Preformed Pairs, \( SU(2) \) Slave-boson Theory, and High \( T_c \)

Superconductors

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Abstract

A preformed-pair model was considered. The quantum disordered phase of the \( d \)-wave superconducting state was obtained by turning on an on-site repulsion. The low energy effective theory of the quantum disordered phase was derived, which was found to be qualitatively equivalent to the low energy effective theory of the \( SU(2) \) slave-boson theory in the staggered-flux phase. Many physical properties of the disordered phase at low energies were obtained, such as the Mott insulator property at zero doping, spin gap and low superfluid density at low doping.
The cuprate superconductors not only contain a high $T_c$ superconducting (SC) phase, they also contain, in the neighborhood of the SC phase, an antiferromagnetic (AF) phase (at and near zero doping), a spin-gap (SG) phase (in underdoped regime), a non-Fermi liquid (NF) phase with a large Fermi surface (near optimal doping), and a Fermi liquid (FL) phase (in overdoped regime). (Of course the last three phases are not really different phases. They can continuously cross over into each other without any phase transition.) There are several important energy scales showing up in the above phases. The most important scale is the charge gap $U \sim 2\text{eV}$ at zero doping. Such a charge gap, as the energy cost for the doubly occupied site, also plays extremely important role in the underdoped regime. The next energy scale is $J \sim 0.1\text{eV} –$ the interaction energy of spins. Since $J \ll U$, the undoped cuprate is a Mott insulator. There is also a spin gap appearing at energy scale $\Delta \sim 0.03\text{eV}$ in the SG phase. The energy scale associated with the superconductivity is given by $T_c \sim 0.003 – 0.01\text{eV}$, whose value depends on the doping concentrations. A theoretical model for the high $T_c$ superconductors (HTS) should address the above energy scales, or at the very least address the large charge gap $U$.

The slave-boson approach (both the $U(1)$ and $SU(2)$ theories) \cite{1} to the HTS takes the large charge gap as the main input. The model imposes a no-double-occupancy constraint, which effectively sets the charge gap $U \to \infty$. This approach leads to an effective theory which contains spinons (spin $1/2$ neutral fermions), holon (spinless charge $e$ bosons), and a gauge field. The spinon, describing the spin degree of freedom, has an energy scale $J$, the spin-gap phase can be explained by the staggered-flux (sF) phase of spinons, which has an energy scale of a fraction of $J$ \cite{1,2}.

After the photoemission experiments \cite{3} which confirmed the spin gap and measured their momentum dependence for underdoped HTS’s, many groups \cite{4} proposed a preformed-pair picture to explain the spin gap. Although the preformed-pair picture is very natural in explaining the spin gap and its momentum dependence at energy scale $\sim 25\text{meV}$, it is not clear how to recover the large charge gap near $2\text{eV}$ within this picture, i.e. it is not clear how to explain the insulating properties at zero doping within the preformed-pair picture.
Historically, a “preformed-pair picture” was first suggested by Anderson and his group under the name of Resonating Valence Bound (RVB) state [1]. The main difference between the RVB state and the above preformed-pair picture, is that the RVB state also imposes the no-double-occupancy constraint. Thus the RVB state is naturally a Mott insulator at half filling.

In this paper, we start from a preformed-pair model with $d$-wave pairing (which addresses the spin gap first), and study the quantum disordered $d$-wave (QDdW) phase through a mathematical trick of promoting the effective XY model (or the $O(2)$ non-linear $\sigma$-model) to an anisotropic $O(3)$ non-linear $\sigma$-model. It is difficult to study the disordered phase of XY model directly, because the vortices, which are important in the disordered phase, are singular objects in the XY model. However, as we will see, regarding the XY model as an anisotropic $O(3)$ non-linear $\sigma$-model can overcome this difficulty. We find that the QDdW phase is described by an effective theory with spin 1/2 neutral fermions, spinless charge $e$ bosons and a $U(1)$ gauge field. The effective theory gives rise to an insulating phase at half filling with a finite charge gap. The optical conductivity $\sigma(\omega) = 0$ for $\omega$ below the charge gap if there is a particle-hole symmetry. Although our calculation is reliable only when the charge gap $U$ is less than the spin gap $\Delta$, the effective theory is well behaved and reasonable even when we push the charge gap well beyond the spin gap. In this limit our effective theory is very similar to effective theories of sF phase obtained from the $SU(2)$ slave-boson approach [2]. The close relation between the QDdW phase and the sF phase of the $SU(2)$ slave-boson theory is not surprising. The underlying physics of the sF phase in the slave-boson theory is the RVB picture (note that the sF phase is gauge equivalent to the $d$-wave paired phase of spinons within the $SU(2)$ slave boson theory [2]). The RVB state is nothing but a liquid of non-overlapping Cooper pairs. It is only natural to see that the liquid of non-overlapping Cooper pairs is also the QDdW phase.

