Theory of Quasi-Particles in the Underdoped High $T_c$ Superconducting State

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The microscopic theory of superconducting (SC) state in the $SU(2)$ slave-boson model is developed. We show how the pseudogap and Fermi surface (FS) segments in the normal state develop into a $d$-wave gap in the superconducting state. Even though the superfluid density is of order $x$ (the doping concentration), the physical properties of the low lying quasiparticles are found to resemble those in BCS theory. Thus the microscopic theory lay the foundation for our earlier phenomenological discussion of the unusual SC properties in the underdoped cuprates.

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It has become clear in the past several years that the underdoped cuprates show many highly unusual properties compared to conventional metals/superconductors, both in the normal and SC states. The most striking of all are the pseudo spin-gap in the normal state and the low superfluid density (of order $x$). The photoemission experiments reveal that the pseudogap is of the same size and $k$ dependence as the $d$-wave SC gap. Furthermore, the pseudogap is essentially independent of doping and the SC transition temperature $T_c$ (which is proportional to $x$) can be much less then the pseudogap in the low doping limit. A phenomenological model was developed to described the above unusual SC properties.

The model is based on two basic assumptions: A) the superfluid density is given by $x$ and $k$ dependence as the $d$-wave SC gap. B) the quasiparticle (qp) dispersion in presence of an external electromagnetic gauge potential has a BCS form:

$$E^{(sc)}_A(k) = \pm \sqrt{\varepsilon^2(k) + \Delta^2(k)} - \frac{A}{c} \cdot j(k)$$

where $j(k)$ is the current carried by the “normal state qp” with momentum $k$. In ref. $\text{[2]}$ $j$ is assumed to be $-ev_F = -e\partial_k \varepsilon$. With these assumptions the model successfully explains the observations that linear temperature dependence of the superfluid density is independent of $x$ and that $T_c \approx x \Delta_0$, a strong violation of the BCS ratio.

It was recently pointed out that in conventional BCS superconductors developed out of a Fermi liquid, the Fermi liquid correction to the qp current appears, so that in general

$$j(k) = -e\alpha v_F$$

For example, if only a single Fourier component of the Landau parameter $F_1$ is important, $\alpha = 1 + F_1/3$, but more complicated anisotropic Landau parameters are generally possible. With the more general assumption $\text{Eq. (2)}$, the phenomenological model now predicts that

$$\rho_s(T) = \frac{x}{ma^2} - \frac{2\ln 2}{\pi} \alpha^2 \left( \frac{v_F}{v_2} \right)^3$$

where $v_2$ is the velocity of the $d$-wave SC qp in the direction perpendicular to $v_F$. We have seen that in order to agree with experiments, $\alpha$ near the nodes is either exactly unity or close to it, and must be independent of $x$. On the other hand, if one attempts to describe the normal state of underdoped cuprates by Fermi liquid theory, one faces the dilemma that the area of the Fermi surface is $1 - x$ while the spectral weight of the Drude peak (which develops into the superfluid density in the SC state) is proportional to $x$. In Fermi liquid theory this can be accommodated by assuming $1 + F_1/3 = x$. From Eq. (3) we see that within this scenario, the $T$ dependence of $\rho_s$ is too small by a factor of $\alpha^2 = x^2$. Thus a proper microscopic theory must explain in a natural way why the spectral weight is $x$ while $\alpha \approx 1$. We believe this requirement is a central issue in the high $T_c$ problem, and lies at the heart of the debate of spin-charge separation $\text{[2]}$ vs Fermi liquid theory in the normal state.

In this paper we show that this requirement is satisfied by the $SU(2)$ slave-boson theory. $\text{[2]}$ The slave-boson theory was developed to satisfy the constraint of no double occupation in the $t$-$J$ model. The electron is decomposed into a fermion and a boson and naturally incorporates the physics of spin-charge separation in the normal state. The charge is carried by the bosons so that assumption A is automatic. The difficulty is that at the mean field (MF) level, the SC state is described by the condensation of slave bosons and the SC qp dispersion is given by the fermion dispersion. Since $A$ couples directly only to the bosons, the shift in the qp spectrum is reduced and in Eq. (2), $\alpha$ is less than one. In fact, in the traditional $U(1)$ formulation, $\alpha = x$ and this theory faces the same difficulty as Fermi liquid theory.

