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Flux Phases in the $t - J$ Model

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After a short review of the case for the $t - J$ model as a suitable low energy model Hamiltonian for CuO_2 planes in the high- T_c superconductors, the renormalized mean field approximation to this model is discussed. At half-filling the reduction to a Hilbert space containing only spin degrees of freedom leads to a wide class of degeneracies in the fermion meanfield description. One particular class of states which has generated much interest in the past year, is that built from one electron Hofstadter states which are eigenstates in the presence of a uniform magnetic flux. The mean field theory of such states in a $t - J$ model is reviewed followed by a discussion of their unusual properties. In conclusion, some comments on the relationship to anyon models and other open questions are given.

1. Introduction

The discovery of high- T_c superconductors has greatly stimulated interest in the properties of strongly correlated electrons. The simplest model that one can use to describe such a system has a single tight-binding band made from a single orbital on each site¹. The strong correlation condition forbids double occupancy of this orbital. At an electron density of exactly 1 electron/site this restriction limits the Hilbert space to spin degrees of freedom only which are coupled with a Heisenberg interaction (J). This simple model on a square lattice is a good description of the low energy spectrum² of the insulating CuO_2 planes which have a formal valence Cu^{2+} . The question of how to describe the removal or addition of electrons (i.e. hole or electron doping) has been the subject of a great deal of discussion. The simplest description was proposed initially by Anderson¹ namely that the extra charge would be carried by formal valence Cu^{3+} or Cu^+ ions which would be spin singlets. The Hilbert space that results for electron count less than 1 per site say, has 3 configurations on each site namely spin up or down and empty. Electrons can transfer on the neighboring empty sites with a matrix element, t . These two terms make up the $t - J$ Hamiltonian which will be the subject of this talk.

The adequacy of the simplest $t - J$ model to describe doped CuO_2 planes is an interesting question which cannot be covered here in detail. The key question is whether the starting Hamiltonian containing $Cu - d$ and $O - p$ orbitals can be reduced to the much smaller Hilbert space with 3 configurations per Cu site. Given that added holes go mainly into O -orbitals, the $t - J$ model requires that the formal Cu^{3+} ion that carries the charge is a tightly bound singlet between the central Cu spin and the hole with spin residing on the four neighboring $O2p$ -orbitals, as discussed by Zhang and Rice ³. Unfortunately there is no small parameter which can be used to formally justify the reduction procedure. In addition there are many terms in the starting Hamiltonian such as direct $O - O$ overlap or the Coulomb repulsion on O -orbitals which complicate the description. There are also questions concerning the values of parameters in the starting Hamiltonian. Recently Hybertsen, Stechel, Schluter and Jennison ⁴ have reported a detailed set of a priori calculations based on the local density functional method to estimate the parameters. They then examined the low energy effective Hamiltonian by comparing to the low energy eigenvalues of the full Hamiltonian obtained by exact diagonalization on a small cluster ⁵. The set of parameter values they obtain agree quite well with the obtained in other calculations and empirically ⁶. The $t - J$ model extended through a small n.n.n. hopping term t' is found to give a good representation for both hole and electron doping. The Heisenberg coupling J estimated ⁴ at $\approx 130\text{ meV}$ agrees very well with experimental values ² on La_2CuO_4 . The n.n. hopping matrix element $t \approx 420\text{ meV}$ is essentially the same for both electron and hole doping ⁴ leading to a value for the ratio $J/t \approx 0.3$. The ratio $t'/t \approx -0.2$ is rather small. Other estimates ⁷ gave a rather larger value for $|t'|$. Nonetheless it seems that the $t - J$ model is the simplest reduced Hamiltonian that can be considered reasonable for the CuO_2 planes.

2. Renormalized Mean Field Theory

This talk will concentrate on only one of the many methods being used currently to tackle the $t - J$ model. The restriction to a reduced Hilbert space complicates the problem considerably, even in meanfield theory as we shall discuss.

