value, indicating an underlying gapless state eg. the Dirac spin liquid which is proximate to both gapped states. Taken from reference B.

known a priori. However, the novel construction they employed utilizes projected entangled pairs (PEPS) which allows for more freedom in tuning the wavefunctions and lowering the energy. Although they do not directly capture the gapless spin liquid, an unusual result is observed - two different gapped spin liquids, the so called Q_1=±Q_2 states [10], are found to have the same (extrapolated) ground state energy (Figure 2b). The authors interpret this as indicating the system is actually in gapless state that can give rise to either one of these gapped phases. Indeed, both those states can be realized by starting from the Dirac spin liquid and condensing pairs of fermions, unlike the other two states which have different energies and are not proximate to the Dirac state. This also highlights the subtle difference between the Dirac and gapped spin liquids the latter being essentially a descendent of the

Dirac spin liquid in the presence of fermion pairing.

There are several questions that remain open - first, the Dirac spin liquid is only observed indirectly in these studies. The finite size gap should decrease with increasing system size, which the current studies do not show systematically at the existing system sizes. Furthermore, it is not clear how to reconcile the observations related to quantum entanglement with a Dirac spin liquid (which have been claimed to be evidence for a gapped Z_2 spin liquid [6]). Also, can we interpret the low energy part of the KQA spectrum entirely in terms of emergent fermions and photons? Finally, what lessons do these studies hold for the Kagome spin liquid candidate Herbertsmithite?

At a broader level, the remarkable complexity contained in such a simply stated problem (ground state of (1) on the Kagome lattice) may be pointing to a fundamental gap in our understanding of quantum many body phenomena that remains to be filled.

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