We recently introduced a new formulation of the slave-boson theory, the $SU(2)$ theory $\text{[2]}$, which incorporates an $SU(2)$ symmetry that is known to be important at half-filling. In that case a fermion doublet $\psi^T = (\psi^\uparrow, \psi^\downarrow)$ was introduced because in the projected subspace, both $\psi^\uparrow$ and $\psi^\downarrow$ represent the removal of an up-spin. We extended this symmetry to finite $x$ by introducing a boson...
SU(2) doublet $b^T = (b_1, b_2)$. The spin-up and spin-down electron operators are given by the SU(2) singlets $c_\uparrow(i) = \frac{1}{\sqrt{2}} b^\dagger(i) \psi(i)$, $c_\downarrow(i) = \frac{1}{\sqrt{2}} b^\dagger(i) \psi(i)$ where $\psi = i r^2 \psi^*$. The advantage of this formulation is that near half-filling, low lying fluctuations which were ignored in the $U(1)$ formulation are included at the MF level. Furthermore, we found that if we go beyond MF theory and include an attraction between the fermions and bosons, the electron spectral function contains qp-like peaks which exhibit a gap near $(0, \pi)$ but appear gapless in a finite region near $(\frac{\pi}{2}, \frac{\pi}{2})$, leaving what we may term a FS segment. These features are in qualitative agreement with the photoemission experiments. It is then natural for us to extend the same treatment to the SC state, and see how the FS segment evolves into $d$-wave SC qp. Then we can study the coupling of these qp to $A$ in order to justify assumption B and determine whether $\alpha = 1$.

The SU(2) slave-boson model is described by the following effective theory at MF level (for details see Ref. [8]):

$$H_{\text{mean}} = H^f_{\text{mean}} + H^b_{\text{mean}}$$

where

$$H^f_{\text{mean}} = J' \sum_{<ij>} (\psi_i^\dagger U_{ij} \psi_j + \text{c.c.}) + \sum_i \psi_i^\dagger a_0(i) \tau^i \psi_i$$

$$H^b_{\text{mean}} = t' \sum_{<ij>} (b_i^\dagger U_{ij} b_j + \text{c.c.}) + \sum_i b_i^\dagger a_0(i) \tau^i b_i$$

where $J' = \frac{3J}{2}$, $t' = \frac{t}{2}$. The fields $\psi^T = (\psi_\uparrow, \psi_\downarrow)$ and $b^T = (b_1, b_2)$ are SU(2) doublets. The MF $d$-wave SC state at $T = 0$ is described by the following ansatz: $U_{\uparrow+\uparrow} = -\sqrt{\tau^3 - \eta^3}$, $U_{\downarrow+\uparrow} = -\sqrt{\tau^3 + \eta^3}$ and $a_0(3)(i) = a_0$, $a_0^{(1,2)}(i) = 0$, $\langle b^0(i) \rangle = (\sqrt{\tau}, 0)$. At higher temperatures ($T > T_c$), boson condensation disappears, $\langle b(i) \rangle = 0$ and $a_0(3)(i) = 0$; the above ansatz describes a normal metallic state with a pseudogap.

The analysis in Ref. [8] indicates that the SU(2) theory contains a soft mode which correspond to rotation from $b_1$ into $b_2$. Such a soft mode was overlooked in the $U(1)$ theory. With the hard core repulsion between the bosons, one can show that the magnitude of quantum fluctuations of bosons is comparable with the magnitude of the condensation. Thus the quantum fluctuations have a potential to completely destroy the boson condensation, or at least they will reduce the the boson condensation by a finite fraction. This leads us to consider two scenarios:

1. Single boson condensation (SBC) where $\langle b_1 \rangle = \sqrt{x_c} < \sqrt{\pi}$, $\langle b_2 \rangle = 0$ and a factor $x - x_c$ of bosons remain incoherent and separated from the condensate by an energy gap $\Delta_b$ due to the Higgs mechanism.