A recent work [3] also started from a preformed-pair model and studied the QDdW phase (which was named the “nodal phase”) through a mathematical trick of duality transformation of XY model. However, due to some unknown reasons, the effective theory obtained
in Ref. [5] for the nodal phase has some physical results which are different from the ones obtained from our effective theory. The most notable difference is that the neutral spin 1/2 fermions do not carry the charge of the gauge field, while in our approach they do carry the charge.

We start with a generalized Hubbard model which contains an on-site repulsion $U$ and a nearest neighbor spin coupling:

$$H = \sum_{\langle ij \rangle} (c_i^\dagger t_{ij} c_j + h.c.) + \frac{U}{2} \sum_i (n_i - 1)^2 + J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

(1)

Note that the Hubbard model can generate the above spin coupling with $J = 4t^2/U$. Here we treat $U$ and $J$ as independent variables. We will limit our discussion at zero temperature. Let us ignore the on-site repulsion $U$ at the moment. The nearest neighbor spin coupling causes an attraction between a spin-up and spin-down electrons. We assume that such an attraction leads to a $d$-wave SC state described by the following mean field theory

$$H = \sum_{\langle ij \rangle} (c_i^\dagger t_{ij} c_j + c_i^\dagger \Delta_{ij} \epsilon_{\alpha\beta} c_j^\dagger + h.c.)$$

(2)

where $\Delta_{ij} = \Delta_{ji}$ is the $d$-wave pairing amplitude. As we turn on the on-site repulsion $U$, the $d$-wave pairing order parameter $\Delta_{ij}$ will have stronger and stronger quantum fluctuations. If we assume the fluctuation is mainly the phase fluctuation at a length scale larger than a few lattice spacing, then the quantum fluctuations may destroy the SC phase without closing the $d$-wave spin gap. This picture may explain the $d$-wave-like spin gap in the normal state of underdoped cuprates. Notice that the on-site $U$ can play two roles a) it increases the superconducting phase fluctuation and destroy the SC state, and b) it opens up a charge gap at zero doping (at least when $U$ is very large). Thus it is natural to guess that, at zero doping, the QDdW phase caused by finite on-site repulsion $U$ is also an insulator with finite charge gap. In the following, we will derive an effective theory for the QDdW phase and argue that this is indeed the case.

In addition to the $SU(2)$ spin symmetry, the Hamiltonian Eq. (1) has another $SU(2)$ symmetry at half filling (when the chemical potential gives $\langle n_i \rangle = 1$), which we call the
pseudo-spin symmetry. The $SU(2)$ pseudo-spin symmetry can be made explicit by introducing the doublet

$$\lambda_i = \begin{pmatrix} \lambda_{i1} \\ \lambda_{i2} \end{pmatrix} = \begin{pmatrix} c_{i\uparrow} \\ (-)^i c_{i\downarrow}^{\dagger} \end{pmatrix}$$

which carries pseudo-spin 1/2. (This symmetry is explicitly broken if we introduce a $-\frac{1}{4} n_i n_j$ term in Eq. (1). We shall consider the effect of such term later.) We would like to stress that although our theory has the pseudo-spin symmetry, it is not essential to our calculations and results. Most results obtained in this paper are still valid even without the symmetry.

