Andreev reflections in the pseudogap state of cuprate superconductors

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(March 24, 2022)

We propose that, if the pseudogap state in the cuprate superconductors can be described in terms of the phase-incoherent preformed pairs, there should exist Andreev reflection from these pairs even above the superconducting transition temperature, $T_c$. After giving qualitative arguments for this effect, we present more quantitative calculations based on the Bogoliubov–de Gennes equation. Experimental observations of the effects of Andreev reflections above $T_c$—such as an enhanced tunneling conductance below the gap along the copper oxide plane—could provide unambiguous evidence for the preformed pairs in the pseudogap state.

Underdoped to slightly overdoped cuprate superconductors exhibit a progressive transfer, as the temperature is lowered, of the low-energy spectral weight to the higher energy region in both the spin and charge channels \[\text{[1,2]}.\] The resulting “pseudogap” begins to appear at a crossover temperature $T^*$, well above the superconducting transition temperature, $T_c$, and the nature of this pseudogap state has been the focus of considerable recent interest. Many proposals have been presented to explain this phenomenon, including various forms of electron pairing \[\text{[3–5]},\] antiferromagnetic fluctuations \[\text{[6,7]},\] and spin-charge separation scenarios \[\text{[8,9]},\] but no consensus on the origin of the pseudogap has emerged. Among the electron pairing scenarios, the phase-incoherent preformed pair (PIPP), or, normal state pair, scenario suggested by Emery and Kivelson \[\text{[3]},\] seems particularly intriguing, since the amplitude of the pairing order parameter is lowered, of the low-energy spectral weight to the phase coherence and hence superconductivity for $T > T_c$. Several earlier experiments, as well as recent terahertz spectroscopy results \[\text{[10]},\] seem to support the idea of the PIPP, but their existence has not been established \[\text{[11]}\]. In the present paper, we show that a crucial test of the PIPP scenario will be the possible Andreev reflection (AR) \[\text{[12,13]}\] from the pseudogap state: We propose that if the pseudogap state contains PIPP, AR will occur and will produce, among other effects, an enhanced conductance even above $T_c$ that should be readily measurable in tunneling conductance experiments.

Two qualitative intuitive arguments suggest that AR should occur from a state containing PIPP. First, AR (or “retroreflection of a hole”) in a normal metal–superconductor (NS) junction occurs because an electron, which is a well-defined elementary excitation (quasiparticle) in the normal metal, is not an elementary excitation of the superconductor. Therefore, an electron from the normal metal, upon entering the superconductor, has to “reconstruct” itself as a linear combination of the quasiparticles of the superconductor, namely, the Bogoliubovons. This requires an electron of momentum $k$ and spin $\sigma$ to find a time-reversed mate electron of momentum $-k$ and spin $-\sigma$ to form a pair. The hole left behind by the mate electron then retraces the path of the incoming electron, which is the AR. Naively, the same underlying physics should apply to the (assumed) preformed pairs in the pseudogap state, because an electron is not an elementary excitation of that state either, once the pairs are formed, independent of their phase coherence. The second heuristic argument involves the phase stiffness. The superfluid density in the static, long wavelength limit, $\rho_s(T)$, which also determines the superconductor’s phase stiffness, $\Theta(T) = h^2\rho_s(T)/kB$, vanishes for $T > T_c$. In the dynamic Kosterlitz-Thouless-Berezinsky (KTB) theory, $\rho_s(\omega,T) \sim \omega\tau_c/(1 + \omega\tau_c) > 0$ as $\omega$ is increased from 0, where $\tau_c$ is the coherence time \[\text{[14]}\]. Precisely this finite frequency phase stiffness, measured by a terahertz spectroscopy, was recently reported to scale as $\Theta_{KTB} = (8/\pi)T_{KTB}$, in accord with the KTB theory of the classical phase fluctuations \[\text{[15]}\]. $T_{KTB} = T_c$ for two-dimensional (2D) superfluids. Importantly, the superfluid density at a finite wavevector ($\omega = 0$), $\rho_s(q,T)$, does not vanish identically above $T_c$ but is given by $\rho_s(q,T) \sim (q\xi_+)^2$, where $\xi_+$ is the phase correlation length for $T > T_{KTB}$ \[\text{[16]}\]. AR probes the superfluid density at the finite wavevector $q \sim 1/\xi$ because it occurs within the pairing correlation length, $\xi$, around the interface between, say, a NS junction. Hence, AR, being a proximity effect, is not particularly sensitive to the long wavelength physics, which determines $T_c$, and is expected to be present above $T_c$ because $\rho(q,T) \sim (\xi_+/\xi)^2 > 0$ for $T^* > T > T_c$.
To provide more quantitative calculations of these qualitative arguments, we will apply the Bogoliubov-de Gennes (BdG) equation [16] with appropriate boundary conditions [17] to a pseudogap state assumed to be described in terms of the PIPP [3]. As expected, we find that the AR is still present well above $T_c$, and its effects may be observed in tunneling experiments. The tunneling conductance, $G = dI/dV$, as a function of the bias voltage, $V$, measured along the in-plane $\{100\}$ direction of $d$-wave superconductors for a small tunneling barrier exhibits a conductance enhancement (CE) inside the superconducting gap [18,19]. It is enhanced by the factor of 2 in the low $T$ and small tunneling barrier limit with an edge at the pairing amplitude [20]. We will show that, if the pseudogap state can be described in terms of the PIPP, this CE will also be present above, as well as below, $T_c$.