2. Boson pair condensation (BPC) where $\langle b_\alpha \rangle = 0$ but $\langle b_\alpha(i)b_\beta(j) \rangle \neq 0$. We note that BPC is sufficient to generate electron pair condensation $(c_\uparrow(i)c_\downarrow(j)) \neq 0$. The boson pairing will also generate an energy gap $\Delta_{bp}$.

We defer a discussion of the motivation and more detailed formulation of the BPC state, but remark at the point that we do not know a priori whether SBC or BPC is favored. Of course neither $b$ nor $\langle bb \rangle$ is gauge invariant and the only real distinction between these scenarios lies in their experimental consequences. In particular, we will show that BPC implies $\alpha = 1$ while SBC implies $\alpha < 1$.

The MF electron propagator is given by the product of the boson and the fermion propagator:

$$G_0(\omega, k) = i \int \frac{d\nu}{(2\pi)^3} G^b(\nu - \omega, q - k) G^f(\nu, q)$$

where $iG^f = \langle \psi \psi^\dagger \rangle$ and $iG^b = \langle bb \rangle$ are $2 \times 2$ matrices. In the normal state, the boson propagator for finite $A$ satisfies $G^b_A(\omega, k) = G^b(\omega, k - \frac{\pi}{2} A)$. Thus the MF electron propagator also shift with $A$ as expected: $G_0, A(\omega, k) = G_0(\omega, k + \frac{\pi}{2} A)$. This is a consequence of the gauge symmetry. However, in the SC state, the bosons may condense according to scenario 1 and the boson propagator contains two terms. The first term, coming from SBC does not shift with $A$. This is because as we continuously turn on a constant $A$, $b$ has to satisfy periodic boundary condition in a box and cannot be changed (unless we want to create a vortex). On the other hand, the second term, coming from non-condensed bosons, shifts with $A$, since the boson dispersion shifts with $A$. Thus for finite $A$, the boson propagator is given by $G^b_A(\omega, k) = -i(b) \langle bb \rangle \delta(\omega, k) + G^b_{in}(\omega, k - \frac{\pi}{2} A)$. Now it is clear that, in the SC state, the poles in the MF electron propagator, coming from the product of the fermion propagator and the first term of the boson propagator, do not shift with $A$. (In RPA, the generation of the fictitious gauge field $a$ by a finite $A$ shifts the fermion dispersion by $\frac{\pi}{2} A$ where $\alpha = x$ as discussed earlier.)

To obtain Eq. (1) we have to go beyond the MF theory. First we assume that not all bosons condense: $\langle b_\alpha(i) \rangle = \sqrt{x_c}$ with $x_c$ less then the total boson density $x$. The non-condensed bosons have small energies and momenta near $k = (0, 0)$, $(\pi, \pi)$, the two bottoms of the boson band. We ignore the gap $\Delta_b$ for simplicity and model $G^b_{in}$ by peaks of finite width near $\omega = 0$ and $k = (0, 0)$, $(\pi, \pi)$. With those assumption, one can show that the MF electron propagator can be approximated by

$$G_0, A(\omega, k) \approx x_c \left[ \frac{(u^f(k))^2}{\omega - E(k) - i0^+} + \frac{(v^f(k))^2}{\omega + E(k) - i0^+} \right] + \frac{x - x_c}{2} \left[ \frac{(u^f(k + \frac{\pi}{2} A))^2}{\omega - E(k + \frac{\pi}{2} A) - i1} + \frac{(v^f(k + \frac{\pi}{2} A))^2}{\omega + E(k + \frac{\pi}{2} A) - i1} \right] + G_{in}(\omega, k + \frac{e}{c} A)$$

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where $E = \sqrt{(\varepsilon f)^2 + (\Delta f)^2}$, $\varepsilon f = -2J'\chi (\cos k_x + \cos k_y) + g_{(3)}^0$, $\Delta f = -2J'y (\cos k_x - \cos k_y)$, $u f = \frac{\alpha}{2\sqrt{2}\Delta} \sqrt{1 + \frac{\varepsilon f}{\Delta f}}$, and $v f = \frac{\alpha}{2\sqrt{2}\Delta} \sqrt{1 - \frac{\varepsilon f}{\Delta f}}$. The first term in $G_{0,A}$ comes from the SBC and does not shift with $A$. The second term comes from the peak in $\text{Im}G_{\text{in}}^b$ which shifts with $A$. The decay rate $\Gamma$ comes from the finite peak width of $\text{Im}G_{\text{in}}^b$ in both $\omega$ and $k$ direction. The last term is the incoherent part.

