Surprises in the *t-J* Model: Implications for Cuprates

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(Received 28 February 2019; revised manuscript received 9 February 2020; accepted 16 March 2020; published 10 April 2020)

Many strongly correlated systems, such as the cuprate superconductors, have the interesting physics of low dimensionality and hence enhanced fluctuation effects. We perform an analysis of the *t-J* model in the slave boson formulation which accounts for strong correlations, focusing on fluctuation effects that have hitherto not received the attention they deserve. We find several interesting results including the instability of the d-wave superconducting state to internal phase fluctuations giving way to a time reversal broken $d + is^*$ superconductor at low doping. This offers an explanation for some recent experimental findings in the cuprate superconductors, including the observation of nodeless superconductivity at low doping. We also suggest further experiments that can validate our claims. On a broader perspective, this work points to the importance of considering fluctuation effects in other two-dimensional strongly correlated systems opening up a plethora of possibilities.

DOI: 10.1103/PhysRevLett.124.147002

The rich phase diagram of the copper oxide high-T_c superconductors has been a major source of inspiration in condensed matter physics [1]. One of the important theoretical offshoots has been the extensive study of strongly correlated model systems like the *t-J* model [2–4]. While this model has been successful in explaining several features of the cuprate phase diagram [5–7], a comprehensive understanding of the low temperature phase in the underdoped region is still being sought [8,9]. Recent experiments like the observation of nodeless superconductivity in the underdoped cuprates [10,11], discovery of s-wave-like gap in the pseudogap phase [12], and clear signatures of breaking of time reversal symmetry [13,14] raise new challenges.

A natural question is how much of this new physics is contained in the *t-J* model? The difficulty in addressing this question is twofold: (1) strong electron correlations, and (2) increased importance of long-wavelength fluctuations because of low dimensionality. Numerical techniques like the variational Monte Carlo (VMC) methods using projected mean field like wave functions [15–17] or projected entangled pair states (PEPS) [9] do a good job of accounting for strong correlations, but miss out on the long-wavelength fluctuations because of finite size limitations [18]. The cluster dynamical mean field theory (DMFT) [19,20] studies on the *t-J* model and the related Hubbard model also have similar issues.

The slave-boson formulation of the *t-J* model [21,22] has a unique advantage in this respect. At the mean field level it agrees qualitatively with the VMC studies [16] indicating that the effect of strong correlations are suitably accounted for. At the same time, being analytically tractable, it provides the framework for a systematic study of the effect of long-wavelength fluctuations beyond the mean field theory. It is worth noting that previous slave-boson studies of the *t-J* model have mostly focused on incorporating the effect of fluctuations of the emergent gauge fields in the finite temperature phases, to better describe the effect of strong correlations [23,24]. The description of the zero temperature phase in these studies are mean-field like and do not account for the fluctuations of the order parameter field even qualitatively. It is this crucial piece of physics that we investigate, leading to a set of intriguing conclusions that offer an understanding of the recent experiments on underdoped cuprates, even while suggesting new avenues for experiments.

With model parameters relevant for cuprate superconductors, we use a self-consistent method [25] to estimate the effect of bond pairing order parameter fluctuations on the mean field ground state. We find that the results of this fluctuation-consistent calculation are surprisingly different from those of their mean field counterparts. One of the key differences is that the d-wave superconducting order (d-SC) becomes unstable to antisymmetric bond pairing phase fluctuations [26] (unrelated to any nonpairing competing order) giving way to a $(d + is^*)$-SC for hole doping $(p) \lesssim 0.12$, where s^* represents an extended s-wave pairing amplitude. While a $(d + is^*)$-SC can naturally account for nodeless superconductivity, it also breaks microscopic time reversal ($\mathcal{T}$) symmetry, a prerequisite for the observation of polar Kerr effect (PKE) [14]. Other salient features of our theory which differ remarkably from the mean field theory are as follows: (1) The value of hole doping on the overdoped side at which the d-SC subsides comes down from its mean field value of $p \sim 0.45$ to around $p \sim 0.33$, which is much closer to the experimentally observed values for cuprate superconductors. (2) On the underdoped side, the $(d + is^*)$-SC order has a large extended s-wave amplitude, but the superfluid stiffness nevertheless approaches zero. This is consistent with the Uemura relation [27] and also accounts for the observation of Nernst effect [28,29] as arising from the physics of preformed pairs. (3) Going further on the underdoped side ($p \lesssim 0.055$), the fluctuation modes (except one) become soft and we find no uniform superconducting order in the d-wave, s^*-wave, or $(d + is^*)$-wave channels. We further propose experiments which can put our claim of $(d + is^*)$-SC in underdoped cuprates to test.