Thus a general Hartree-Fock-Bogoliubov wavefunction $|\Psi_{HFB}\rangle$ needs to be projected on to the reduced Hilbert space so that the actual mean field wavefunction is

$$|\Psi_{MF}\rangle = P_d |\Psi_{HFB}\rangle; \quad P_d = \prod_i (1 - n_{i\uparrow} n_{i\downarrow}). \quad (1)$$

One approximation scheme which is reasonably accurate when compared to numerical calculations and used by Zhang et al ⁸, replaces the projection operator by a renormalization factor calculated according to Gutzwiller's prescription i.e. one replaces

$$\begin{aligned} H_{t-J} &= P_d \left\{ -t \sum_{\langle ij \rangle \sigma} d_{i\sigma}^+ d_{j\sigma} + h.c. + J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j \right\} P_d \\ &= P_d \{ H_t + H_J \} P_d \end{aligned} \quad (2)$$

by the simpler form

$$\tilde{H}_{t-J} = g_t H_t + g_J H_J, \quad (3)$$

where g_t, g_J are numerical factors which depend on the average densities of \uparrow and \downarrow -spin electrons. For paramagnetic translationally invariant states⁸

$$g_t = 4\delta(1+2\delta)^{-1} \quad g_J = 4(1+2\delta)^{-2} \quad (4)$$

where $n_\uparrow = n_\downarrow = 1/2 - \delta$. (2δ is the hole concentration). This approximation has been shown by Vollhardt and coworkers⁹ to be exact in infinite dimensions and was shown by Kotliar and Ruckenstein¹⁰ to be expressible as a slave boson meanfield theory.

At half-filling ($\delta = 0$) the $t - J$ model reduces to a Heisenberg model and it is now generally agreed that this has a antiferromagnetically ordered ground state with a sublattice magnetization reduced to 60% of the Neel value due to quantum fluctuation. The purely spin-problem is best described by the spin operators $\{\vec{S}_i\}$ which operate in a Hilbert space containing 2^L configurations, (L : Number of sites). But we are interested in representing it in the much larger fermion Hilbert space which applies for $\delta \neq 0$. This introduces a tremendous redundancy since the unprojected $|\Psi_{HFB}\rangle$ are vectors in 4^L Hilbert space. Anderson, Affleck and coworkers^{1,11} were the first to point out that this results in local SU(2) gauge invariance. Thus if we on any set of sites $\{i\}$ make a transformation

$$\begin{aligned} d_{i\sigma}^+ &\longrightarrow \alpha_i d_{i\uparrow}^+ + \beta_i d_{i\downarrow} \\ d_{i-\sigma} &\longrightarrow -\beta_i^* d_{i\uparrow} + \alpha_i^* d_{i\downarrow}; \quad [|\alpha_i|^2 + |\beta_i|^2 = 1] \end{aligned} \quad (5)$$

we change the unprojected wavefunction $|\Psi_{HFB}\rangle$ drastically but after projection of wavefunction which is now purely a spin wavefunction is the same. In the fermion mean field theory this redundancy has the consequence that a large class of meanfield solutions are degenerate at $\delta = 0$, even though they ostensibly represent fermion states with quite different characteristics. For example two especially interesting states are the d -wave superconducting state (or d -wave RVB state) and the Affleck-Marston¹² state. These are represented by quite different diagonal and off-diagonal expectation values in the unprojected states i.e. ($\tau = x$ or y)

$$\begin{aligned} \tilde{\Delta}_\tau &= \langle d_{i\uparrow}^+ d_{i+\tau\downarrow}^+ - d_{i\downarrow}^+ d_{i+\tau\uparrow}^+ \rangle \\ \chi_{i,i+\tau} &= \sum_\sigma \langle d_{i,\sigma}^+ d_{i+\tau,\sigma} \rangle \end{aligned}$$

take values

$$\tilde{\Delta}_x = -\tilde{\Delta}_y = \chi_{i,i+x} = \chi_{i,i+y} = 0.339 \quad (6)$$

$$\tilde{\Delta}_x = \tilde{\Delta}_y = 0; \quad \chi_{i,i+\tau} = 0.479 \exp(\pm i\pi/4) \quad (7)$$

in the d -wave RVB and Affleck-Marston states respectively, yet when projected onto the reduced Hilbert space these two states are identical.

These two states are of special interest because within this class of mean field solutions they give the best expectation value of H_t when a small number of holes are introduced. To leading order in δ they give the same value⁸ for the kinetic energy per added hole. These states do not have long range AF order and since they are written as fermion wavefunction are easily generalized to finite doping. At $\delta = 0$ Gros¹³ found numerically an energy of -0.64 J/site which is several percent higher than current estimates¹⁴ of an AF ordered spin state -0.67 J/site. Lee and Feng¹⁵ have shown that by introducing a long range AF into these states that their energy can be lowered to values much closer to that obtained with spin wavefunctions. Introducing holes suppresses the AF long range order and they find the generalizations of the d -wave RVB state are stable against AF ordering beyond 5% doping. Therefore we will concentrate on the generalizations of the paramagnetic wavefunctions at finite doping and ignore the AF ordered states.

