SU(2)-symmetry in a realistic spin-fermion model for cuprate superconductors

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(Dated: January 21, 2015)

We consider the Pseudo-Gap (PG) state of high-$T_c$ superconductors in form of a composite order parameter fluctuating between $2p_F$-charge ordering and superconducting (SC) pairing. In the limit of linear dispersion and at the hotspots, both order parameters are related by a SU(2) symmetry and the eight hotspot model of Efetov et al. [Nat. Phys. 9, 442 (2013)] is recovered. In the general case however, curvature terms of the dispersion will break this symmetry and the degeneracy between both states is lifted. Taking the full momentum dependence of the order parameter into account, we measure the strength of this SU(2) symmetry breaking over the full Brillouin zone. For realistic dispersion relations including curvature we find generically that the SU(2) symmetry breaking is small and robust to the fermiology and that the symmetric situation is restored in the large paramagnon mass and coupling limit. Comparing the level splitting for different materials we propose a scenario that could account for the competition between the PG and the SC states in the phase diagram of high-$T_c$ superconductors.

Reflecting our rather poor understanding of the physics of cuprate superconductors, two kinds of theories are still debating wether the final solution for this problem will be a “bottom-up” approach based on a strong coupling theory [1, 2] or rather a “top-down” approach at weaker coupling, where symmetries and proximity to a Quantum Critical Point (QCP) plays a dominant role [3, 4]. The recently proposed Eight Hot Spots (EHS) model is a promising “top-down” approach to cuprate superconductors [5, 6]. It drastically simplifies the Fermi surface of the compounds by keeping only eight points in the anti-ferromagnetic (AF) zone boundary, the so-called hot spots and the effect of long-range AF fluctuations between them. When the velocity is linearized at the hot spots, one observes surprisingly that an SU(2) symmetry relating the $d$-wave SC channel (Cooper pairing) to the $d$-wave bond order, or Quadrupolar Density Wave (QDW), (charge channel) is present. Moreover, an imposant pre-emptive instability (of order of 0.6 J, where J is the AF energy scale) in the form of a composite SU(2) order parameter emerges, that has been identified as a good candidate for the pseudo-gap (PG) state of those compounds [6–9]. Motivated by an impressive set of new experimental results [10–19], this theory points out to the emerging idea that charge order is most certainly a key player in the physics of cuprate superconductors, in addition to AF order, $d$-wave SC state and the Mott insulator phase. Recent angle-resolved photoemission spectroscopy (ARPES) experiments confirm as well the presence of modulations in the SC state for underdoped Bi2201 [20, 21] and has been interpreted either in terms of charge order or Pairing Density Wave (PDW) inside the PG phase [22–25].

The idea of an emerging SU(2) symmetry belongs to a wide class of theories which explain the PG phase of the cuprates through the notion of degenerate symmetry states between the $d$-wave SC order and another partner. Maybe the most famous attempt to such a unification has been the SO(5) theory which relates the $d$-wave SC state to the AF order [26]. Not less famous is the SU(2) symmetry which relates the SC $d$-wave order to the $\pi$-flux phase of orbital currents [1]. In both cases, the key question was to argue that the energy splitting between the two orders was small enough so that thermal effects would restore the symmetry above $T_c$ and below $T^*$, which are the SC and the PG critical temperatures. The same question holds here for the SU(2) symmetry relating $d$-wave and QDW order. Although the EHS model in its linearized version verifies the symmetry exactly, it is not clear if a more realistic Fermi surface, including curvature and the whole band structure, will induce small or large energy splitting. Moreover, the EHS model relies on long-range AF fluctuations which mediate the interactions, but the experimental observation points out to short-range AF correlations which potentially will gap a whole part of the Fermi surface, as depicted in Fig. 1a). A theory for “hot regions” instead of “hot spots” is thus needed.