In terms of $\lambda$, the $d$-wave effective Hamiltonian Eq. (2) can be rewritten as

$$H = \sum_{\langle ij \rangle} \left( \lambda_i^\dagger (t_{ij} - (-)^i (i \text{Im}\Delta_{ij}\sigma_1 + i \text{Re}\Delta_{ij}\sigma_2))\lambda_j + \text{h.c.} \right)$$

The dynamics of the $O(2)$ superconducting order parameter ($\text{Re}\Delta_{ij}, \text{Im}\Delta_{ij}$) is described by a 2D XY model, whose disordered phase contains vortices. To avoid this difficulty, we promote the $O(2)$ order parameter to an $O(3)$ order parameter $\Delta_{ij}^d(n_{ij}^1, n_{ij}^2, n_{ij}^3)$:

$$H = \sum_{\langle ij \rangle} \left( \lambda_i^\dagger (t_{ij} - i \Delta_{ij}^d n_{ij} \cdot \sigma (-)^i)\lambda_j + \text{h.c.} \right) + \sum_{\langle ij \rangle} \frac{1}{2g}(n_{ij})^2.$$  

Here $\Delta_{ij}^d$ is real and is the gap function for a constant $d$-wave order parameter, $n_{ij}$ is a unit vector. We have included the quadratic $(n_{ij})^2$ term to implement the constraint, and the bare value of $1/g$ is $\Delta^2/2J$. Note that in the presence of the pseudo-spin symmetry, the ground state is described by the $O(3)$ order parameter $n_{ij}$ instead of the $O(2)$ superconducting order parameter. $n_{ij}$ is a pseudo-spin vector and Eq. (5) has the same pseudo-spin rotation symmetry as in Eq. (1).

$n_{ij}^{1,2}$ describe the phase fluctuations of the $d$-wave order parameter. $n_{ij}^3$ describe a new kind of fluctuation. To have a better understanding about the $n_{ij}^3$ fluctuations, let us rewrite Eq. (5) in terms of the electron $c_i$ operators:

$$H = \sum_{\langle ij \rangle} \left( c_{i\alpha}^\dagger (t_{ij} - i(-)^i \Delta_{ij}^d n_{ij}^3) c_{j\alpha} + \text{h.c.} \right)$$

$$+ \left( c_{i\alpha}^\dagger \Delta_{ij}^d (n_{ij}^2 + i n_{ij}^1) \epsilon_{\alpha\beta} c_{j\beta}^\dagger + \text{h.c.} \right) + \sum_{\langle ij \rangle} \left( \frac{1}{2g}(n_{ij})^2 \right).$$  

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It is clear that the \( n_{ij}^3 \) fluctuations correspond to staggered flux fluctuations.

To understand the dynamics of \( n_{ij} \), we also need to know its temporal part which is generated from the coupling to the fermions. Since \( n_{ij}^{1,2} \) carry electric charge \( \pm 2e \), the temporal part has the following form as required by the electromagnetic gauge invariance and the pseudo-spin symmetry:

\[
L_b = \sum_{\langle ij \rangle} \frac{a^2}{16\chi} \left[ (\delta_{ab} \partial_t + 2eA_0 T_{ab}) n_{ij}^b \right] (\delta_{ab} \partial_t + 2eA_0 T_{ab}^f) n_{ij}^f \tag{7}
\]

where \( T = \begin{pmatrix} i\sigma_2 & 0 \\ 0 & 0 \end{pmatrix} \), \( a \) is the lattice constant, and \( \chi \) is the compressibility identified from the coefficient of \((eA_0)^2\), \( eA_0 \) being the chemical potential. The compressibility can be obtained by integrating out the electron degree of freedom and is given by the integral

\[
\frac{a^2}{16\chi} = \frac{a^2}{2\pi} \int d^2k \frac{\Delta_k^2}{(\epsilon_k^2 + \Delta_k^2)^{\frac{3}{2}}} \tag{8}
\]