Model.—The t-J model written in terms of the electron creation ($c^\dagger_{i\sigma}$) and annihilation operators ($c_{i\sigma}$) is,

$$H_{tJ} = P\left[-\sum_{\substack{i,\delta \\ \sigma}} t(\boldsymbol{\delta}) c^\dagger_{i+\delta\sigma} c_{i\sigma} + J \sum_{\langle i,j\rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j\right)\right] P, \tag{1}$$

where P is a projection operator that restricts H_{tJ} to the no-double-occupancy sector of the Hilbert space. $\mathbf{S}_i$ and n_i are, respectively, the electron spin and number operators on the site i. $t(\boldsymbol{\delta})$ is the hopping amplitude from a site i to a neighbor at site $i + \boldsymbol{\delta}$. In our calculations we shall use the nearest neighbor hopping amplitude t, and, the next nearest neighbor hopping amplitude, $t' = -0.3t$. We shall also set the nearest neighbor exchange interaction energy, J, to $0.3t$.

Fluctuation-consistent saddle point.—Within the U(1) slave-boson formulation of the t-J model one can obtain the grand partition function of the system as a coherent state path integral over the holon (slave-boson) and the spinon (slave-fermion) field configurations with the constraint that there is exactly one slave particle per site. It is well known that this formulation of the t-J model introduces a (local) gauge redundancy [5]. However, at zero Kelvin and finite values of hole doping, the holons are condensed to realize a deconfined Higgs phase of the internal gauge fields wherein the local constraint becomes irrelevant [30,31], and one can rewrite the grand partition function as a path integral over gauge invariant degrees of freedom [24,32–34] comprising a set of gapped fields and an electronlike fermionic field with only a global chemical potential. For the analysis of the low temperature phase one can drop the gapped degrees of freedom, and introduce Hubbard-Stratonovich fields in the particle-particle and particle-hole channels to deal with the quartic terms in the fermion field. A straightforward integration over the quadratic fermion field gives the grand partition function as a path integral of only the Hubbard-Stratonovich fields.

The possibility of superconductivity in the t-J model can now be analyzed by studying the saddle point configurations of the Hubbard-Stratonovich fields along with the number equation

$$N(1 - p) = -\frac{\partial \Phi}{\partial \mu}, \tag{2}$$

where N is the number of sites in the square lattice with periodic boundary conditions, p is the hole doping above half-filling, Φ is the grand canonical free energy and μ is the chemical potential. Typically, one replaces Φ in Eq. (2) by its saddle point estimate (Φ^{SP}) ignoring the contribution from the fluctuations about the saddle point. A more accurate and yet tractable way, which we employ in this work, is to include the effect of Gaussian fluctuations of the Hubbard-Stratonovich fields [25] (about their saddle point values). Furthermore, at zero Kelvin the fluctuations in the particle-hole channel get gapped out because of the Anderson-Higgs mechanism operative on the holon condensate and the internal gauge fields [24]. And thus, in the overdoped and moderately underdoped regions of the phase diagram where the phase of the holon condensate is sufficiently stiff, fluctuations in the pairing order parameter are arguably the most relevant ones in the Gaussian fluctuation corrected grand free energy, which we denote as Φ_{GF} [34].

Results.—The results obtained by solving self consistently the saddle point equations along with the number equation Eq. (2), with Φ replaced by Φ_{GF} are plotted in Fig. 1 as a function of the hole doping p. All the quantities shown are in units of the nearest neighbor hopping amplitude t. The dashed line in the plots shows the usual saddle point results, i.e., when Φ in Eq. (2) is replaced by Φ^{SP}, while the points show the results for the fluctuation-consistent saddle point. Figure 1(a) shows the pairing amplitude and its different components. $\Delta_{\circ d}$ is the d-wave pairing amplitude when the fluctuation effects are not included, i.e., the usual slave-boson mean field result. Δ_d and Δ_s, indicated respectively by purple crosses and black squares, are the d-wave and extended s-wave components of the $d + is^*$ pairing amplitude when fluctuation effects are included self-consistently. Interestingly, we find that there is a phase transition from a d-wave