When there is BPC, the electron will have a non-vanishing off-diagonal propagator. In scenario 1 SBC automatically generates BPC $\langle b_{a}(i) b_{b}(j) \rangle = x_c \delta_{a1} \delta_{b3}$. This yields an off-diagonal electron propagator $-i(c_{\uparrow}c_{\downarrow})$:

$$F_{0,A} \simeq \frac{x_{pc} u f v f}{2} \left[ \frac{1}{\omega - E - i\Gamma_b} - \frac{1}{\omega + E - i\Gamma_b} \right] (7)$$

where $x_{pc} = x_c$ and $\Gamma_b \rightarrow 0^+$. More generally, with or without SBC, the bosons can form pairs with size $l_b$. We shall show later that, in scenario 1, the BPC is characterized by $\langle b_{a}(i) b_{b}(j) \rangle = \frac{x_c}{2} f(x - j)(\delta_{a1} \delta_{b3} + (-1)^{x-j} \delta_{a3} \delta_{b1})$. Despite a different form of BPC, the off-diagonal electron propagator still takes the same form Eq. (7) with $\Gamma_b \sim \frac{x_c}{l_b}$, as long as $l_b$ is much larger than the lattice spacing. Note that $F_{0,A}(\omega, k)$ does not depend on $A$, since the BPC $\langle bhf \rangle$ cannot depend on $A$.

A second ingredient in going beyond MF theory is to calculate the electron propagator through a ladder diagram to include effects of pairing between the boson and the fermion caused by the $SU(2)$ gauge fluctuations. The gauge fluctuations induce the following effective interaction $\frac{1}{2} V \psi^d \bar{\psi} b \bar{b} = V c^\dagger c - V \frac{1}{2} \psi^d \bar{\psi} b \bar{b}$ with $V > 0$. Here we will only use the first term $V(c^\dagger c + c^\dagger c)$ because an analytic calculation is possible. The more general interaction will not modify our results qualitatively. The resulting electron propagator is given by

$$G_A(\omega, k) = \left[ \begin{array}{cc} -i(c^\dagger c^\dagger) & -i(c^\dagger c) \\ -i(c c^\dagger) & -i(c^\dagger c) \end{array} \right] = \left[ \begin{array}{cc} G_{0,A}(\omega, k) & F_{0,A}(\omega, k) \\ F_{0,A}(\omega, k) & -G_{0,A}(-\omega, -k) \end{array} \right]^{-1} - Vf^3 \right]^{-1} (8)$$

Let us assume for simplicity $\Gamma = \Gamma_b = 0^+$. We first consider scenario 3 where there are no SBC, $x_c = 0$. For $A = 0$, the poles of $G_{11}(\omega k)$ come in pairs of opposite signs, just as in BCS theory. However the total residue is $\frac{2\alpha}{\sqrt{(\omega + \Delta)^2}}$, significantly reduced from the BCS value. There are two positive branches which determine the qp excitations

$$E_{\pm}^{(sc)}(k) = \sqrt{\tilde{E}_{\mp}^2 + \left( \frac{x_{pc}\Delta}{x} \right)^2} (9)$$

where

$$\tilde{E}_{\pm} = \pm \sqrt{(\varepsilon - \hat{\mu})^2 + \Delta^2 - \left( \frac{x_{pc}\Delta}{x} \right)^2} - \hat{\mu} (10)$$

