

Magnetism and Superconductivity in the Pseudogap Phase of Underdoped Cuprates

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Abstract. The theoretical description of the anomalous properties of the pseudogap phase in the underdoped region of the cuprate phase diagram lags behind the progress in spectroscopic and other experiments. A phenomenological ansatz, based on analogies to the approach to Mott localization at weak coupling in lower dimensional systems, for the single particle propagator in the pseudogap phase has been proposed by Yang, Rice and Zhang. This ansatz has had success in describing a range of experiments, especially spectroscopies such as ARPES and aspects of STM results. Recently this approach has been extended to successfully interpret the magnetic excitations in the spin response response. In the charge channel, d-wave cooperon excitations accompany the opening of the pseudogap and they generate an additional d-wave attraction for quasiparticles at the remnant nodal Fermi surfaces.

1. Introduction

The phase diagram of the cuprates is by now quite well established. The two limits of a standard Landau Fermi liquid metallic state at strong overdoping and an AF ordered Mott insulator in the parent stoichiometric compound, are well understood. In between the full Fermi surface at overdoping shrinks as the doping is reduced, before finally disappearing at zero doping. In an intermediate density range four disconnected Fermi arcs, centered on each nodal direction, are observed in ARPES experiments [1]. These Fermi arcs lead to only a partial gapping of the Fermi surface, hence the name pseudogap. This pseudogap phase at underdoping is the most puzzling and anomalous region of the phase diagram. One much debated question is whether this partial gapping of the Fermi surface is a consequence of some form of superlattice order in this underdoped region. Certainly there are a number of examples of superlattice instabilities in underdoped cuprates e.g. the static stripe phase in $\text{La}_{2-x}\text{Ba}_x\text{Cu}_2\text{O}_4$ at $x = 1/8$ [2] with antiphase modulated superconductivity coexisting with charge and spin density waves. However no superlattice instabilities have been reported in the cleanest and best ordered examples of underdoped cuprates in the pseudogap phase at zero magnetic field, e.g. the double chain cuprate $\text{YBa}_2\text{Cu}_4\text{O}_8$ [3] and O-chain ordered Ortho II- $\text{YBa}_2\text{Cu}_3\text{O}_{6.5}$ [4]. This absence leads us to argue that the partial truncation Fermi surface is not driven by a superlattice instability. Rather, the appearance of superlattices in certain underdoped cuprates



like the d-wave superconductivity at lower temperatures reflect instabilities of the underlying pseudogap phase. Some years back Anderson[5] advocated the interpretation of the pseudogap phase as a well defined, but ultimately unstable, fixed point, similar to the Landau Fermi liquid in standard metals. The key issue then is to understand how such a highly anomalous phase can come about as the cuprates evolve from the full Fermi surface Landau Fermi liquid at overdoping, to a Mott insulator at stoichiometry. Although the basic model that describes the cuprates, namely a single band Hubbard model on a 2D square lattice, looks deceptively simple a direct 'a priori' approach is very challenging. We are looking for an anomalous phase stabilized by short range order, in a system of strongly interacting fermions. Some years ago Yang, Rice and Zhang[6] proposed a phenomenological approach which seeks to give a consistent description of the key anomalous electronic properties that characterize the pseudogap phase. The YRZ approach was based on a generalization of the well studied case of multi-leg Hubbard ladders to the case of a 2D square lattice. In particular, in two model ladder systems, a partial truncation of the Fermi surface is found at light doping already the weak coupling - namely, wider Hubbard ladders with an even number of legs[7] and a 2D array of 2-leg Hubbard ladders with long range interladder hopping[8]. In both systems there only short range correlations predominantly in the antiferromagnetic (AF) and d-wave pairing (dSC) channels. Their general properties are consistent with the original proposal for a resonant valence bond (RVB) phase proposed by Anderson very soon after the discovery of the cuprate superconductors[9]. We will not go into details here about the considerations that led to the phenomenological form for the single particle propagator and refer the reader to a recent review[10] which covers both the reasoning behind the proposed form and the comparison to a range of experiments. It is worth noting however that an alternative derivation starting from the strong coupling coupling t - J model was recently given by Lee[11]. Following on an earlier paper by Ng[12], he pointed out that in the factorization approach with spinons and holons, if the hole hopping term is treated as a source of attraction which leads to spinon-holon bound state, a form similar to YRZ follows for the propagator. For more details see the recent paper by James *et al*[13]. The YRZ ansatz [6] for the coherent part of a single particle Green's function $G^{YRZ}(\mathbf{k}, \omega)$ in a doped RVB spin liquid takes the form