In this paper we address carefully all these issue by evaluating the SU(2) splitting on realistic Fermi surfaces, for the two distinct components of the composite order parameter: the $d$-wave $\chi$-field in the charge sector (which forms the QDW order in the EHS model) and the $d$-wave $\Delta$-field describing the SC pairing sector. We find that the splitting of the SU(2) symmetry increases with the mass of the paramagnons, but decreases with the strength of the coupling constant between AF fluctuations and conduction electrons. This opens a wide regime of parameters where the splitting is minimal – of the order of a few percents – and where the SU(2) symmetry is expected to be recovered through thermal effects in a regime of temperatures $T_c < T < T^*$. Above the PG temperature $T^*$ all traces of the short-range charge and SC field have disappeared. Of course the SU(2) symmetry holds in the whole temperature range between $T_c$ and $T^*$, hence subleading charge instabilities which occur below $T^*$ do have their SU(2) partners in the form of Pairing Density Waves (PDW) [27, 28]. We also study the effects of the Fermi surface shape in breaking the SU(2) symmetry – which is only preserved in the EHS model with a linearized dispersion. We find that the splitting is marginal away from the points where $\chi$ and $\Delta$ are maximal. In the physical situation of a large paramagnon mass and also strong coupling, the maximum of $\chi$ moves towards the zone edge...
leading to bond order parallel to the x-y axes. All these findings point to the realization that, while being a secondary instability to AF ordering, charge order is a key player in the physics of the PG phase of the cuprates.

We start from the spin-fermion model \([5, 6, 27]\) with Lagrangian

\[
L = L_\psi + L_\phi,
\]

where

\[
L_\psi = \bar{\psi} \left( \partial_t + \epsilon_\sigma + \lambda \phi \sigma \right) \psi,
\]

\[
L_\phi = \frac{1}{2} \phi D^\dagger \phi + \frac{u}{2} \left( \phi^2 \right)^2.
\]

The fermionic field \(\psi\) describes the electrons which are coupled via \(L_\psi\) to spin waves described by the bosonic field \(\phi\).

The effective spin-wave propagator is \(\hat{G}_{k}^{-1} = g(\omega) + |k|^2 + m\) where \(m\) is the paramagnon mass which vanishes at the QCP and \(g\) a phenomenological coupling constant. For notational reasons we also write \(k = (i\omega, \mathbf{k})\), where \(i\omega\) are fermionic matsuabara frequencies. Neglecting the spinwave interaction \((u = 0)\) one can formally integrate out the bosonic degrees of freedom. The partition function then writes \(Z = \int D[\psi] \exp(-S_0 - S_1)\) with

\[
S_0 = \sum_{k, \sigma} \bar{\psi}_k G_{0,k}^{-1} \psi_k,
\]

\[
S_1 = -\sum_{k, q, \sigma, \sigma'} J_q \bar{\psi}_{k, \sigma} \psi_{k + q, \sigma'} \bar{\psi}_{k', \sigma'} \psi_{k' - q, \sigma},
\]

where the bare propagator is

\[
\hat{G}_{0,k}^{-1} = \text{diag}(i\omega - \epsilon_k, i\omega - \epsilon_{-k-p}, i\omega - \epsilon_{k+p}, i\omega - \epsilon_{-k}),
\]

and the spinor field \(\Psi_k = (\psi_k, \bar{\psi}_{k-p}, \psi_{k+p}, \bar{\psi}_{k-\mathbf{Q}})^T\). Furthermore, \(J_q^{-1} = 4D_q^{-1}/3\lambda^2\), \(\sigma \in \{\uparrow, \downarrow\}\) labels the spin, \(\mathbf{Q} = (\pi, \pi)^T\) is the AFM ordering vector and \(p\) stands for the 2\(p_F\) vector, as depicted in Fig. 1a). Note that the chemical potential \(\mu\) is implicitly subtracted from the dispersion \(\epsilon_k\).