In a paired state, the quasiparticles (Bogoliubovons) can be written in terms of a two-component spinor as

$$
\psi(x) = \begin{pmatrix} f(x) \\ g(x) \end{pmatrix},
$$

where $f(x)$ and $g(x)$ are, respectively, the electron and hole components and obey the BdG equation [14]. Inspection of the BdG equation shows that $\psi(x)$ oscillates on a length scale of $k_F^{-1}$, where $k_F$ is the Fermi wavenumber, so we introduce the transformation

$$
\begin{pmatrix} f(x) \\ g(x) \end{pmatrix} = e^{i k_F \cdot x} \begin{pmatrix} u(x) \\ v(x) \end{pmatrix},
$$

where $u(x)$ and $v(x)$ now vary on a much longer length scale than $k_F^{-1}$. For $k_F \xi \gg 1$ the BdG equation then becomes [21,22]

$$
\begin{align*}
Eu(x) &= -\frac{i}{m} \mathbf{k}_F \cdot \nabla u(x) + \Delta(k_F, x)v(x), \\
Ev(x) &= \frac{i}{m} \mathbf{k}_F \cdot \nabla v(x) + \Delta^*(k_F, x)u(x).
\end{align*}
$$

We write the pairing order parameter as

$$
\Delta(k_F, x) = \Delta_k \exp[i \theta(x)] \Theta(x),
$$

where $\Delta_k = \Delta_d \cos(k_x a) - \cos(k_y a)$, a the lattice constant of a copper oxide plane, and $\Theta(x)$ is the step function. $x = (x, y, z)$ is a 3D vector, where we take $x$ to be normal to the interface and $z$ parallel to the interface and normal to the copper oxide plane. The $x > 0$ and $x < 0$ sides correspond, respectively, the paired and normal states. In the PIPP scenario, the Cooper pairs are formed above $T_c$, but the phase fluctuations of the pairing order parameter destroy phase coherence and hence superconductivity above $T_c$. Such phase fluctuations are taken to be thermal and static as in the previous works [3,22]. Other kinds of phase fluctuations such as quantum or temporal ones were argued to be less important [3,22]. The thermal fluctuations destroying superconductivity above $T_c$ are due to a plasma of unbound vortices and antivortices, and are described by the 2D XY model [10]. Each vortex is surrounded by a circulating supercurrent which is related with the order parameter phase $\theta(x)$ by $\nu_s(x) = \hbar \nabla \theta(x)/(2m)$, where $\nu_s(x)$ is the local superfluid velocity.