$$\begin{aligned} G^{YRZ}(\mathbf{k}, \omega) &= \frac{g_t(x)}{\omega - \xi(\mathbf{k}) - \Sigma^{RVB}(\mathbf{k}, \omega)}; \\ \Sigma^{RVB}(\mathbf{k}, \omega) &= \Delta_R^2(\mathbf{k})/(\omega + \xi_0(\mathbf{k})) \end{aligned} \quad (1)$$

where

$$\begin{aligned} \xi(\mathbf{k}) &= \xi_0(\mathbf{k}) - 4\bar{t}'(x) \cos k_x \cos k_y - 2\bar{t}''(x)(\cos 2k_x + \cos 2k_y) - \mu_p \\ \xi_0(\mathbf{k}) &= -2\bar{t}(x)(\cos k_x + \cos k_y) \\ \Delta_R(\mathbf{k}) &= \Delta_0(x)(\cos k_x - \cos k_y) \end{aligned} \quad (2)$$

The renormalized hopping coefficients $\bar{t}(x)$, $\bar{t}'(x)$ and $\bar{t}''(x)$ contain Gutzwiller factors and the RVB gap function decreases linearly with increasing hole density x as $\Delta_0(x) = \Delta_0(1 - x/0.2)$. These approximate strong coupling forms are taken from the earlier renormalized mean field theory for the $t - J$ model. The key ingredient in $G^{YRZ}(\mathbf{k}, \omega)$ is that the RVB pairing gap opens not on the Fermi surface as in a BCS superconductor, but is pinned by Umklapp scattering processes to the fixed surface in $\mathbf{k}$ space where $(\cos k_x + \cos k_y)$ vanishes - the U- surface which coincides with reduced zone in the case of simple AF ordering. At stoichiometry the RVB gap on a fixed surface in reciprocal space leads to an insulating state. Finite doping causes 4 closed hole pockets to appear centered on the nodal directions and lying inside this U-surface. The spectral weight of the quasiparticles varies strongly around the pockets which causes them to

appear as the 4 nodal arcs observed in ARPES experiments. Recent ARPES experiments by the Brookhaven group on underdoped BSCCO samples in the normal pseudogap phase are a stronger test of this Green's function.[14, 15]. They used the finite temperature broadening of the signal to extract the quasiparticle dispersion not only below, but also up to an energy roughly $3kT$ above the Fermi energy. They observed clear evidence of a coherent quasiparticle dispersion through the Fermi level but with particle-hole asymmetry arising from back bending of the quasiparticle dispersion at positive energy to form a closed pocket in agreement with the YRZ form. More details on these very interesting and innovative experiments can be found in the talk by Peter Johnson. Additionally, earlier spectroscopic STM experiments reported quasiparticle Fermi arcs consistent with the pocket front surface, i.e the surface nearest the zone center, where the spectral weight is largest[16]. All told these experiments agree nicely with the quasiparticle dispersion and the interpretation of the 4 disconnected Fermi arcs proposed by YRZ. These spectroscopic experiments are the most explicit test of the RVB form for the propagator. The predictions that follow for a range of other experiments were worked out by a number of groups, especially by Carbotte, Nicol and their collaborators [17, 18, 19, 20] and by Valenzuela and Bascones[21]. These range from measurements of the specific heat, infrared conductivity, Raman scattering, to the temperature and doping dependence of the superconducting penetration depth. Again the overall agreement between the phenomenological theory, when generalized to describe also a d-wave superconducting state, and experiment is quite satisfactory. One feature that these experiments test is the relative weak dependence of a number of low temperature properties on the hole density. In the theory there is not much change in properties that are sensitive to the near nodal parts of the Fermi arcs, such as the low temperature specific heat and the low temperature variation of the penetration depth. More discussion on this topic can be found in the recent review[10]and the papers quoted therein. Here we concentrate on two recent studies of the collective modes in the spin and charge sectors in the pseudogap phase.

