Spin liquid Groundstates ?

Z. Y. Meng, T. C. Lang, S. Wessel, F. F. Assaad, and A. Muramatsu, "Quantum spin-liquid emerging in two-dimensional correlated Dirac fermions," Nature **464**, 847 (2010).
S. Yan, D. A. Huse, and S. R. White, "Spin liquid ground state of the S=1/2 Kagome Heisenberg Model," arXiv:1011.6114.

Recommended with a commentary by S. A. Kivelson
Department of Physics, Stanford University

In the beginning – or at any rate, soon after the discovery of high temperature superconductivity – there was a period of intense excitement concerning the existence of exotic spin-liquid phases. Various physical arguments made their existence seem all but inevitable, and numerous mean-field and variational calculations found ever more exotic spin-liquid solutions of the Hubbard and related models. Experiments on the antiferromagnetism in the undoped cuprates, which revealed a conventional Neel ordered groundstate, somewhat damped that initial enthusiasm, and sober studies of obvious spin-liquid candidates, such as the spin 1/2 triangular lattice antiferromagnet, likewise found that magnetic order was unexpectedly robust. There followed a long period in which an anthropic proof of the non-existence of spin liquids ("I can't find it, therefore it doesn't exist!") underlay a widespread dismissal of the entire notion.

This response was not universal. There were those who continued to be obsessed by spin-liquids: Special reverse engineered models were found which have exact spin-liquid groundstates including various forms of the quantum dimer model and the Kitaev model. The relation between gapped spin-liquid states and topological quantum field theories was elucidated.[1] Various improved mean-field theories were explored. As numerical methods for studying strongly interacting quantum systems were developed, they were applied – often with disappointing results – to the search for "realistic" models with spin-liquid phases. Spin liquids even appear as a major topic in the condensed matter physics text book by Fradkin[2] – but most serious accounts of the state of the field have treated spin liquids as a form of "exotica." What has been lacking to revive more general interest in the subject was a clear experimental sighting in a laboratory material and a theoretically established case in which a spin-liquid groundstate occurs in a model that was not artificially constructed for the purpose.

In the last year, two different state of the art numerical studies have reported evidence of the existence of a fully gapped spin-liquid state in two distinct, natural models of strongly interacting electrons in two spatial dimensions. The first paper is a quantum Monte-Carlo study of the Hubbard model on the honeycomb lattice, where evidence is presented of the existence of a fully gapped phase at intermediate values of U (of order the bandwidth), which is identified by the authors as a spin-liquid. The second paper is a density matrix renormalization group (DMRG) study of the spin 1/2 Heisenberg model on the Kagome lattice, where, the authors conclude, there is a fully gapped spin-liquid state that appears to have Z_2 topological order.

A. Hubbard model on a honeycomb lattice:

Because the honeycomb lattice is bipartite, quantum Monte-Carlo calculations are not vexed by fermion minus sign problems so long as the band is half filled (one electron per site). According to Murphy's Law, this should guarantee that nothing interesting occurs in this model. Meng *et al*[3] were able to obtain groundstate information on systems up to $L = 18$ sites across. (That's 648 sites – wow!) In the absence of interactions, the system is a semimetal, with the Dirac nodal spectrum so touted in studies of graphene. A familiar RG analysis shows that the semimetal is a stable phase for a non-vanishng range of interaction strengths, U. At large U, the model maps to the spin 1/2 Heisenberg model, which is well known to exhibit a magnetically ordered Neel state. Both of these states have gapless spin excitations, and the semimetal has gapless charge excitations, as well.

Unexpectedly, Meng *et al* found that for $3.5 < U < 4.3$ (in units in which the hopping matrix t=1), there appears to be an intermediate phase that is fully gapped. The inferred spin-gap is small, $\Delta_s \simeq 0.03t$, presumably implying a longish correlation length and correspondingly large finite size effects. Indeed, finite size scaling must be used to extract $\Delta_s \equiv \lim_{L\to\infty} \Delta_s(L)$; even for $L = 18$, $\Delta_s(L)$ is more than a factor of 2 larger than the extrapolated value Δ_s. However, the two transitions appear relatively sharply defined. A followup paper, by another group[4], has reached the same conclusions.

The identification of the fully gapped phase as a spin-liquid is still more complicated. The existence of both a charge and spin gap already rules out many possible phases, including any gapless spin-liquid phase. The authors undertook a heroic search for evidence of any form of broken symmetry which could be responsible for the spin-gap in this phase, including time reversal symmetry, which would accompany an anomalous quantum Hall phase, and translation symmetry, which would accompany a valence bond crystal phase. From the fact that they found no evidence of any broken symmetry, the authors concluded that the intermediate phase must be a spin-liquid.