The next task is to obtain the effective theory for the QDdW phase of Eq. (5). One way to obtain the effective theory is to set \( n_i = 0 \) in Eq. (5) since \( \langle n_i \rangle = 0 \) in the disordered phase. However the effective theory obtained this way is not a good description of the disordered phase in our mind. The disordered phase that we considered has the following picture. The vector \( n_i \) varies slowly in space and time. Thus locally \( n_i \) can be treated as a constant vector which gives rise to a finite spin gap in fermionic quasi-particles spectrum even in the disordered state. Thus it is better to do an expansion in the power of \( \partial n \) instead of in the power of \( n \). The new expansion can be achieved through a “local rotation”, which makes the \( \partial n \) dependence explicit. This “local rotation” has been used to study the disordered phase of the antiferromagnetic state. [6]

The local rotation can be realized in the following way. We first parameterize \( n_{ij} \) in Eq. (5) as \( n_{ij} = \frac{1}{2} (n_i + n_j) \). (This parameterization ignore some short wavelength fluctuations.) Note that in long wavelength approximation, \( n_i \) and \( n_j \) point to approximately the same direction as \( n_{ij} \), since they are nearest neighbors, therefore the \( n_{ij} \) thus constructed can still be treated as a vector of unit length. Next we apply a local rotation at each site \( i \)
such that \( n'_i \)'s are all rotated to the \( z \)-direction. This is done by introducing two new fields \( z_i \) and \( \psi_i \) [6]:

\[
n_i = z_i^\dagger \sigma z_i, \quad z_i^\dagger z_i = 1
\]

\[
\lambda_i = U_i \psi_i
\]

where \( U_i = \begin{pmatrix} z_{i1} & -z_{i2}^* \\ z_{i2} & z_{i1}^* \end{pmatrix} \), and \( n_i \cdot U_i^\dagger \sigma U_i = \sigma_3 \).

Now we can rewrite \( n_{ij} \cdot \lambda_i^\dagger \sigma \lambda_j = \frac{1}{2} \psi_i^\dagger \{ \sigma_3, U_i^\dagger U_j \} \psi_j \). Even when \( n_i \) is very close to \( n_j \), \( z_i \) and \( z_j \) can still differ by a finite \( U(1) \) phase. Thus, to the lowest order approximation, the main difference between \( z_i \) and \( z_j \) is the \( U(1) \) phase. Define

\[
a_0^i = -iz_i^\dagger \partial_t z_i
\]

and

\[
\psi_i^\dagger \{ \partial_t - ia_0 \sigma_3 \} \psi_i
\]

Next we look at the boson part

\[
L_b = -\frac{1}{2g} (n_{ij})^2 = -\frac{1}{2g} (1 + n_i \cdot n_j)
\]

where \( n_i \cdot n_j \) can be rewritten in terms of \( z_i \) as

\[
n_i \cdot n_j \simeq 2 \left( z_i^\dagger e^{-ia_{ij}} z_j + c.c. \right) - 1
\]

Although \( L_b \) does not contain it, a temporal term for \( z_i \) can be generated by integrate out the fermions. Eq. (10) and Eq. (11) define a \( CP^1 \) model (coupled to fermions) on the lattice. Using the standard approach to the disordered phase of \( CP^1 \) model [7], we obtain the following effective Lagrangian (for the QDdW phase)

\[
L_{eff} = \sum_i i\psi_i^\dagger (\partial_t + ia_0 \sigma_3) \psi_i
\]

\[
-\sum_{\langle ij \rangle} \left( \psi_i^\dagger \left( t_{ij} - i \left( -\right)^i \Delta_d \sigma_3 \right) e^{ia_{ij} \sigma_3} \psi_j + c.c. \right)
\]

\[
+ \sum_i \frac{1}{g'} \left( \left( (\partial_t - ia_0 - ieA_0 \sigma_3) z_i \right)^2 - \Delta_c^2 z_i^\dagger z_i \right)
\]

\[
- \frac{2}{g} \sum_{\langle ij \rangle} \left( z_i^\dagger (e^{-ia_{ij}} - \frac{1}{2} A_{ij} \sigma_3 - \delta_{ij}) z_j + h.c. \right) + ... \]

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where $1/g' = a^2/2\chi$, and the $z_i^\dagger z_i$ term serves as the Lagrange multiplier which frees the $z_i$ field from the $z_i^\dagger z_i = 1$ constraint, it is also this term that gives the charge gap $\Delta_c$ in our effective theory. The $|(\partial_t - ia_0 - ieA_0\sigma_3)z_i|^2$ term comes from the $(\partial_t n_{ij})^2$ term in Eq. (7). The above low energy effective Lagrangian for the QDdW phase is the main result of this paper.