2. Magnetic Excitation Spectrum

We start with the interpretation of the magnetic excitation spectrum that is observed in the pseudogap phase. A series of neutron scattering experiments on several cuprates have found an unusual spectrum which, in keeping with the enhanced AF response, is centered at the wavevector (π, π) . It has been named as a hourglass spectrum consisting of two components: a triplet mode centred at (π, π) which disperses upward symmetrically around (π, π) , and lower frequency legs which stretch down to zero energy at a ring of wavevectors displaced slightly away from the central wavevector (π, π) . These have an incommensurate intercept at zero energy [22]. There has been much discussion in the literature on the interpretation of this unusual spectrum. Here we concentrate on a recent series of calculations by James, Konik and Rice [13] based on the YRZ ansatz for propagator in the pseudogap phase. They used a RPA scheme to calculate the spin response

$$\langle \mathbf{S} \cdot \mathbf{S} \rangle_{YRZ}(\omega, \mathbf{k}) = -\frac{3}{\pi} \frac{\chi_{YRZ}(\omega, \mathbf{k})}{1 - J(\mathbf{k})\chi_{YRZ}(\omega, \mathbf{k})}, \quad (3)$$

where χ_{YRZ} is simply a particle-hole bubble obtained using the YRZ propagators. To describe the spin response in the superconducting state an additional d-wave pairing amplitude is included in the Green's function. The parameters in the propagator have values appropriate for the description of underdoped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$. The energy scale of the magnetic response is largely determined by the RPA exchange interaction J . An appropriate choice of J allows one to obtain a common magnetic response for several underdoped cuprates as illustrated in Fig. 1.

The hourglass in both theory and experiment has strong incommensurate response at lowest energies concentrated at four points displaced slightly from the wavevector (π, π) along the axes at wavevectors, $(\pi, \pi \pm \delta)$ and $(\pi \pm \delta, \pi)$. As the energy is initially increased this response evolves inwards towards (π, π) and simultaneously becomes more isotropic in its distribution

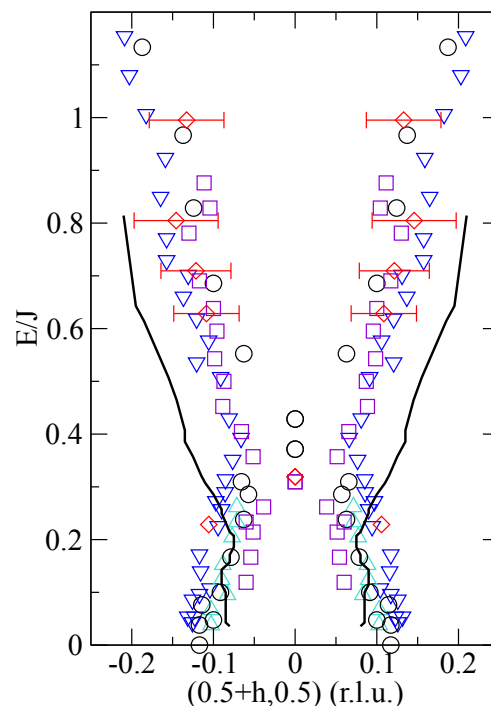


Figure 1. Hourglass dispersion of the resonance near the central wavevector (π, π) . The thick black line is the position of the maximum intensity peak in the RPA calculations[13]. Experimental data points (appropriately rescaled) are taken from experiments on a number of underdoped 214 and YBCO cuprates - for details see James *et al* [13]