Eq. (1) can be solved by taking

$$
\begin{pmatrix} u(x) \\ v(x) \end{pmatrix} = e^{i k_F \cdot x} \begin{pmatrix} u e^{i \theta/2} \\ v e^{-i \theta/2} \end{pmatrix}
$$

to yield a Doppler-shifted local quasiparticle excitation spectrum of

$$
E = k_F \cdot \mathbf{v}_s(x) + \sqrt{(k_F \cdot \mathbf{k}/m)^2 + \Delta_k^2}.
$$

In writing Eq. (3), we have assumed that the phase $\theta(x)$ varies slowly on the scale of a single pair size $\xi$ in the sense that it is meaningful to specify the energy vs. wavevector relation of a quasiparticle at the position $x$. This condition can be written as $k_F \cdot \mathbf{v}_s(x) < \Delta_d$, which is satisfied in the pseudogap state as estimated by Franz and Millis [22], as we will discuss later. The change in the local quasiparticle excitation spectrum of Eq. (3) will affect the spectral properties of the superfluid in that a physical observable must be averaged over the positions of the fluctuating vortices. A similar situation arises, as noted by Volovik [23] in the mixed state of a $d$-wave superconductor where the superflow around the field-induced vortices leads to the residual DOS proportional to $\sqrt{T}$. This contributes $\sim T \sqrt{\xi}$ to the electronic specific heat, and leads to general scaling relations [24]. This suggests that the semiclassical approximation can be justified in the mixed state. In the present case, we consider a plasma of thermally induced vortices instead of a regular Abrikosov lattice of field-induced vortices. The essential physics, however, remains unaltered because we are interested in the $q \sim 1/\xi$ scale physics.

To determine how the AR will affect physical observables, we begin with the current, $I$, which is given by

$$
I = \text{Im} \left[ e \psi^* \nabla \psi \right] = \text{Im} \left[ e \left( f^* \nabla f + g^* \nabla g \right) \right].
$$

To obtain the quasiparticle wavefunctions $\psi$ of a NS junction, we follow Blonder et al. [17] and write

$$
\psi_N(x) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{i k_e \cdot x} + A \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{i k_o \cdot x} + B \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{i \mathbf{k}_e \cdot x}
$$

for the normal metal, where $\mathbf{k}_e = (-k_{ex}, k_{ey}, k_{ez})$, and

$$
\psi_S(x) = C \begin{pmatrix} u_+ e^{i \theta/2} \\ v_+ e^{-i \theta/2} \end{pmatrix} e^{i \mathbf{q}_s \cdot x} + D \begin{pmatrix} u_- e^{i \theta/2} \\ v_- e^{-i \theta/2} \end{pmatrix} e^{i \mathbf{q}_s \cdot x}
$$

for the paired state. Here, $\mathbf{k}_e = (k_F + k)\hat{e}_F$, $k = m E/k_F$, $\mathbf{k}_o = k_F + \mathbf{k}'$, $\mathbf{q}_s = \mathbf{k}_F + \mathbf{q}$, and $\mathbf{q}_h = \mathbf{k}_F + \mathbf{q}'$. When the surface is along the $\{100\}$ direction, one can show from the BdG equation that $u_+ = u_- = u_0$ and $v_+ = v_- = v_0$, where

$$
\begin{align*}
u_0 &= \left[ \frac{E - \eta + \sqrt{(E - \eta)^2 - \Delta_0^2}}{2(E - \eta)} \right]^{1/2}, \\
v_0 &= \left[ \frac{E - \eta - \sqrt{(E - \eta)^2 - \Delta_0^2}}{2(E - \eta)} \right]^{1/2}.
\end{align*}
$$
Here, $\eta = k_F \cdot \mathbf{v}_s$ and $\Delta_\phi = \Delta_d \cos(2\phi)$ because we consider the $\{100\}$ surface, where $\phi = \tan^{-1}(k_{Fy}/k_{Fx})$. The energy dispersion relation of Eq. (3) determines only the components of the momenta along the $k_F$ direction of the incoming electrons such that $\mathbf{q} \cdot k_F/m = -E$, $\mathbf{q} \cdot k_F/m = \sqrt{(E - \eta)^2 - \Delta^2_F}$, and $\mathbf{q} \cdot k_F = -\mathbf{q} \cdot k_F$. The components normal to $k_F$ are determined by the boundary conditions, as can easily be seen.