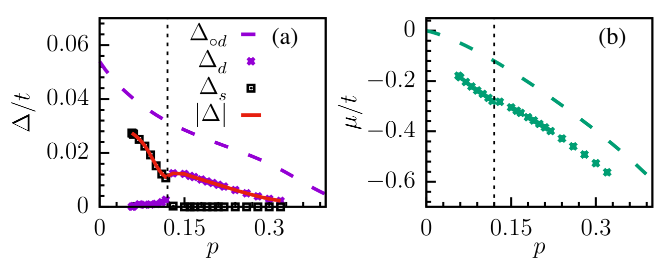

FIG. 1. Fluctuation-consistent saddle point. Panel (a) shows the pairing amplitude ($|\Delta| = \sqrt{\Delta_d^2 + \Delta_s^2}$) and its d-wave and extended s-wave components, Δ_d and Δ_s, respectively, as a function of doping p. Panel (b) shows the variation of the chemical potential μ with doping p. In both these plots, the corresponding quantities in the usual saddle point theory (i.e., without the fluctuation corrections) are shown for comparison by dashed curves. The dotted vertical lines mark the doping value ($p_c \sim 0.12$) where the fluctuation-consistent theory has a phase transition.

superconductor for $p > p_c$ to a $d + is^*$ superconductor with predominantly extended s-wave character for $p < p_c$, at $p_c \sim 0.12$ (marked by a vertical dotted line). Within our fluctuation-consistent theory this transition is a first order phase transition. $|\Delta| = \sqrt{\Delta_d^2 + \Delta_s^2}$, the magnitude of the pairing amplitude with the effect of fluctuations included, is shown by the solid red line. Figure 1(b) shows the chemical potential μ as a function of p, with the dashed line depicting the usual saddle point values, and the green crosses depicting the fluctuation-consistent saddle point results.

To understand better the phase transition at $p_c \sim 0.12$ we analyze the slow and long-wavelength collective modes of the pair condensate. This is done by analyzing the inverse fluctuation propagator in the slow and long-wavelength limit ($q \to 0$). Generically, this system has two phase modes and two amplitude modes corresponding to the complex valued fluctuations of the pairing field on the unique x and y bonds associated with each lattice site. For $p > p_c$, where there is only d-wave pairing, the normal modes at $q = 0$ are given by the symmetric and antisymmetric combinations of the phase and amplitude modes: the symmetric phase mode (P_s mode, which is also the Goldstone mode of the d-SC order and is gapless in the absence of coupling to the electromagnetic gauge field), the antisymmetric phase mode (P_a mode), the symmetric amplitude mode (A_s mode), and the antisymmetric amplitude mode (A_a mode) [26]. In the underdoped region where $d + is^*$ pairs stabilize, the P_s mode and the A_a mode continue to be normal modes in the $q \to 0$ limit, while the P_a mode and the A_s mode combine to give two new normal modes. We continue to use the old nomenclature for these new modes; the mode whose gap parameter [40] (M) connects with the P_a mode of the d-wave condensate at the transition point is still called the P_a mode, and the A_s mode of the $d + is^*$ condensate is defined in an analogous way.

Figure 2 shows the relevant properties of the collective modes of the pair condensate as a function of p obtained from our theory. The vertical dotted lines in all these plots are at $p_c \sim 0.12$ where Fig. 1(a) shows the phase transition. Figure 2(a) shows the *stiffness* (ρ_s) of the P_s mode which is the gapless Goldstone mode. It is remarkable that ρ_s goes to zero at $p \sim 0.055$, consistent with the spirit of the Uemura relation observed in experiments on the cuprates. In Fig. 2(b) we show the gap parameter, M_{P_a}, of the P_a mode; in Fig. 2(c) the gap parameter of the A_a mode, M_{A_a}; and, in Fig. 2(d), the gap parameter, M_{A_s}, of the A_s mode. The phase transition at p_c from d wave superconductivity to $d + is^*$ superconductivity is marked by the vanishing gap parameter of the P_a mode [Fig. 2(b)]. Such a feature would usually indicate a continuous phase transition, but the inclusion of fluctuation effects turn it into a first order phase transition with the *actual gap* [41] in the P_a mode remaining finite at p_c (see Fig. S3.4 of [34]). Furthermore, we find that below $p \sim 0.055$ there is no stable uniform