around (π, π) . Whether this inward dispersion reaches (π, π) depends in the observations on the particular cuprate that is being examined. At an energy of order $J/5$ the dispersion reverses and moves outwards from (π, π) and is more isotropically distributed about (π, π) . The low energy part of the spectrum in this theory is caused by quasiparticle-hole excitations between opposite near-nodal pockets. This interpretation of the low energy part of the spectrum as particle-hole excitations agrees with neutron scattering experiments performed on $\text{YBa}_2\text{Cu}_3\text{O}_{6.5}$ -OrthoII samples. This cuprate is among the best ordered underdoped cuprates and has the advantage that large single crystals are available. The experiments of Stock *et al* [23] show a clear suppression of the low energy spectrum as T drops below T_c consistent with a suppression of the low energy particle-hole excitations as the superconducting gap opens up on the nodal Fermi arcs. Note, the calculations of James *et al* are for clean materials. The presence of impurities, even nonmagnetic impurities such as Zn, introduce local moments [24], so that a mixture of itinerant and local moments will occur in most cuprates. Recently the spin response at higher energies has been measured by RIXS experiments with enhanced resolution by Le Tacon *et al* [25]. Interestingly the calculations of James *et al* also reproduce the key features of these experiments [13].

3. Superconductivity in the Pseudogap Phase of the Cuprates

Turning to the charge response, we can divide theories of the pseudogap phase that do not rely on some form of superlattice into two classes. One proposes that the pseudogap results from an extended region of enhanced superconducting fluctuations above a transition temperature which is lowered by strong phase fluctuations. These are a consequence of reduced

phase stiffness, which in an underdoped Mott insulator is determined by the hole doping rather than the electron density. This theory implies that when thermal fluctuations are suppressed in the superconducting groundstate, a standard d-wave gap opens over the full Fermi surface, as in overdoped cuprates. However as pointed out by Deutscher[26], the large difference in the Andreev tunneling signal between overdoped and underdoped cuprates is difficult to rationalize in this scenario. The YRZ proposal for the pseudogap phase belongs to the second class which assumes an insulating pseudogap appears as a precursor to Mott insulating behavior at stoichiometry - a proposal which agrees with the Andreev results[27]. Some years back Norman, Pines and Kallin[28] raised the interesting question of whether the associated reduction in the Fermi surface area simply weakens the d-wave superconductivity. There are however a number of strong arguments in favor of a more nuanced effect of the pseudogap on superconductivity. This can occur if a low energy cooperon resonance accompanies opening of the antinodal pseudogap. The analogy between the physics underlying the pseudogap and Hubbard ladder discussed earlier is a reason to explore this possibility.

