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Quantum spin liquid: a tale of emergence from frustration

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Abstract. I give a review of the current status of the quantum spin liquid, emphasizing the connection to lattice gauge theory, de-confinement and the emergence of novel particles and gauge fields in the low energy effective theory

The study of quantum spin liquid and frustrated magnetism is a field in many-body theory which has attracted a great deal of attention in recent years, due both to theoretical advances and the fact that promising candidate systems have been found experimentally. I would like to review some of the recent progress, but first begin with a bit of historical perspective. Louis Néel proposed the possibility of antiferromagnetic order back in 1936,[1] and by now Néel order is ubiquitous and seems second nature to condensed matter physicists. It is difficult for us to comprehend that Néel's ideas was initially met with skepticism and Landau was among the doubters. This was briefly mentioned in the obituary for Néel written by Jacques Friedel.[2]

... Werner Heisenberg's work on exchange had just shown that short-range effects should be expected. Between 1931 and 1933, Néel observed those effects in the susceptibility of iron and alloys and in the specific heat of nickel. Then, assuming that short-range interactions could be antiparallel, Néel developed the concept of anti ferromagnetism, in which two interpenetrating atomic lattices are treated in a molecular field approximation. ... To describe anti ferromagnetism Lev Landau and Cornelius Gorter suggested quantum fluctuations to mix Néel's solution with that obtained by reversal of moments. ... Néel's difficulties with anti-ferromagnetism and inconclusive discussions in the Strassbourg international meeting of 1939 fostered his skepticism about the usefulness of quantum mechanics; this was one of the few limitations of this superior mind.

To paraphrase Friedel, we can say that Landau's objection is that unlike a ferromagnet, Néel's up-down arrangement of spins is not an eigenstate of the Heisenberg exchange Hamiltonian, because the mutual spin flip term will reduce the sublattice order and may eventually disorder the Néel state. After all, Néel's solution is an uncontrolled mean-field theory, and the only exact solution known at the time is Bethe's solution of the Heisenberg spin chain,[3] which does not show long range order. Therefore in the absence of direct experimental evidence, one has reasons to be skeptical. Well, Nature has sided with Néel, and except for one dimensional spin systems, almost all experimental spin systems find a way to order at low temperatures. (Disorder and random exchange may lead to spin freezing, but let us leave spin glass out of this discussion.)

The possibility of quantum fluctuations destroying Néel order was raised again in 1973 by P.W. Anderson.[4] He focused on the singlet formation between two spins with energy gain of


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$-S(S+1)J$. The origin of the factor unity in $(S+1)$ is quantum mechanics and $S=\frac{1}{2}$ enjoys the greatest energy gain. In a spin chain, a trial wave function of singlet dimers yields an energy of $-\frac{3}{8}J$ per bond, which is lower than the Néel value of $-\frac{1}{4}J$. Indeed, we now understand Bethe's solution as a linear superposition of singlets with varying range. Anderson suggested that a similar superposition may hold for higher dimensions, which he called the resonating valence bond (RVB) state. He further proposed that frustrated lattices such as the triangular lattice may help stabilize the RVB state vs Néel order. Unfortunately it was found that the Heisenberg model can partially relieve frustration by forming 120 degrees order.[5] The field laid dormant until 1987, when soon after the discovery of high temperature superconductors, Anderson argued that upon doping, the RVB state naturally forms a superconductor because the singlet pairs are now mobile and can be viewed as Cooper pairs.[6] This suggestion launched a great deal of theoretical activities. While there remains no consensus on the theory of high temperature superconductors, there has been a great deal of development in the "easier" problem of quantum disordered spin states, which we call spin liquids. The requirement for a spin liquid is that it is a charge insulator with an odd number of electrons per unit cell (i.e. a Mott insulator) which does not exhibit Néel order down to zero temperature, despite the presence of antiferromagnetic exchange. We now know that the spin liquid is more than just the absence of order. Theory predicts the emergence of new excitations such as particle carrying $S=\frac{1}{2}$ and no charge, called spinons. Spinons may be fermions or bosons, and the excitation may gapped or gapless. Furthermore, the spinons do not live by themselves, but are coupled to an emergent gauge field, which may be $U(1)$ or $Z2$. Current analytic theory is not powerful enough to tell us which of these possibilities is realized for a given Hamiltonian, but the different possibilities can be classified and their nature fully described. As we shall see, the spin liquid problem is closely related to lattice gauge theory coupled to matter field, and the spin liquid states correspond to the deconfined phases.

