Phase diagram of the triangular lattice Hubbard model

Observation of a chiral spin liquid phase of the Hubbard model on the triangular lattice: a density matrix renormalization group study
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Despite decades of study, the ground state properties of the celebrated electronic Hubbard model are, in general, poorly understood in spatial dimension d > 1. The minimal version of the model considers spin-1/2 electrons on a lattice with nearest neighbor hopping t and an on-site electron-electron repulsion U. When there is, on average, 1 electron per lattice site, in the large-U regime (U >> t), the model describes a Mott insulator. This insulator has local moments coupled together by antiferromagnetic superexchange interactions, typically leading to long range Neel order.

On a 2d square lattice it is known that even for weak U << t the ground state is an antiferromagnetic insulator driven by an instability of the perfectly nested Fermi surface. The story is more interesting on non-bipartite lattices such as the triangular lattice which is the subject of the highlighted paper. Then for U >> t, deep in the Mott insulator, the antiferromagnetic exchange is frustrated by the triangular geometry. The ground state is nevertheless known, from numerical calculations, to have a non-collinear antiferromagnetic order where on any triangle the three sites have spins rotated relative to each other by 120 degrees. For weak U << t, the Fermi surface is nearly circular and not nested. There is no instability (other than the Kohn-Luttinger superconductivity at ultra-low temperatures) and for all practical purposes the model can be taken to be a Landau Fermi liquid.

The evolution, on the triangular lattice, between the weak U Fermi liquid and the large-U Mott insulator is a rather fundamental question which has received tremendous attention in the last 15 or so years. Much of this interest is due to the relevance of the triangular lattice Hubbard model to quasi-two dimensional organic salts such as k-(ET)2Cu2(CN)3 and EtMe3Sb[Pd(dmit)2]2` which show many fascinating phenomena (see, eg, Ref [1] for reviews, and below). Prior numerical treatments of the model indicated that the insulator in the immediate vicinity of the Mott transition is non-magnetic. These include Density Matrix Renormalization Group (DMRG) studies on a 2-leg triangular Hubbard ladder[2], exact diagonalization of spin models obtained in a systematic t/U expansion[3], and DMRG studies on wider ladders on simplified spin models that kept 2-particle and 4-particle ring exchanges[4] In other words as t/U is increased the 120 degree magnetic order is destroyed within the insulating phase. Further, these studies provided evidence that the resulting non-magnetic insulator is an exotic phase of matter (known as a quantum spin liquid) with a gapless fermi surface of emergent neutral spin-1/2 fermionic excitations (known as spinons).

The highlighted paper by Szasz et al revisits this triangular lattice Hubbard model with large scale DMRG calculations on ladders with widths upto 6 legs. Introduced originally as an efficient way to numerically solve 1d models, increasingly DMRG on ladders has become a powerful tool for exploring the properties of quantum many body systems in 2 dimensions. It has been used to great effect in studying models of interacting quantum spins, for quantum Hall problems, and for the Hubbard model itself. Szasz et al used a version of the method known as infinite- system DMRG (iDMRG) that studies the system on a lattice on an infinite cylinders of finite circumference. Further they used a recent technical innovation[5] – to work in a basis of states which are momentum eigenstates along the circumferential direction (the y-direction) and local position eigenstates along the cylinder length (the x-direction) . This allows them to fix the momentum ky and study the ground state in different ky sectors. Further this trick increases the computational efficiency and enables them to access wider ladders than had been previously possible.

Their resulting DMRG simulations confirm the expected large-U Mott insulator with 120 degree magnetic ordering (adapted to the quasi-1d setting) as well as the small-U Fermi liquid. Furthermore in agreement with previous results, a non-magnetic insulator is found sandwiched in between these two limits. The surprise is in the nature of this non-magnetic insulator. First it appears to break time reversal symmetry as evidenced by a non-zero value of the scalar spin chirality order parameter $S \cdot S \times S$ where the product is taken over the three sites i,j,k of an elementary triangular plaquette. Second it appears to be gapped. Finally the paper provides good evidence that it is a specific state known as a chiral spin liquid which supports anyonic excitations that carry fractional spin-1/2.

The chiral spin liquid is a spin analog of a fractional quantum Hall state. It has shown up in recent numerical studies of frustrated quantum magnets with extended further neighbor interactions (see, eg, Ref [6]). It's appearance in the weak Mott insulating phase of the triangular lattice Hubbard model is interesting and raises a number of further questions.

The extensive studies reported by Szasz et al represent tremendous progress in numerical treatment of the ground state of this important model. These results are sure to be scrutinized closely by other methods in the future. They contradict previous DMRG studies of the same model on a 2-led ladder[2] which instead found a gapless spin liquid. They are also possibly in tension with an exact diagonalization study[3] of a spin model obtained by a high order truncation of the t/U expansion of the Hubbard model. It might be interesting to directly study this spin model by DMRG and compare the results with the Hubbard model.

A further source of tension is with experiments on nearly isotropic triangular lattice organic salts[1]. These have long been known to be non-magnetic Mott insulators. Though their exchange scale is about 250 K, they apparently have gapless spin-carrying excitations at least down to temperatures of 1 K. The low-T spin susceptibility is a constant and the heat capacity is linear in T, with a Wilson ratio close to 1. Further in at least one material, the heat conductivity is metallic at even lower-T and is magnetic field dependent. These phenomena fit the expectations of a neutral fermi surface. It remains to be seen if they can be reconciled with the chiral spin liquid found in the recent iDMRG calculations. The chiral spin liquid will have a finite temperature Ising phase transition, and at low-T, a quantized thermal Hall conductance. Neither of these have been reported in experiments on the organics. The authors suggest that this could be due to domain formation which may be hard to align with a magnetic field due to the weakness of orbital coupling in a Mott insulator. These calculations should stimulate a new wave of experiments revisiting the possibility of broken time reversal symmetry in these materials.

On the technical side, it is clear that the iDMRG had converged to the chiral spin liquid for the ladders studied in this paper. But perhaps this is not the true ground state? It is known that the DMRG method tends to favor states with low quantum entanglement. Compared to the gapless spin liquid states the chiral spin liquid indeed has lower quantum entanglement. The authors however point out that their simulations converge to the Fermi liquid in the weak-U regime which is expected to have larger entanglement (at least as measured by the entanglement entropy) than the gapless spin liquid.

Finally theoretically the possibility that the chiral spin liquid resides in between the Fermi liquid and the strong-U insulating antiferromagnet raises fascinating questions on the nature of the resulting quantum phase transitions which are currently not understood.

References

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