3. Flux States

The name flux states has been applied to the Affleck-Marston (AM) state¹² and generalizations thereof built from wavefunctions that describe electrons in an external magnetic field or flux. The relevance of these wavefunctions was clarified recently by the following conjecture¹⁶. Consider a system of non-interacting electrons (density ν electrons/site) moving in a square lattice described by a n.n. tight-binding matrix element ($-t$) but we introduce a phase factor $e^{i\varphi_{ij}}$ for each n.n. bond (ij). If we seek a solution with uniform density and choose the phases to derive from a vector potential corresponding to a uniform magnetic flux (in units of the flux quantum) $\Phi = (2\pi)^{-1} \sum_{\square} \varphi_{ij}$ in each lattice square, then according

to this conjecture the ground state is not given by $\Phi = 0$ (i.e. Bloch states) but by the choice $\Phi = \nu$. The eigenvalues of the uniform flux problem on a square lattice were studied extensively by Hofstadter¹⁷ who found a complex spectrum $\{\varepsilon_l\}$ with many bands which depend on the commensurability of the flux Φ . The choice $\Phi = \nu$ corresponds to placing the Fermi level in the large gap between the 1st and 2nd Landau-Hofstadter bands. Clearly energy is gained by having an energy gap at the Fermi energy. However the Hofstadter spectrum is compressed overall relative to the Bloch spectrum so that the question of whether

$$E_G(\nu, \Phi) < E_G(\nu, \Phi = 0); \quad E_G(\nu, \Phi) = \sum_l^{\text{occ}} \varepsilon_l \quad (8)$$

depends on which of these two factors is dominant. Hasegawa et al¹⁶ and Montambaux¹⁸ and Nori¹⁹ have made a series of numerical calculations which support this conjecture. $E_G(\nu, \Phi)$ has a cusp minimum as a function of Φ at $\Phi = \nu$. Note $E_G(\nu, \Phi = \nu)$ seems to be a continuous function of ν without obvious structure at commensurate values of ν ¹⁸.

Earlier this year Anderson, Shastry and Hristopoulous²⁰ proposed generalizations of the AM-state and in particular a variational state which can be written as

$$|\Psi_{ASH}\rangle = P_d \prod_{l,l'}^{\text{occ}} d_{l\uparrow}^+ d_{l'\downarrow}^+ |\text{vac}\rangle, \quad (9)$$

where $d_{l\sigma}^+$ creates a Hofstadter state $\{l\sigma\}$. Lederer, Poilblanc and Rice ²¹ (LPR) showed that this state can be used to minimize the energy of the exchange term H_J when the flux in the Hofstadter problem is chosen to be commensurate with density of \uparrow (or \downarrow) spin electrons i.e. $\Phi = n_\uparrow = n_\downarrow$. Consider just one term in the Heisenberg interaction, then we may write

$$\langle \Psi_{ASH} | S_i^+ S_j^- | \Psi_{ASH} \rangle = \langle \Psi_{ASH} | e^{i\varphi_{ij}} d_{i\uparrow}^+ d_{j\uparrow} \cdot e^{-i\varphi_{ij}} d_{j\downarrow}^+ d_{i\downarrow} | \Psi_{ASH} \rangle \quad (10)$$

and the expectation value factors into \uparrow and \downarrow expectation values. Introducing the phase factor simplifies the problem when we choose the phase φ_{ij} to be the same as in the one-electron Hamiltonian used to generate the Hofstadter eigenvalues. This choice allows us to express each expectation value simply as a sum over occupied Hofstadter eigenvalues and using the singlet character of the wavefunction and the renormalization approximation LPR get

$$\langle \Psi_{ASH} | H_J | \Psi_{ASH} \rangle = -\frac{3J}{16} g_J \left(\frac{1}{L} \sum_l^{\text{occ}} \epsilon_l \right)^2. \quad (11)$$

This energy is then minimized by the choice of the commensurate flux $\Phi = n_\uparrow$, leading to the name commensurate flux phase (CFP) for this choice. The fact that H_J describes an exchange process whereby \uparrow and \downarrow -spin electrons interchange positions allowed us to introduce a phase factor to the hop for \uparrow and \downarrow -spin separately and this in turn allowed us to introduce a fictitious flux for each species determined by the other species. Note since the Hofstadter eigenvalues depend only on the flux and not on gauge in which this flux is represented, this property carries over to the H_J -term.