and $\hat{\mu} = -\frac{2V}{(1 - s \Gamma_b)}$. In order to interpret those results, let us first consider the normal state which is recovered by setting $x_{pc} = 0$ in Eq. (10) and Eq. (10), yielding the normal state dispersion $E_{\pm}^N = \tilde{E}_{\pm}(x_{pc} = 0)$. This corresponds to a massless Dirac cone initially centered at $(\pm \pi/2, \pm \pi/2)$ when $V = 0$ which is the MF fermion spectrum of the staggered-Flux (s-Flux) phase. The effect of $V$ (the boson-fermion pairing) is two-fold. The $\tilde{\mu}$ inside the square-root shift the location of the node towards $(0, 0)$ by a distance $\Delta k = -\tilde{\mu}/v_F$ while the last term shift the spectrum upwards. The cone intersects the Fermi energy to form a small Fermi pocket with linear dimension of order $x$. As shown in Fig. 1a, the spectral weight is concentrated on one side of the cone, so that only a segment of FS on the side close to the origin carries substantial weight. This is the origin of the notion of “FS segment” introduced in Ref. [33].

![Fig. 1. Schematic illustration of the qp dispersion (the pole locations of $G$) for (a) normal state, and SC state with (b) $0 < x_{pc} < x$ and (c) $x_{pc} = x$. The line thickness indicates the size of residue of $G_{11}$, and dash line indicates vanishing residue. The momentum scan is along the straight line in (d) where the curved segment is the FS segment in the normal state.](https://example.com/fig1.png)

Now let us see what happens in the SC state when $x_{pc} \neq 0$. Eq. (10) takes the standard BCS form if $\tilde{E}_{\pm}$ is interpreted as the normal state dispersion. However, $\tilde{E}_{\pm}$ differs from the normal state spectrum $E_{\pm}^N$ by the appearance of the term $-x_{pc}\Delta/x^2$ in Eq. (10). Close to the node this term is small so that qualitatively the spectrum develops from the normal state in a BCS fashion, as shown in Fig. 1b. This is particularly true if the higher energy gap between the two branches is smeared by lifetime effects. Thus we see that the “FS segment” is gapped in a BCS-like fashion. However, the velocity $v_2$ in the $(1, -1)$ direction, being proportional to $x_{pc}/x$, does not extrapolate to the gap at $(0, \pi)$ (which is essentially independent of $x_{pc}$), but cross-over to it at the edge of the FS segment. It is worth remarking that in the special case $x_{pc} = x$, $E_{\pm}^{(sc)}$ reduces to the standard BCS form with the normal state dispersion $\varepsilon(k)$, a chemical potential $2\tilde{\mu}$ and a SC gap $\Delta(k)$. The high energy gap closes and spectral weight on one branch vanishes, yielding a BCS spectrum as shown in Fig. 1c. It is easy to see that Eq. (10) is proportional to the BCS Green function in this special case.
We have also calculated the effect of constant $A$ on the qp dispersion, to linear order of $A$. This adds a term $\frac{i}{2} j_{\pm} \cdot A$ to Eq. (1) where $j_{\pm}$ is interpreted as the current carried by the qp. We recall that in standard BCS theory, the current is given in terms of the normal state spectrum by $\varepsilon A = \varepsilon \partial E$ because $A = \varepsilon(k + \frac{i}{2} A)$. Remarkably this is almost true in our case in the sense that $j_{\pm}$ is given by $\varepsilon A \partial E_{\pm} A$, where $\partial E_{\pm} A$ is obtained by replacing $k$ by $k + \frac{i}{2} A$ in $\varepsilon$, $\mu$ and $\Delta$ everywhere in Eq. (10) except for the term $(\frac{i}{2} \sqrt{\Delta})^2$, which is kept independent of $A$. Near the node, $\Delta$ is negligible so that the current is very close to $\varepsilon \partial E \simeq \varepsilon \partial E_N$ (which becomes exactly $\varepsilon \partial E$ along the diagonal), thus reproducing Eq. (1). We have checked numerically that even away from the node in the region of the “FS segment”, the current is remarkably close to $\varepsilon \partial E_N$, which can be quite different from the BCS value $\varepsilon \partial E$ near the edge of the FS segment.