The field of spin liquids received a powerful boost several years ago with the discovery of promising experimental candidates. They include the organic molecular compounds and a mineral called Herbertsmithite, which is a $S=\frac{1}{2}$ Kagome lattice that can be synthesized in the laboratory.[7] The $S=\frac{1}{2}$ Kagome lattice is a highly frustrated two dimensional lattice which has long been suspected to harbor a spin liquid ground state based on numerical work.[8] What is interesting is that in addition to using frustration to stabilize the spin liquid as proposed by Anderson, the organic materials have taught us a second route, i.e., the proximity to the Mott transition. The two families of organic material consist of molecular dimers (called ET and dmit as abbreviation) which carry a single electron each, and form an approximate triangular lattice. It can be modeled as a Hubbard model on a triangular lattice with one electron per unit cell.[9, 10] Deep in the Mott insulator regime, the low energy physics is described by a nearest-neighbor Heisenberg model and the system is expected to order into the 120 degree phase. The spin liquid materials turn out to be insulators which turn into a metal (dmit) or superconductor (ET) under modest pressure. The proximity to the Mott transition means that while the low energy excitations may still be described by the spin degrees of freedom, the Hamiltonian is much more complicated than the nearest-neighbor Heisenberg. For example, ring exchange terms may be important.[9] We therefore focus on the nature of the ground state, and leave aside the question of what spin Hamiltonian can stabilize it.

These two quite distinct spin liquid candidates share the common feature that they both appear to be gapless. In the organic system, the spin susceptibility goes to a constant and the specific heat has a linear T term,[11] both characteristic of a metal with a Fermi surface, and most uncommon for an insulator. Thermo-conductivity κ was measured and it is found at least for the dmit salts that κ/T goes to a constant at low temperature.[12] All these strange properties are consistent with the emergence of fermonic spinons which form a Fermi surface. The situation with Herbertsmithite is less clear because there exists a significant amount of local

moments between the Kagome planes which obscure the low temperature behavior. Recently a single crystal large enough for neutron scattering was grown.[13] The data show that the spin excitation is gapless and rather featureless as a function of energy and has been argued to support the picture of gapless spinons.

Now we describe how the Heisenberg model $H = J\sum_{<ij>} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$ is mapped onto a lattice gauge theory. It is convenient to introduce fermions $f_{i\alpha}$ which carry spin index α on site and write the spin operator as

$$\boldsymbol{S}_i = \tfrac{1}{2} f^\dagger_{i\alpha} \boldsymbol{\sigma}_{\alpha\beta} f_{i\beta}. \tag{1}$$

The fermions must be subject to the constraint

$$f^\dagger_{i\uparrow} f_{i\uparrow} + f^\dagger_{i\downarrow} f_{i\downarrow} = 1, \tag{2}$$

which excludes empty or doubly occupied fermions. A similar representation can be made by introducing spin carrying bosons called Schwinger bosons instead of fermions. However, with bosonic representations, the mean field theory yields either Néel order or gapped spin liquid states and gapless spin liquid requires fine tuning to a quantum critical point. On the other hand, we will see that fermionic representation naturally accommodates gapless phases. Since the experimental systems observed so far appear to be gapless, we will use the fermionic representation. The Heisenberg term is quartic in the fermion operator and is given as[14]

$$\boldsymbol{S}_i \cdot \boldsymbol{S}_j = -\tfrac{1}{4} f^\dagger_{i\alpha} f_{j\alpha} f^\dagger_{j\beta} f_{i\beta} - \tfrac{1}{4}\left(f^\dagger_{i\uparrow} f^\dagger_{j\downarrow} - f^\dagger_{i\downarrow} f^\dagger_{j\uparrow} \right)\left(f_{j\downarrow} f_{i\uparrow} - f_{j\uparrow} f_{i\downarrow} \right) + \tfrac{1}{4} f^\dagger_{i\alpha} f_{i\alpha} \tag{3}$$

Eq.(2) invites mean field decoupling in the particle-hole and particle-particle channels

$$\chi_{ij} = < f^\dagger_{i\alpha} f_{j\beta} > \quad \text{and} \tag{4}$$

$$\Delta_{ij} = \langle (f_{j\downarrow} f_{i\uparrow} - f_{j\uparrow} f_{i\downarrow}) \rangle \,. \tag{5}$$