In the presence of holes we have to examine also the kinetic energy, H_t . Introducing the phase factor again into the expectation value gives again a sum over Hofstadter eigenvalues but now the phase factor is not compensated so that

$$\langle \Psi_{ASH} | H_t | \Psi_{ASH} \rangle = 2t g_t L^{-1} \sum_l^{\text{occ}} \epsilon_l \cdot \langle \cos \varphi_{ij} \rangle_{\text{ave}} \quad (12)$$

but now the average over all bonds depends on the gauge in which the flux is represented. This degree of freedom can be used to minimize the energy. LPR defined a function $K(\Phi) = \max \langle \cos \varphi_{ij} \rangle_{\text{ave}}$ where the maximum is taken w.r.t. the choice of gauge and also there is a discrete degree of freedom since a unit flux may be added or subtracted from a square in the magnetic supercell. This gauge dependence shows up clearly in the case of $\Phi = 1/2$ (AM-state) where a Landau gauge give $1/2$ but a choice with alternating fluxes $\pm 1/2$ on neighboring squares and $|\varphi_{ij}| = \pi/4$ gives $K(\frac{1}{2}) = 1/\sqrt{2}$. Also $K(\Phi \rightarrow 0) = 1$ but in between, $0 < \Phi < 1/2$, $K(\Phi)$ varies with a lower bound of $2/\pi$. This function shows up also in the study of Josephson junction arrays and it has been extensively studied ²² in that context. It is clear that these values of $K(\Phi)$ represent a considerable cost in kinetic energy in the CFP-states.

This kinetic energy cost shows up as a limitation on the stability of the CFP for $J/t < 1$. This in the renormalized mean field theory it has the consequence that for $2\delta = 1/8$ the state with $\Phi = 7/16$ requires a value of $J/t \gtrsim 1.8$ to be stabilized. This unfavorable cost in kinetic energy is not just a consequence of the renormalized mean field theory. Poilblanc, Hasegawa and Rice ²³ examined a 4×4 cluster with 2 holes (i.e. $2\delta = 1/8$) by exact evaluation of the ASH-states and by exact numerical diagonalization. Again the choice $\Phi = 7/16$ is not favored for $J/t < 1$ but smaller commensurate flux values (e.g. $\Phi = 1/16$) can occur. The overall comparison to the exact energies is not bad. There are many interesting aspects to this comparison for small clusters which cannot be covered here such as the role of the broken translation symmetry and the introduction of hole-hole repulsion.

Liang and Trivedi ²⁴ have reported a series of exact numerical evaluations on quite large clusters (20×20) which agree in their overall conclusion that relative large values of J/t are required to stabilize the CFP.

There is another generalization of the AM-state namely a staggered flux phase (SFP) with alternate values $\pm \Phi$ on neighboring squares. Such states were proposed by Harris, Lubensky and Mele ²⁵ and their energies were considered in some detail by Poilblanc and Hasegawa ²⁶. Such states do not have a gap at the Fermi energy but they gain energy through the splitting of the van Hove singularity at the Bloch band center. The analogous $K_S(\Phi)$ -function which appears in the kinetic energy H_t -term is however much larger since a continuous choice $|\varphi_{ij}| = \pi\Phi/2$ is now possible so that $K_S(\Phi) \geq K(\Phi)$. Thus the overall energy is improved for $J/t < 1$, relative to CFP. Poilblanc and Hasegawa ²⁶ find in their exact studies on small clusters that the kinetic energy term favors SFP over CFP in this region. There remains however the possibility that introducing further correlations in the wavefunctions or additional terms in the Hamiltonian might change this.

4. Properties of Flux States and Relation to Anyons

In this part the CFP will be emphasized although SFP are clearly of interest too. The first property that is clearcut is the chiral spin order in these states. Following Wen, Wilczek and Zee ²⁷ the chiral spin order expectation value on a square can be expressed as

$$\langle E_{123} + E_{134} + E_{124} - E_{234} \rangle = -4Im \{ \langle \chi_{12} \chi_{23} \chi_{34} \chi_{41} \rangle - \langle \chi_{14} \chi_{43} \chi_{32} \chi_{21} \rangle \} \quad (13)$$

with $E_{123} \equiv \vec{\sigma}_1 \cdot (\vec{\sigma}_2 \times \vec{\sigma}_3)$. The r.h.s. depends directly on the value of $\sin(2\pi\Phi)$ so that for $\Phi \neq 1/2$ (i.e. except AM-state), it is nonzero and such states have a chiral spin order.

