The Complexity of the t-J Model

"Competing states in the t-J model: uniform d-wave state versus stripe state"
P. Corboz, T. M. Rice, and Matthias Troyer – arXiv:1402.2859

Recommended with commentary by Steven Kivelson, Stanford University

Let me start by making one thing perfectly clear – it is not that I think that the Hubbard or t-J models are "realistic" models of the cuprates (or any other particular material for that matter). It is not even that they are the same model – the t-J and Hubbard models are only the same model in any precise sense in the limit of $t/U \sim J/t << 1$ – the regime of ferromagnetism. However, in the intermediate coupling regime $U \approx 8t$ or $J \approx t/2$ they have become the paradigmatic models of doped antiferromagnetic (Mott) insulators; the Hubbard and t-J models are to the field of highly correlated electron systems as the Ising model is to statistical mechanics. The difference, however, is that there is far from an established understanding of even the zero temperature phase diagram of the Hubbard or t-J models.

In a recently posted paper, Corboz *et al* have found the "best" variational solution of the 2D t-J model on the square lattice to date – best in the technical sense that they have obtained the lowest variational energy. The nature of the states used in this study are interesting in their own right – they have constructed variational tensor product states for the system in the thermodynamic limit, *i.e.* there are no issues of finite size effects. These states generalize the matrix product states that are at the core of density matrix renormalization group calculations that have already been enormously successful in elucidating the properties of these models in one-dimensional geometries. While there is always the danger with variational studies that the true ground state could have properties that are incompatible with the assumed form of the states considered, the only obvious prejudice of the present study is that it favors states with relatively lower quantum entanglement. Given this and the large number of variational degrees of freedom (determined by the bond dimension of the tensors), it is quite plausible that the present results can be taken at face value.

The results obtained by Corboz *et al* are interesting and astonishing, and I think suggest that there is a deeper understanding (not yet achieved) that is possible. What they find is that for the range of parameters studied – i.e. J/t between 0.2 and 0.8 and "doped hole concentration" x between 0 and 0.16 – that three states with distinct patterns of broken symmetry all have energies that are, to a high degree of accuracy, equal to each other. (By definition $x = 1-n$, where n is the number of electrons per site.) The reason for this robust near-degeneracy between three distinct phases is presently unclear. (Also interesting is that all of these three phases have been plausibly suggested to exist in the cuprate phase diagram.)

The simplest of the three phases is the uniform d-wave superconducting phase (USC). For $x < x_c$ (where $x_c = 0.1$ for $J/t=0.4$) this has coexisting antiferromagnetic Neel type magnetic order. As the "uniform" in the name suggests, this phase has uniform charge density on all sites and uniform expectation of the pair-field creation operator, Ψ.

The next most complex phase (CDW+SC) has coexisting charge density wave (CDW) and d-wave superconducting order. This is a "striped-phase" which spontaneously breaks translational and spin rotational symmetry through unidirectional CDW and spin-density order (SDW) order. It also has superconducting order, *i.e.* it has a non-zero expectation value of Ψ. Naturally, the value of Ψ is spatially modulated with the same period as the CDW, but its average over space is non-zero, and indeed, while it is "d-wave like" in that it changes sign under spatial rotation by $\pi/2$, its sign is unchanged by arbitrary spatial translations.

The most exotic phase is the "pair density wave" (PDW), which has similar stripe order as the CDW+SC phase, but with superconducting order, Ψ, that changes sign under translation by the CDW period, resulting in a superconducting state in which the spatial average value of Ψ is exactly zero. Indeed, the superconducting component of the PDW state has its maximum amplitude at the nodes of the SDW order and vanishes where the SDW amplitude is maximal. It is a close relative of the famous Larkin-Ovchinikov state, with the difference that there is no net ferromagnetic component of the state.

Naturally, it is not true that these three distinct phases are *exactly* degenerate; the CDW+SC phase achieves the lowest variational energy. However, the ground-state energy per site of the CDW+SC is lower than the PDW only by roughly $\Delta E = 0.001$ t x, and than the USC by roughly $\Delta E = 0.01$ t x. These differences are so small that it is not clear that they are significant (within the accuracy of the variational ansatz), and in any case one would expect that small changes to the model could easily tip the balance one way or the other. At the rough intuitive level, this near degeneracy reflects the fact that locally, all three phases look pretty similar in that they all look like a uniform d-wave superconductor, with or without coexisting antiferromagnetism depending on the local doped hole concentration. However, why the energy differences are so extraordinarily small and why this apparent coincidence persists over a broad range of parameters seems mysterious.

A few other aspects of the results are significant as well: 1) The periodicity of the CDW order either of the striped phases is *not* determined by Fermi surface nesting features; rather the preferred density of holes per unit length of stripe, n_s, is a function of the value of J/t (*i.e.* is determined by the strength of the interactions), ranging from about n_s=0.35 for J/t=0.2 to n_s=1 (corresponding to insulating stripes) for J/t=0.8. 2) There is a clear energetic preference for vertical or horizontal stripes over diagonal stripes; moreover, when the periodicity of the state is chosen to favor diagonal stripes, the energy is minimized by insulating stripes with n_s=1. 3) Since the variational states are always assumed to be periodic, the only possible stripe states are commensurate; calculations were carried out for CDW periods equal to 4, 5, 7 and 9 lattice constants. In all cases the energetically preferred stripes were found to be site centered. However, there is no indication that there is any significant commensurability lock-in energy, and for incommensurate stripes, no sharp symmetry distinction between site and bond centered order exists. 4) The SDW component of the order suffers a p phase shift across the row of sites at which the CDW order is maximal; thus, for even period CDW order, the SDW period is twice that of the CDW (which is the same as the period of the SC order in the case of the PDW), while for odd period CDW order, the SDW period is equal to that of the CDW. 5) For the range of x less than about 0.08, the energy per hole is almost independent of x; thus, it is unclear whether or not the stripe phase is stable with respect to phase separation in this range – phase separation at small x was recently inferred in a somewhat different high quality variational study of the Hubbard model[Y. Yamaji and M. Imada, arXiv:1306.2022]. 6) In the context of the cuprates, there has been considerable discussion of whether striped states or checkerboard states (bidirectional CDW states that preserve the C_4 rotational symmetry of the underlying lattice) are preferred; however, the failure of an earlier version of the present calculation [P. Corboz, S. R. White, G. Vidal, and M. Troyer, Phys. Rev. B **84**, (2011) 401108]to find such checkerboard phases given a variational ansatz that would have permitted it stands as moderately compelling evidence that this form of order does not arise naturally.