We select the SC and the 2\(p_F\) channel by introducing the two order parameters

\[
\Delta_k = (\psi_{k, \sigma} \bar{\psi}_{-k, \sigma}), \quad \chi_k = (\psi_{k, \sigma} \bar{\psi}_{k+p, \sigma}).
\]

The interaction \(S_1\) is now decoupled by means of a Hubbard-Stratonovich transformation. The partition function becomes (up to a normalization factor)

\[
Z = \int D[\psi] D[\Delta, \chi] \exp[-S_0 - S_{1, eff}].
\]

The effective interaction is

\[
S_{1, eff} = \sum_{k, q, \sigma} \left[J_q^{-1} \chi_{k+q} \chi_{k+q} + J_q^{-1} \Delta_k \chi_{k+q}\right] - \sum_{k, \sigma} \psi_{k, \sigma} M_{k, \sigma} \psi_{k},
\]

with \(\mathbf{k} = \mathbf{k} + \mathbf{Q}\) and the matrix \(M\) is

\[
M_{k} = \left(\begin{array}{cc}
-\Delta_k & -\chi_k \\
-\chi_{-k} & -\Delta_{k+p}
\end{array}\right),
\]

The fermions in Eq. (5) can now be integrated out so that the partition function becomes

\[
Z = \int D[M] \exp\left[-\frac{1}{2} \sum_{k, q} \text{Tr} J_q^{-1} M_{k+q, \sigma} M_k + \frac{1}{2} \sum_k \text{Tr} \log \hat{G}^{-1}_{k}\right],
\]

with \(\hat{G}^{-1} = \hat{G}^{-1}_{0} - \hat{M}\). After functional differentiation of the free energy \(F = -T \ln Z\) with respect to \(M_k\) we obtain the MF equations in matrix form

\[
\hat{M}_k = \sum_{k'} J_{k-k'} \hat{G}_{k'}.\]

The matrix equation can now be projected onto the different components. We will consider here the case of two competing order parameters which can not be non-zero at the same point in \(k\) space. Therefore, we consider the equation for \(\Delta\) with \(\chi = 0\) and vice versa. The gap equations follow as

\[
\Delta_k = T \sum_{\alpha', k'} J_{k-k'} \frac{\Delta_{k'}}{\Delta_k + \epsilon_{k'}^2 + \omega' \tau},
\]

\[
\chi_k = -\Re T \sum_{\alpha', k'} \langle i\omega' - \epsilon_{k'} - i\omega' - \epsilon_{k'+p}\rangle \frac{\chi_{k'}}{\Delta_{k'} + \epsilon_{k'}^2 + \omega' \tau}.\]

To solve these equations numerically, \(\epsilon_k\) is parametrized in tight-binding approximation with the following parameters: YBCO [29] (parameter set tb2), Bi2201 [30], Bi2212 [31] and Hg1201 [32] and for electron doped cuprates [33]. The momentum sums in Eq. (10) are then carried out by discretizing the \(k\)-space by rectangular and equidistant grids. To keep the numerical computations tractable we neglect the frequency dependence of \(\chi\) and \(\Delta\). The Matsubara sums are
then carried out exactly in the limit $T \to 0$ and the momentum sums are performed over $400 \times 400$ points and over two Brillouin Zones (BZ) in order to include the interference with the hotspot from the neighbouring BZ. Moreover, note that the $2p_F$ vector which connects two opposed FS points at $\pm p/2$ is only properly defined on the FS. For arbitrary points in the first BZ we therefore use the $2p_F$ vector of the nearest FS point. Throughout this article, we use 10% hole filling (respectively 10% electron filling in the electron doped case) and the bandgap is $10^4$. To evaluate the strength of the SU(2) symmetry, we study the level splitting $|\chi - \Delta|/\Delta$. This parameter afford the study of the relative amplitude between the QDW and SC order parameter, $\chi$ and $\Delta$. It vanishes for a perfect SU(2) symmetry and becomes closer to one for a complete SU(2) symmetry breaking.