From the definition of $z_i$ and $\psi_i$ in Eq. (9), we note that $z_i$ carries pseudo-spin 1/2, and $\psi_i$ carries pseudo-spin zero. For the spin and the charge, $z_i$ carries spin zero and charge $-e$ (or $e$), while $\psi_i$ carries spin 1/2 (with $S_z = +1/2$) and charge zero. We see that $\psi_i$ and $z_i$ are very much like the spinon and the holon in the $SU(2)$ slave-boson theory.

Also, our theory is originally expressed in terms of physical variables $n_i$ and $\lambda_i$. Rewriting the theory in terms of $\psi_i$ and $z_i$ introduces unphysical degree of freedom. The theory is invariant under the local transformations

$$z_i \rightarrow e^{-i\theta_i(t)}z_i, \quad \psi_i \rightarrow e^{i\theta_i(t)\sigma_3}\psi_i$$

because $n_i$ and $\lambda_i$ are invariant under those transformations. Thus it is not surprising to see that the effective theory $L_{eff}$ is a $U(1)$ gauge theory, and is invariant under the gauge transformation Eq. (14) and

$$a_{ij} \rightarrow a_{ij} + \theta_i - \theta_j, \quad a_{0i} \rightarrow a_{0i} - \partial_t \theta_i$$

It is also clear that the gauge field $a_\mu$ carries no spin, charge and pseudo-spin quantum numbers.

We would like to discuss the above effective Lagrangian in more detail.

**A)** The term $\sum_i iz_i^\dagger(\partial_t + ia_0 - ieA_0\sigma_3)z_i$ cannot appear in the effective Lagrangian. Note that our theory Eq. (13) is invariant under a 90° rotation followed by $n_{ij} \rightarrow -n_{ij}$ (or $n_i \rightarrow -n_i$) transformation. (Note $\Delta_{ij}$ changes sign under the 90° rotation.) Thus the effective theory Eq. (13) should be invariant under a 90° rotation followed by $z_i \rightarrow i\sigma_2 z_i^\dagger$ transformation. The linear time derivative term $\sum_i iz_i^\dagger \partial_t z_i$ changes sign under the above transformation and cannot appear in the $L_{eff}$. 

B) The effective Lagrangian Eq. (13) is invariant under the $SU(2)$ spin rotation $W$:

$$
\begin{pmatrix}
\lambda_{1i} \\
(-)^i \lambda_{2i}^\dagger
\end{pmatrix} \rightarrow W \begin{pmatrix}
\lambda_{1i} \\
(-)^i \lambda_{2i}^\dagger
\end{pmatrix}
$$

(16)

moreover, when $A_\mu = 0$, it is also invariant under the $SU(2)$ pseudo-spin rotation:

$$z_i \rightarrow U z_i$$

(17)

Under the pseudo-spin rotation, $A_\mu$ transform as a component of a pseudo-spin vector. Thus $A_\mu$ only couple to operators with pseudo-spin quantum number $(\tilde{S}, \tilde{S}_z) = (1, 0)$. This result has an important consequence. The ground state of the quantum disorder phase is a pseudo-spin singlet. Since $\psi$ is a pseudo-spin singlet, all the pseudo-spin 1 states have finite energy gaps. The electromagnetic field $A_\mu$ only connect the ground state to pseudo-spin 1 excited states. Thus the conductivity $\sigma(\omega)$ is zero when $\omega$ is less the energy gap for the pseudo-spin 1 excitations which is finite. Hence the quantum disorder phase is an insulator with finite charge gap. The value of the charge gap is given by $\Delta_c$ in $L_{\text{eff}}$. The argument should still hold even if some small pseudo-spin breaking terms are introduced.