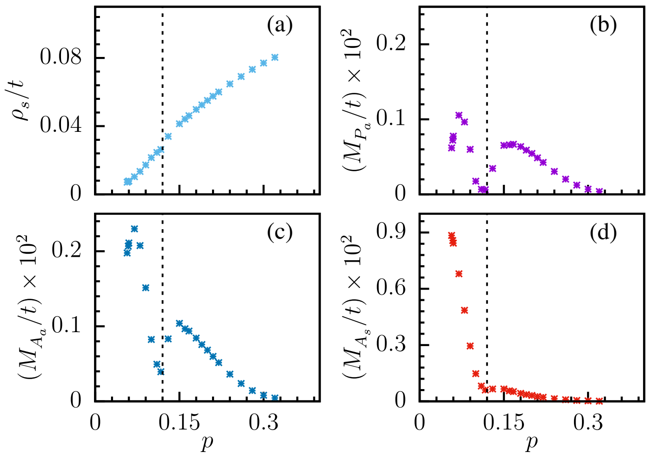

FIG. 2. Properties of the collective modes. All the data presented are obtained at the fluctuation-consistent saddle point and the vertical dotted line marks the doping (~0.12) where the fluctuation-consistent theory hosts a phase transition. Panel (a) shows the stiffness of the P_s mode. Panel (b) has the gap parameter of the P_a mode. Panel (c) depicts the gap parameter of the A_a mode. And panel (d) has the gap parameter of the A_s mode.

superconducting phase in any of the pairing channels, extended s, d, and $d + is^*$, that we explore. This is marked by the vanishing stiffness of the P_s mode and by the softening of the P_a mode and the A_a mode.

Discussion.—As described in the previous paragraphs, there are four distinct doping regions which emerge out of our calculations: (1) the overdoped ($p > 0.14$), (2) the moderately doped ($0.1 < p < 0.14$), (3) the underdoped ($0.055 < p < 0.1$), and (4) the deeply underdoped ($p < 0.055$) regions.

We begin with a discussion of our results on the overdoped side *vis-á-vis* other theories of the t-J model and the large-U Hubbard model, along with the experimental observations in cuprate superconductors. In this region the stiffness of the holon condensate is expected to be large and, therefore, our fluctuation-consistent theory would also be expected to be most dependable in this region. Here, the d-wave pairing gap is known to grow as p decreases in both VMC [16] (cf. the variational parameter Δ_{var}) and slave-boson mean field theory [5]. In contrast, our fluctuation-consistent results are that the d-wave pairing gap [41] first increases and then attains a plateau around $p \sim 0.15$. Interestingly, this behavior of the d-wave pairing gap in the overdoped region agrees qualitatively with cluster DMFT studies of the t-J model [19] and of the closely related Hubbard model [20,42]. It is also in qualitative agreement with a large-$\mathcal{N}$ theory that we had presented in a similar setting [26]. Most importantly, ARPES experiments on the cuprate Bi2212 [10] and STM experiments on several cuprates [43] do find results consistent with such a behavior of the superconducting gap in the overdoped region. All these results put together clearly suggest that the pseudogap [44], which increases monotonically with decreasing doping, is distinct from the pairing gap, at least in this region. Yet another quantitative improvement that our theory provides over the slave-boson mean field theory is the reduction in the value of doping at which the d-SC dies out, from the rather large value of $p \sim 0.45$ to a realistic value of $p \sim 0.33$ [see Fig. 1(a)]. The latter compares favorably with the observed behavior in overdoped cuprate superconductors.

In the moderately doped region our results are remarkably different from those of other theories of the t-J model. We find that on approaching this regime from the overdoped region, the d-SC makes a transition [45] to a $(d + is^*)$-SC at $p_c \sim 0.12$. The difference from other numerical theories like cluster DMFT and variational calculation using PEPS is, most likely, arising because of their severe finite size limitations, and, hence, their inability to include the effects of long-wavelength fluctuations which are crucial to stabilize the $(d + is^*)$-SC. Our fluctuation-consistent theory does not have this limitation. We also point out that we evaluate all the momentum sums as Brillouin zone integrals, and hence, capture the contribution of all long-wavelength Gaussian fluctuations correctly in the infinite system size limit [46,47].