Applying the boundary conditions at $x = 0$,

$$\psi_N(x = 0) - \psi_S(x = 0) = 0,$$

$$\frac{\partial \psi_N}{\partial x}(x = 0) - \frac{\partial \psi_N}{\partial x}(x = 0) = 2mV_0 \psi_N(x = 0),$$

where $V_0$ is the barrier potential energy at the boundary, we obtain for $\{22\}$ tunneling

$$A = \frac{\cos^2 \theta}{D_0},$$

$$B = \frac{1}{D_0} \left[ (1 - \Gamma^2) \left\{ Z(Z + i \cos \theta + (\bar{\eta}/2)^2 \cos^2 \theta \right\} 
+ \frac{1}{v_0} (\bar{\eta}/2)^2 \cos^2 \theta \right],

D_0 = (1 - \Gamma^2) \left[ Z^2 + (\bar{\eta}/2)^2 \cos^2 \theta \right] + (1 + \bar{\eta}) \cos^2 \theta,$$

where $\Gamma = v_0/u_0$, with $u_0$ and $v_0$ given by Eq. (3), $\theta$ the tunneling angle, and $Z$ the dimensionless barrier strength given by $Z = mV_0/k_F$. In deriving Eq. (4), we have made the approximation $\bar{\eta}_x \equiv m v_{sx}/k_F \approx \eta/(2\epsilon_F) \approx \bar{\eta}$. The average over the tunneling angle was performed with an equal probability appropriate for small $Z$ (26). Inserting Eq. (3) into Eq. (4), we find that the tunneling current is given by $I(E) \propto 1 + |A|^2 - |B|^2$. This current must be averaged over the phase fluctuations of the order parameter in the pseudogap state as $I(V) = \int d\eta P(\eta) I(V, \eta)$, where $P(\eta)$ is the probability distribution of $\eta$ given by $P(\eta) = \delta(\eta - k_F \cdot \mathbf{v}_s(x))$. The angular brackets indicate thermodynamic average over the phase fluctuations governed by the 2D $XY$ model (22). In the cumulant expansion, $P$ yields a Gaussian distribution of the form

$$P(\eta) = \frac{1}{\sqrt{2\pi W}} e^{-\eta^2/(2W)},$$

where $W$ is given by

$$W \approx 3.48(\alpha_L + \alpha_T)\Delta_d^2(T/T_c).$$

It is crucial to note that $P(\eta)$ was evaluated above $T_{KTB}$ so that we are in the non-superconducting pseudogap state. The $\alpha_L$ comes from the longitudinal fluctuations and will be strongly suppressed in a realistic model by the Coulomb interaction, while $\alpha_T$ comes from the transverse fluctuations due to vortices (23). Franz and Millis found $\alpha_T \approx 0.1$ (22) by fitting Eq. (11) to the scanning tunneling spectra (24). We use this value below. The width of the phase fluctuation given by Eq. (11) and (11) is $\sqrt{W} \approx 0.6\Delta_d$ which means that $\eta < \Delta_d$ is satisfied in the pseudogap state of the cuprates. We, therefore, expect that there will exist AR and residual CE, as shown explicitly below. If, on the other hand, the phase fluctuations are too strong in the sense that $\eta \gg \Delta_d$, then the semiclassical approximation employed to write Eqs. (3) and (4) is not valid, and AR will be washed away.

From the current we can calculate the tunneling conductance, $G = dI/dV$, which after averaging over the phase fluctuations, is given by

$$G(V) = \frac{1}{\pi} \int_{-\pi/2}^{\pi/2} d\theta \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi W}} e^{-\eta^2/(2W)} G(V, \eta, \theta),$$

$$G(V, \eta, \theta) = \frac{e}{\pi} \int_{-\infty}^{\infty} dE \frac{\partial f(E - V)}{\partial V} [1 + |A|^2 - |B|^2],$$

where $A(E, \eta, \theta)$ and $B(E, \eta, \theta)$ are, respectively, the coefficients for the Andreev and normal reflections, and are given by Eqs. (2) and (3). In Fig. 1, we show the normalized tunneling conductance, $G(V)/G_n(V) = \pi(1 - Z/\sqrt{1 + Z^2})^{-1}G(V)$, where $G_n$ is the tunneling conductance at the normal state for $T > T^*$ averaged over the angle $\theta$, calculated with Eqs. (8) and (12), as a function of the bias voltage. The curves are (from above) for $T = 1, 1.5, 2$, and $3 Tc$. We take $W = 0.3 \Delta_d^2(Tc/T_c)$ and $\Delta_d = 0.04 eV$ for the underdoped $Tc = 84 K$ BSCCO analyzed by Franz and Millis (22), with $\epsilon_F/\Delta_d = 10$. $Z$ is to be regarded as a fitting parameter to experimental data; we have taken $Z = 0.1$ as a representative value for low barrier tunneling experiments like the point contact spectroscopies (18, 19). The calculated conductance is not very sensitive to the precise parameter values. Note that, as anticipated, the contribution to the tunneling conductance from the AR does not vanish upon averaging over the phase fluctuations because we average $|A|^2$ and $|B|^2$. In Fig. 1, there is a strong CE due to the non-vanishing pairing amplitude, which is clearly seen up to the highest temperature and arises from the AR off the PIPP. At $T = 3 Tc$, $G(0)/G_n(0) \approx 1.46$, for the parameters given above. Without the normal state pairing, $G(0)/G_n(0)$ would be equal to 1 above $Tc$.