Next we briefly comment on what happens under scenario 1. The main difference is that the current carried by qp is no longer equal to $ev_F$, but reduce from it depending on $x_c$. It is clear that in the extreme case of $x - x_c = G_{\alpha A} = 0$, $G_{\alpha A}$ and $F_{\alpha A}$, and hence $G_A$ do not depend on $A$, so that $j = 0$. As $x_c$ varies from $x_c$ to $x$, $\alpha$ interpolates between 0 and 1. (Note $v_F$ is defined as the normal state Fermi velocity in the $(1,1)$ direction, $v_F = \partial E_N$. It is also exactly equal to the qp velocity in the $(1,1)$ direction at the SC nodes.) Due to strong quantum fluctuations of bosons, $x - x_c$ is of order $x$ and hence $\alpha$ is order unity. The main question is whether $\alpha$ is exactly 1. According to our model, whether $\alpha = 1$ depends on whether there is a SBC. Thus it is very interesting and important to determine $\alpha$ experimentally.

From Eq. (3), the temperature dependence of the London penetration depth gives a direct measurement of $\alpha^2 \frac{\partial \Delta}{\partial T}$. Density of states measurements using the $T^2$ coefficient of the specific heat yields $v_F v_2$. The Fermi velocity can be estimated from transport measurements or high resolution photoemission experiment. Thus in principle the quantities $\alpha$, $v_F$ and $v_2$ can be measured. It is of course of great interest to establish how close $\alpha$ is to 1, or whether $v_2$ is reduced with respect to that extrapolated from the energy gap at $(0, \pi)$ measured by photoemission or tunneling.

We may regard $\alpha = 1$ as a signature of spin-charge recombination, ie the boson and fermion binds (through the ladder diagram) into an electron which responds fully to A. We have so far focussed our discussion to low energy excitations near the nodes. At higher energy away from the Fermi surface, the binding may become unimportant and the electron spectrum is given by the convolution of the fermion and boson spectrum. In the BPC state, an energy gap $\Delta_{bp}$ arises in the boson spectrum, which should lead to a shift of the electron spectral function in the SC state relative to the normal state by the energy $\Delta_{bp}$ towards higher binding energy.

Finally we comment on finite temperature behaviors. In addition to the reduction of superfluid density due to thermal excitation of qp, $\Delta_{bp}$ we expect $x_{pc}$ to decrease with increasing $T$, leading to a reduction of $v_2$: $v_2(T) = \frac{x_{pc}(T)}{x_{pc}(0)} v_2(0)$. As $T$ reaches $T_c$, $x_{pc} = v_2 = 0$ and the nodes of $E^{sc}$ become the “FS segment” while the spin gap near $(0, \pi)$ remain finite. We see that $x_{pc}$ plays the role of the order parameter of the transition, so that the temperature dependence of $x_{pc}$ is described by a Ginzburg-Landau theory near the transition.

We complete our discussion by giving a more microscopic motivation for the notion of BPC. It was pointed out recently that one way of capturing the physics of strong boson fluctuation is to attach flux tube of opposite sign to $b_1$ and $b_2$ (in s-Flux gauge), converting them to fermions. This has the advantage that at the MF level, time reversal symmetry is not broken. In the s-Flux gauge, the massless gauge field is simply a $U(1)$ gauge field which couple to $b_1$ and $b_2$ with opposite gauge charge. This problem was treated by Bonesteel et al [1] who found that there is a instability towards boson pairing with $\langle b_1 b_2 \rangle \neq 0$. Thus it is natural to assume that, in the s-Flux gauge, only $\langle b_1 \rangle = \langle b_2 \rangle$ is non-zero in the BPC. After transformed to the $d$-wave gauge, $\langle \delta b^T \rangle$ becomes the one that we used below Eq. (3). We expect the energy gap $\Delta_{bp}$ to scale with the effective “Fermi” energy, ie $x$.

In summary we develop a theory for quasiparticles in the high $T_c$ superconducting state. Our theory reproduces both small superfluid density $\rho_s \sim x$ and large $\alpha \sim 1$, as required by experiments.

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