Konik, Rice and Tsvelik [29] examined an array of coupled 4-leg Hubbard ladders near half-filling. In wider ladders the bands pair up on a hierarchy of energy scales with the pairing of the outermost and innermost bands having the largest gap [7]. This band pair exhibits enhanced responses similar to the half-filled 2-leg Hubbard ladder. For a suitable parameter choice, the larger energy gap causes this band pair to be half-filled and insulating in an initial finite density range but supporting a cooperon collective excitation. Under these conditions, a pairing attraction is generated on the Fermi pockets in the central band pair through coupling in the Cooper channel to the cooperon of the insulating band pair. Although this is clearly an artificial model, Konik et al [29] proposed it as a tractable model which contains the essential features of the cuprates, namely *d*-wave pairing on remnant Fermi pockets supported by coupling to the cooperon excitation living on the remaining gapped bands. There have been a number of reports of enhanced, even giant, penetration lengths for d-wave superconductivity into nonsuperconducting phases of underdoped cuprates [30, 31, 32]. Bozovic *et al* [31] reported a giant proximity effect in uniform trilayer junctions of high temperature superconductors at temperature T above the superconducting transition temperature T_c of the spacer underdoped cuprate layer in the pseudogap phase. These reports motivated Huang and coworkers[33] to model this system using the YRZ form for the normal state propagator of the lower T_c underdoped spacer cuprate layer. They found that this normal phase when modeled by YRZ propagators with a d-wave attraction in line as expected at low energies from renormalization results for the Hubbard model[10], had a cooperon pole in the pairing propagator. The excitation energy of this cooperon goes unstable at T_c . A cooperon excitation in the barrier leads to an enhanced penetration of the superconductivity into the spacer layer in the trilayer junction. Choosing input parameters that reproduced the transition temperatures in the trilayer, Huang *et al* [33] could reproduce the giant proximity effect reported by Bozovic and coworkers[31] quite accurately as illustrated in Fig. 2. The contribution of the cooperon excitation can be deduced from the distribution of the Josephson current in momentum space of the underdoped sample (doping $x \approx 0.1$). A detailed examination of origin of the enhancement shows that the contribution from the cooperon excitation is significant and may be comparable with that from the quasiparticles in the nodal regions of k -space. Note that an alternative explanation of the enhanced penetration depth[31] based on a model with strong phase fluctuations has been given by Marchand *et al*[34]. There are also experiments on $YBCO/Y_xPr_{1-x}Ba_2Cu_3O_7/YBCO$ superstructure, which also report a very large proximity length at $x < 0.55$ [30, 32]. However these strong proximity effects need a different explanation.

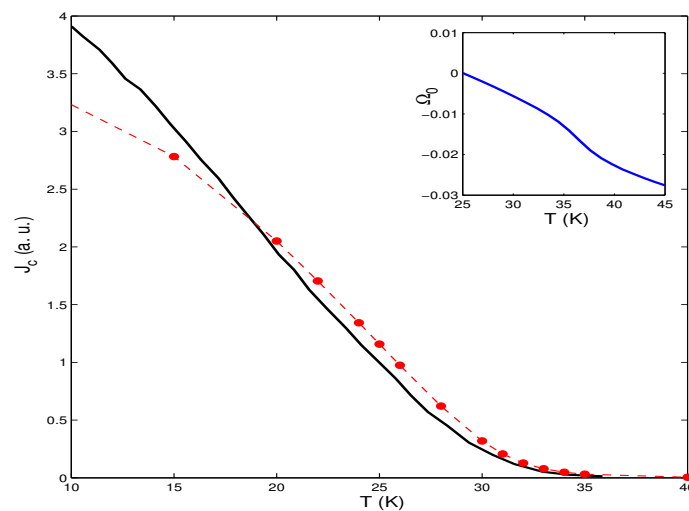


Figure 2. The critical Josephson current in a trilayer junction through a underdoped spacer layer. The black curve is the experimental data of Bozovic *et al* [31]. The red dots are the results of Huang *et al*[33] using the YRZ propagator for the spacer layer. The inset shows the calculated temperature dependence of the cooperon excitation energy above the T_c of the underdoped spacer layer.

4. Conclusions

At present, in the study of the cuprate superconductors there is a lack of consensus on the theory side, to put matters politely. On the experimental side there is continuing strong progress in improving resolution, samples, experimental techniques etc. This situation calls for a phenomenological approach which seeks to develop a theory which consistently explains all, or at least many of the anomalous data taken on the cuprates. The approach described above is motivated by a desire to fill this gap. It certainly has had a number of clear successes but there are still some open issues. The most glaring and most puzzling issue is the explanation of the quantum oscillations observed in underdoped cuprates at high magnetic fields and low temperatures.

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