What is the experimental situation, and what further improvements in or extensions to the theory should be considered? First, experimentally, no CE has yet been reported in tunneling experiments above $Tc$. Our results strongly suggest a more systematic search for CE for $T > Tc$ in heavily underdoped and high quality clean samples. In the heavily underdoped materials, $Tc$ is substantially reduced, which implies that the pseudogap phenomenon can be probed at the relatively low temperature where the thermal fluctuations are suppressed. Similarly, high quality clean samples will also help to observe the CE because the increased electron mean free path will enhance the AR (27). Second, here as in most previous calculations, the pairing gap and the wavefunctions of corresponding quasiparticles were not determined self-consistently, because the previous non-self-consistent solutions of the BdG equation produced satisfactory results.
for the tunneling conductances $\xi$. A main consequence of self-consistent solutions is that the pairing amplitude varies smoothly from 0 to a bulk value over the correlation length $\xi$ unlike non-self-consistent case where the pairing amplitude changes abruptly from 0 to the bulk value at the interface. The phase of the pairing order parameter, however, remains to be describable in terms of the 2D XY model, and will be insensitive to a particular way in which the pairing amplitude is varied, and hence to the self-consistency. It will nevertheless be of interest to study the modifications produced by including self-consistency. Finally, our result that a CE can be caused by the AR from the PIPP, which are a particle–particle (pp) condensate, suggests that one consider possible AR from other forms of condensates. AR is novel in that it can distinguish pp from particle–hole (ph) condensates, unlike the most spectroscopic and transport measurements. For a charge density wave (CDW) or spin density wave (SDW) (both ph condensates), we again anticipate Andreev-like reflections because an electron is not an elementary excitation once the condensate is formed. We expect the effects of AR from any ph condensate to be a dip, rather than a peak, around zero bias voltage in the tunneling conductance because the Andreev-reflected particles are electrons for ph condensate. We are currently exploring this effect and other potential experimental signatures that may distinguish among models of the pseudogap state.

To summarize, we have proposed the Andreev reflection as an unambiguous test of the phase incoherent preformed pair scenario of Emery and Kivelson, which was substantiated by the quantitative analyses based on the Bogoliubov-de Gennes equation. Experimental observation of the Andreev reflection above $T_c$, such as the enhanced tunneling conductance around zero bias voltage along {100} direction, could provide a convincing evidence for the preformed pairs in the pseudogap state. In order to provide more robust argument for our proposal, we are currently solving, without assuming the semiclassical approximation, the Bogoliubov-de Gennes equation with the phase dynamics included fully self-consistently. This will be reported in a separate paper.

We thank Sasha Balatsky, David Pines, Laura Greene, Chandra Varma, Chi Hoon Choi, and Jaejun Yu for valuable comments and discussions. We acknowledge support from KOSEF through grant No. 1999-2-114-005-5 (H.Y.C. and Y.K.B.), the KOSEF 1998 USA Exchange Program (H.Y.C.), and the US NSF under grant No. DMR-97-12765 (D.K.C.). We also thank the Department of Physics, UIUC, and the CNLS, Los Alamos National Laboratory, for their hospitality.

[1] T. Timusk and B. Statt, Rep. Prog. Phys. 62, 61 (1999).
Figure Caption

The normalized tunneling conductance along \{100\} direction as a function of the bias voltage $V$ in units of the pairing amplitude for $Z = 0.1$. The curves are, from above on the $V = 0$ axis, for $T = 1, 1.5, 2, \text{ and } 3 \ T_c$. The conductance enhancement due to the Andreev reflections appears as $G(V = 0)/G_n(V = 0) > 1$. 

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