ARPES [10,11] finds a nodeless superconductor in underdoped cuprates which has, however, been attributed to several possible causes [11,48–52]. Interestingly, the $(d + is^*)$-SC that our theory finds within the t-J model is such a nodeless phase arising from the interplay of strong correlation effects and long wavelength fluctuations. We are unaware of any phase sensitive experiments which probe the order parameter symmetry (Josephson junction interferometry experiments [53,54] and ring magnetometry experiments [55]) that have been performed in the doping range where nodeless superconductivity is observed [56]. Our theory provides a concrete suggestion for such experiments with a prediction that the nodeless superconducting state observed in underdoped cuprates has a $d + is^*$ symmetry. We point out that in the presence of defects a $d + is^*$ superconductor would generate spontaneous magnetization. By producing controlled defects, this fact can also be used to distinguish a $d + is^*$ superconductor from a d-wave superconductor [57].

We have also computed the transverse conductivity, $\sigma_{xy}(\mathbf{k} = 0, \omega)$, and find that its imaginary component is zero for all ω and for all dopings of our interest. This implies that the $d + is^*$ state, although it breaks time reversal symmetry, will not by itself contribute to the polar Kerr effect signal seen in experiments on the cuprates. This is so because the uniform $d + is^*$ state preserves $\mathcal{TR}$, where $\mathcal{T}$ is the time reversal operator and $\mathcal{R}$ rotates the system anticlockwise by 90°. The experimental observation that the polar Kerr effect onset temperature coincides with the onset of charge density wave correlations [13] is an evidence for the role of broken $\mathcal{R}$ in this physics. It is a matter for further investigation whether the $(d + is^*)$-SC in the presence of charge density wave correlations can give rise to PKE. However, given the range of doping over which PKE is observed in the cuprates it is unlikely that the $(d + is^*)$-SC that we find in our study of the t-J model can alone account for all of it, and investigations regarding the possibility of time reversal broken pair density waves might be relevant in this context [58,59].

With further underdoping, our theory predicts that the extended s component of the pairing gap increases to significantly higher values, while the d component diminishes completely by $p \sim 0.055$. Another outstanding feature of our theory is that the superfluid stiffness ρ_s vanishes at around the same value of hole doping (~0.055), which is consistent with the Uemura relation observed in experiments on several underdoped cuprates [27]. This would imply that if the pseudogap phase in underdoped cuprate superconductors has a contribution from preformed pairs, those pairs are likely to be of the extended s type rather than of d type. Further investigations will be required to see whether this scenario can help explain aspects of the observed Nernst effect in the pseudogap phase of the cuprates [28,29]. Furthermore, the mass parameters corresponding to the P_a mode and the A_a mode also approach zero around the same doping (~0.055). Consequently, uniform superconductivity does not survive in any of the pairing channels investigated, namely, d, extended-s or $d + is^*$, below this doping. This, again, is consistent with experiments on cuprates and leaves scope for other nonsuperconducting phases observed close to half filling. It must be noted that fluctuations of the internal gauge fields will become important with underdoping, and may lead to qualitative modifications of our results in the underdoped and the deeply underdoped regimes. Addressing this issue is outside the scope of this Letter.

To conclude, the results of our fluctuation-consistent theory seem to agree better with experiments on cuprate superconductors compared to the mean field slave-boson theory and numerical methods, like VMC and cluster DMFT methods. This is indeed encouraging and interesting. However, we note that our method has an uncontrolled approximation (no small parameter), and hence a mathematical proof of the correctness of our results is presently unavailable. Even so, from a physical perspective this may be a strong indication of weak vertex corrections (see Refs. [60–62]). It would also be worth investigating whether a similar fluctuation-consistent calculation gives a better description for other interesting two dimensional systems like the iron pnictide superconductors. In the context of cuprates, we would like to end with a set of questions which our study throws up and whose answers can be very insightful: What is the nature of the state at finite temperatures in the underdoped region in the presence of the $d + is^*$ pairing with predominantly extended-s character? What, if any, features of the cuprate pseudogap may be understood within this scenario [63]? How do the nonpairing competing or intertwined orders seen in cuprates, which are typically most pronounced close to p_c, fit in? What happens in the deeply underdoped regime? What lies beyond the Gaussian fluctuations which our theory accounts for? We hope this work will prompt further research towards addressing some of these questions.

AVM thanks Subhro Bhattacharjee and Sumilan Banerjee for useful comments and suggestions, and P. Corboz, M. Capone, A. Ghosal, T. V. Ramakrishnan, A. M. Tremblay, P. Phillips, and G. Baskaran for useful discussions. We also acknowledge support from the following funding agencies of Government of India: Shyama Prasad Mukherjee Fellowship/CSIR and DST.

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