A second property concerns orbital currents. Since the current on an individual bond varies as $\sum_{\sigma} \langle d_{i\sigma}^+ d_{i-x,\sigma} - d_{i-x,\sigma}^+ d_{i\sigma} \rangle$ it will be proportional to $\sin(\varphi_{ij})$ so that there will in general be a current pattern in the magnetic supercell when $\delta \neq 0$. The detailed current pattern will depend on the flux Φ and the gauge. Thus these states are in the category of orbital magnets discussed in the classification of

diagonal long range order by Halperin and Rice ²⁸. The CFP-states are characterized by a particular orbital current pattern which in turn will generate spatially varying magnetic fields in the sample. Note these fields are not to be confused with the flux generated selfconsistently through the meanfield treatment of the correlated motion. The real magnetic fields are much smaller in magnitude since they are proportional to the density of holes through the g_t -factor. However they should still be quite measurable ²⁹ in NQR, NMR, μ SR and other experiments which are sensitive to small internal magnetic fields.

The most interesting properties of the CFP are their superconducting properties discussed by LPR. Since the expectation value of the kinetic energy, (H_t -term) depends directly on the gauge in which the flux is represented, these states have a collective gauge coordinate. This was used by LPR ²¹ to construct a Ginzburg-Landau-like expansion for the energy as a function of an applied e.m. field. The coupling between the gauges for \uparrow and \downarrow -spin electron implied by the factorization in Eq. (10) leads to a gauge coupling similar to that in usual BCS-states and to flux quantization with a charge $2e$. The cusp property of exchange energy, (H_J -term) as a function of the flux, Φ leads to a rigidity of the wavefunction w.r.t. a small external e.m. flux so that this will be screened out by a surface current i.e. a Meissner effect. The question of the compressibility of this state is trickier since the function $K(\Phi)$ is not differentiable ²² w.r.t. to Φ at all rational values of Φ leading to an incompressible state. However as discussed out by Lederer and Rice ³⁰, various perturbations such as lattice imperfections, impurities or interlayer coupling etc. may smooth out the cusps in $K(\Phi)$.

The CFP described above have a number of properties in common with the anyon gas model. This model for the superconductivity in the cuprates is based on Laughlin and Wiegmann's proposal that the charge carrying holes are particles which obey 1/2-statistics ³¹. This proposal has led to many papers on the properties of the free anyon gas ^{27,37,33}. Such a gas may be represented as a system of spinless fermions which carry a fraction of a flux quantum leading to long range interactions due to the resulting vector potential. If these are treated in a mean field approximation the parallel to the mean field CFP is quite close. In the anyon gas model there are two species of holes labelled by isospin which as free particles in a fictitious flux such that each species exactly fills its lowest Landau level ³³. Such an anyon gas has been shown to exhibit a Meissner effect and to have a Goldstone mode characteristic of superfluidity ^{37,33}. Further Halperin et al ³³ show that a net orbital moment results on each CuO_2 plane. In addition to this diagonal long range order they show that there is an off diagonal long range order defined by adding and removing two nearby holes with the accompanying flux at large distances.

There is a close parallel between the CFP and the anyon gas as regards the diagonal long range order but although it is plausible that CFP also have ODLRO this remains to be shown explicitly. One important difference is the role of the underlying lattice. In the anyon gas model, it determines only the effective mass of the anyons and none of the commensurability effects associated with cusps in $K(\Phi)$ appear.

5. Conclusions

The past year has seen a lot of progress in the understanding of flux phases and the closely related anyon models and their fascinating properties. Clearly there remains many open questions in this subject especially regarding the relative stability of the commensurate and staggered flux phases and the d -wave RVB state at finite doping levels. In this connection, Zhang ³⁴ has recently reported that the staggered flux phase when treated in the Gutzwiller approximation is unstable towards d -wave pairing. The interrelationship between the mean field theory for the $t - J$ model discussed above and the anyon gas models needs to be clarified further. A word of caution however is in order since very recent reports ³⁵ of μ SR experiments stimulated by the prediction of Halperin et al ³³ give a preliminary limit on the magnetic field at the muon sites which is much below values estimated from an orbital magnetic moment. The definitive results on this point will be a crucial test of the diagonal long range order in the CFP or anyon gas models.

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