For simplicity, let us ignore the pairing channel and consider χ_{ij} only. Note that at the mean field level, the fermion acquires dynamics and is now free to hop on the lattice. Formally we introduce the Hubbard-Stratonovich field χ_{ij} and the Lagrange multiplier λ_i to enforce the constraint Eq.(2).

$$Z = \int d\chi d\lambda df df^\dagger e^{-S} \tag{6}$$

$$\begin{aligned} S &= \int d\tau \left[\sum_i \left[f^\dagger_{i\alpha} \partial_\tau f_{i\alpha} + i\lambda_i \left(f^\dagger_{i\alpha} f_{i\alpha} - 1 \right) \right] \right. \\ &+ \left. \sum_{<ij>} J \left[\chi_{ij} \left(f^\dagger_{j\alpha} f_{i\alpha} + h.c. \right) + 2|\chi_{ij}|^2 \right] \right] \end{aligned} \tag{7}$$

The saddle point describes the mean field theory. Fluctuations around the saddle point are dominated by the phase fluctuation of χ_{ij} which becomes the compact $U(1)$ gauge field a_{ij} on link ij while $i\lambda$ becomes the time component. The low energy theory of Eq.(1) becomes a compact $U(1)$ lattice gauge theory coupled to fermions hopping on a lattice.[15]

It is not surprising that a gauge theory should result from a representation subject to constraints. Because the fermions introduced extra degrees of freedom, we see that there is a gauge redundancy in Eq.(1), i.e., $\boldsymbol{S}$ is invariant under a local gauge transformation $f_i \longrightarrow f_i e^{i\phi}$. Therefore a gauge theory must emerge.

Several mean field solutions are notable. If χ_{ij} is a constant, we will have a half-filled band with a Fermi surface. Another interesting class is called the flux phases where nonzero gauge fluxes penetrate the plaquettes. π-flux for the square lattice[16] and π flux through the hexagons in the Kagome lattice yield massless Dirac fermions.[17] Note the time reversal symmetry is preserved with π fluxes. If we include pairing we can gap the Fermi surface in a variety of ways. We do not know which mean field theory is closer to the truth for a given Hamiltonian, but we can discuss the consequences of each state and compare with experiments. This is why the availability of experiments is crucial for the advancement in the field. Recent advances in numerical methods such as DMRG[18] and projected wave functions plus Lanczos[19] are making important contributions to ascertain the domain of stability of spin liquids for a given Hamiltonian.

The enemy of the spin liquid is confinement. If the gauge theory is in a confined phase, the low lying degrees of freedom remain those of spin excitations, and the system is typically Néel ordered. On the other hand, if we are in the deconfined phase, the fermion and gauge fields emerge as new particles and fields at low energies. The fictitious fermions which we introduced as a formal device and had no dynamics at high energy and short distance take on a life of their own at low energies. This is a prime example of the notion of emergence. There are now several exactly solvable examples which show that this scenario plays out in certain spin Hamiltonians.[20, 21] The reader should not be concerned that the fermions are not gauge invariant. After all the electrons in our world are also not gauge invariant but we have no trouble thinking of them as real objects. The difference between electron and spinon is a qualitative one: the electrons are weakly coupled to the gauge field with a small fine structure constant whereas spinons couple with strength unity. Another difference is that in solids the electron velocity v_F is much less than the speed of light and the coupling to electric field is stronger than the coupling to magnetic field. In spin liquids both velocities are given by J and transverse gauge fluctuations which are unscreened become dominant. For example, for $U(1)$ spin liquids this gives rise to the prediction that the specific heat $\sim T^{2/3}$, i.e., non-Fermi liquid behavior,[22] a subject under intense studies today.[23, 24, 25, 26]

Pure gauge theory is always confining in two dimensions due to instanton fluctuations.[27] The coupling to matter fields can change that. It was shown that coupling to N components of Dirac spinons can suppress instantons if N exceeds a critical N_c.[28] In the π-flux state $N = 4$, and deconfinement is quite possible. In the case of the Fermi sea, it has been shown that there are so many gapless degrees of freedom that it is analogous to infinite N and deconfinement is always possible.[29]

In conclusion, the field of quantum spin liquid is entering an exciting new phase where dialogs between theory and experiment are possible. We can look forward to exciting discoveries ahead.

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