However, if it is a spin-liquid, one might expect to see evidence of topological order in the form of a near ground-state degeneracy which depends only on the topology of the system, with an energy splitting that vanishes exponentially with increasing system size. The authors looked unsuccessfully for such a signature of topological order. It is not, presently, clear to me whether this implies that the intermediate phase is not topologically ordered, or if this is a technical issue associated with finite size effects or the method of calculation

B. Spin 1/2 Heisenberg antiferromagnet on a Kagome lattice

The DMRG study of Yan *et al*[5] on Kagome cylinders is a tour-de-force, both as an exercise in DMRG (cylinders with circumferances as large as $L = 12$ lattice sites were studied, which must be a new record for DMRG) and as an exercise in clever finite size analysis. Studies were carried out for a range of different geometries, with various boundary conditions, and, at times, in the presence of different types of "weak" symmetry breaking fields.

On the basis of these studies, Yan *et al* reached a number of conclusions concerning the ground-state properties of the Kagome antiferromagnet: **1)** The ground-state is a spin-singlet, and there is a small "spin-gap," Δ_s, defined to be the excitation energy of the lowest lying spin 1 state. The value of Δ_s shows sufficient variation with L and the form of the boundary conditions that the authors do not venture to estimate its value in the thermodynamic limit. However, it appears to be smaller than the spin-gap inferred from earlier exact diagonalization studies[6], in which the spin-gap on the largest (36 site) system studied was $0.164J$, where J is the strength of the exchange interaction. **2)** In the thermodynamic limit there is an even smaller "singlet gap," Δ_0, separating the ground-states from the lowest spin-0 excited state. Yan *et al* estimate that Δ_0 is approximately $0.05J$, with uncertain error bars on this estimate. This differs qualitatively from inferences obtained in exact diagonalization studies, in which a large number of low energy spin-0 states were found, suggesting that the state is gapless. For example, for a 36 site system on a torus,[6] the singlet gap is less than 0.01J, and there are of order 50 states with energy lower than $0.05J$. Yan *et al* have attributed this discrepancy to a peculiarity of the boundary conditions in this small-size system. **3)** Yan *et al* conclude that the correlation length governing finite size effects is short (a couple of lattice constants), which they infer from the rapid convergence they find in measured quantities (such as the ground-state energy) as a function of L. I am somewhat surprised by this finding, as I would have thought the small value of Δ_0 would translate to a long correlation length, $\xi \sim (J/\Delta_0)^{1/z}$ with dynamical exponent $z = 1$ or 2. **4)** The ground-state is most probably a spin-liquid. Moreover, there is suggestive evidence that the ground-state is two-fold degenerate on extrapolation to large L, as is expected for a spin liquid with Z_2 topological order.

It is the uncontrived character of the model analyzed by Yan *et al* that makes their result so appealing. Nevertheless, it is interesting to ask whether there is any reverse engineered model on the Kagome lattice which has an exact spin-liquid ground state. A solvable spin 3/2 model on the Kagome lattice with strong spin-orbit coupling was recently analyzed by Chua *et al*[7], and found to have both gapped and ungapped chiral spin-liquid phases - *i.e.* phases that spontaneously break time-reversal symmetry. While the absence of additional ground-state degeneracies makes it seem unlikely that the state found by Yan *et al* breaks time-reversal symmetry, this has not been explicitly tested by them. A construction for engineering Hamiltonians on the square lattice with exact short-range resonating-valence bond spin-liquid ground-states was recently introduced by Cano and Fendley.[8] An analogous construction might be possible for the Kagome lattice. It might be interesting to study a family of models that interpolate between such an engineered model and the Kagome antiferromagnet to test whether the ground-states are adiabatically connected.

[1] For a particularly clear exposition, see T. H. Hansson, V. Oganesyan, and S. L. Sondhi, Annals of Phys. **313** 497 (2004).

[2] E. Fradkin, "Quantum Field Theories of Condensed Matter Systems," (Perseus Books, 1991)

[3] Z. Y. Meng, T. C. Lang, S. Wessel, F. F. Assaad, and A. Muramatsu, Nature **464**, 847 (2010).

[4] D. Zheng, C. Wu, and G-M. Zhang, arXiv:1011.5858 (2010).

[5] S. Yan, D. A. Huse, and S. R. White, arXiv:1011.6114 (2010).

[6] Ch. Waldtmann, H-U. Everts, B. Bernu, C. Lhuillier, P. Sindzingre, P. Lecheminant, and L. Pierre, Eur. Phys. J. B **2**, 501 (1998).

[7] V. Chua, H. Yao, and G. A. Fiete, arXiv:1010.1035.

[8] J. Cano and P. Fendley, Phys. Rev. Lett. **105**, 067205 (2010).