C) The $L_{\text{eff}}$ in Eq. (13) is very similar to the effective Lagrangian of the $SU(2)$ slave-boson theory in the sF(staggered flux) phase. They both contain spinons and holons. In the sF phase, the $SU(2)$ gauge field in the $SU(2)$ slave-boson theory break down to a $U(1)$ gauge field which is just the $U(1)$ gauge field in $L_{\text{eff}}$. Also, both the $SU(2)$ slave-boson theory and the $L_{\text{eff}}$ contain two kinds of holons. It is very satisfying to see that the $SU(2)$ slave-boson theory derived in the limit charge-gap $> \text{spin-gap}$ smoothly connects to our effective theory $L_{\text{eff}}$ derived in the limit charge-gap $< \text{spin-gap}$.

We would like to stress that the above results can be valid even without the exact $SU(2)$ pseudo-spin symmetry. For example the term $\sum_{ij}(n_i - 1)(n_j - 1)V_{ij} = 4 \sum_{ij} \tilde{S}_{iz}\tilde{S}_{jz}V_{ij}$ breaks the $SU(2)$ pseudo-spin symmetry (Here $n_i$ is the particle number operator). However, the term is invariant under the particle-hole transformation which is realized by the $180^\circ$ pseudo-spin rotation around the $x$-axis. The gauge potential $A_\mu$ is odd and $\psi$ is even under such a transformation. Thus we can use the same symmetry arguments as done earlier,
but this time employing particle-hole symmetry instead of pseudo-spin symmetry, to show that $\sigma(\omega) = 0$ for small $\omega$ at half filling. One can also show that $\sigma(\omega) = 0$ even for non-zero chemical potential, as long as the ground state remains to be the half filled state. Although it breaks the particle-hole symmetry, the chemical potential term commutes with the Hamiltonian and cannot change any matrix elements. Hence the chemical potential term cannot change $\sigma(\omega)$ as long as the ground state is not changed.

Now let us consider the situations with finite doping. First we note that a finite hole density can be generated only when the chemical potential is larger than the gap: $|eA_0| > \Delta_c$. Second, when $|eA_0| \sim \Delta_c$, the $z_i$ field has a low frequency solution which represent the low energy excitations. Let us assume $eA_0 \sim \Delta_c$ and replace $eA_0$ by $\Delta_c + eA_0$ (now $A_0$ is small). Expanding the temporal term $|\partial_t - ia0 - i(\Delta_c + eA_0)\sigma_3)z_i|^2 - \Delta_c^2 z_i^\dagger z_i$, we get

$$2i\Delta_c z_i^\dagger \sigma_3(\partial_t - ia0 - ieA_0\sigma_3)z_i$$

after dropping the $|\partial_t - ia0)^2$ and $A_0^2$ term which are small as far as the low energy excitations are concerned. Now the effective Lagrangian Eq. (13) can be rewritten as

$$L_{eff} = \sum_i i\psi_i^\dagger (\partial_t + ia0\sigma_3)\psi_i - \sum_{ij} \left( \psi_i^\dagger (t_{ij} - i\Delta_{ij} \sigma_3(-)^{ij})e^{ia_{ij}\sigma_3} \psi_j + h.c. \right)$$

$$+ \sum_i \left( \frac{i}{g} \Delta_c z_i^\dagger \sigma_3(\partial_t - ia0 - ieA_0\sigma_3)z_i \right)$$

$$- \frac{2}{g} \sum_{ij} \left( z_i^\dagger (e^{-ia_{ij} - i\epsilon_A_{ij}\sigma_3} - \delta_{ij})z_j + h.c. \right) + ... \quad (18)$$

which can be regarded as the effective theory for finite doping. We see that $z$ now behaves as an ordinary (non-relativistic) boson field. A finite density of $z$ can lead to a boson condensation which gives us the $d$-wave superconducting state. The form and the physics of Eq. (13) are identical to that of the $SU(2)$ slave-boson theory at low energies. Many results for the $SU(2)$ slave-boson theory [48] also apply to our effective theory here. In particular, our effective theory (Eq. (13), Eq. (18)) explains the Mott insulating behavior at half filling, as well as the spin gap, low superfluid density, and the positive charge carriers above $T_c$ for underdoped samples. It is highly non-trivial to recover the above properties within a single
consistent theory.

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