In order to test the effect of the curvature on the level degeneracy, we have plotted in Fig. 1b) the variation of the maxima of $\chi$ and $\Delta$ with the paramagnon mass $m$ for a fixed value of the coupling constant $\lambda$. We observe a similarity between the various compounds that we have tested. In a wide range at low value of the mass, the SU(2) degeneracy between $\chi$ and $\Delta$ is verified within a few percents. The existence of such a regime is an indication that a PG driven by SU(2) symmetry is possible in cuprate superconductors. As the mass is increased we progressively lose the level degeneracy with the parameter $\chi$ abruptly dropping down while the paring $\Delta$ is asymptotically going down to zero when the mass increases. Of all the compounds tested, the ones for which the SU(2) symmetry is the weakest are the electron doped and Hg1201 which experimentally show much weaker signs of charge order[19, 34]. In Fig. 1c) the level splitting is directly shown for all the compounds and the two regimes, the one at low mass where the SU(2) symmetry is obtained and the higher mass regime where $|\chi - \Delta|/\Delta$ becomes of order one are clearly seen. Within the non linear $\sigma$-model associated to the present theory[6], the SU(2) regime is a signature of the PG of the system, while the energy splitting of the two levels is associated to the superconducting $T_c$. We see that Fig. 1b) mimics the generic phase diagram of the cuprates where the PG line $T^*$ abruptly plunges inside the SC dome at some value of oxygen doping.

Although it is very encouraging to see that the SU(2) regime has a non-zero probability to exist, one can wonder whether the paramagnon mass in realistic cuprate superconductors is small, since typically the AF correlation length is of few lattice constants[35]. The issue is addresses in Fig. 1d), where the values of $\chi$ and $\Delta$ are shown for a fixed mass as a function of the coupling constant $\lambda$. Here again a generic pattern emerges. For small $\lambda$ the SU(2) symmetry is broken, but surprisingly, above a certain threshold of $\lambda$, the SU(2) symmetry is almost completely restored. As seen in Fig. 1c), the bigger the mass is, the stronger the coupling constant needs to be for the symmetry to be restored. This result could not be anticipated analytically and serves as a good criterion for understanding the electron doped compounds. In those compounds...
the coupling between AF modes and conduction electrons is believed to be weaker than for the hole doped case, which leads to an absence of SU(2) symmetry and a much lower PG line.

The SU(2) symmetry is not only broken due to the curvature of the Fermi surface at the hot spots, but it is typically broken in the BZ away from the eight hot spots. Figure 2 shows the typical shape of $|\chi|$ and $|\Delta|$ for the five compounds under investigation for small values of the mass and coupling constant. We observe well defined peaks at the hot spots with the exception of Bi2212 where for the chosen values of the parameters the peaks are extended towards the zone edge. The level splitting is shown as a density plot in the bottom. It is rather small almost everywhere in the BZ with maxima around the “shadow” Fermi surface. The main learning from these plots is that the variations of the Fermi surface geometry gives a rather small departing from the SU(2)-degeneracy for a various range of compounds.

In Fig. 3 we place ourselves in the more realistic strong coupling and strong mass regime and plot the variation of $|\chi|$, $|\Delta|$ and $|\chi - \Delta|/|\Delta_{\text{max}}|$ in the first BZ for YBCO. The parameters are similar to Fig. 2 but with coupling $\lambda = 160$ and mass $m = 1$.

In conclusion, this paper gives firm ground to the intuition that the charge sector is a key player in the physics of cuprate superconductors. While the main instability is still the AF ordering, the $d$-wave bond order relates to the $d$-wave pairing through an SU(2) symmetry. We have shown that there exists a wide range of parameters where the SU(2) degeneracy is fulfilled, which gives a natural explanation for the large PG regime observed in certain compounds. We argue that compounds like electron doped cuprates or the La-serie are outside the regime of SU(2) degeneracy, and the more pronounced energy splitting is the reason for the weaker PG regime.

We acknowledge discussions with A. Chubukov, S. Kivelson, H. Alloul, P. Bourges, Y. Sidis, A. Sacuto, and V. S. de Carvalho. We thank the KITP, Santa Barbara and the IIP, Natal for hospitality during the elaboration of this work. This work is supported by the grant EXCELCIUS of the Labex PALM of the Université Paris-Saclay, of the ANR project UN-ESCOS ANR-14-CE05-0007, as well as the grant Ph743-12 of the COFECUB which enabled frequent visits to the IIP, Natal. This research was carried out with the aid of the Computer System of High Performance of the IIP and UFRN, Natal, Brazil.

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