A model and calculation of evolving tunneling spectra for the gap and pseudogap in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$

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Abstract.
By the intrinsic tunneling spectroscopy in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (Bi2212), it is found that the superconducting coherence peak becomes greater and sharper and the pseudogap peak diminishes with the increase in doping. It is also found that these changes are accompanied by a significant almost exponential increase in the maximum Josephson current density $J_c$. In order to explain the experimental results, we propose a model, in which mobile carriers reside only in limited areas in the $k$-space, and are closely correlated with the $d$-wave superconducting order parameter. The range of the area in which mobile carriers reside depends on the doping level. Outside these areas the density of states is absent at the chemical potential and a semiconducting gap is assumed. Based on this model, the tunneling spectra are calculated at various doping levels to obtain the result that the superconducting peak increases from a cusp at the shoulder of the pseudogap to a dominantly strong peak as the doping increases. The results are in qualitatively good agreement with the experimental tunneling spectra observed.

1. Introduction
The pseudogap, most visibly observed in tunneling spectra [1] in its literal meaning and in other physical properties [2] in less direct form, is a still unexplained phenomenon in high temperature (high-$T_c$) superconductors. It is commonly accepted that the elucidation of the pseudogap origin leads to a clue to the mechanism of the occurrence of high-$T_c$ superconductivity. There have been attempts to explain the pseudogap phenomena. In a preformed boson model [3, 4, 5], it is assumed that incoherent pairs (preformed bosons) above $T_c$ becomes coherent below $T_c$ and gives rise to a finite stiffness. Consequently, the pseudogap must connect smoothly with the superconducting gap at $T_c$. In an optimally doped Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (Bi2212), it appears that this occurs.

On the other hand, however, it is also argued that the pseudogap can originate from some kind of ordered state [6]. In this case, the pseudogap is distinct from the superconducting gap. In some tunneling spectra, the pseudogap peak is seen to coexist with the superconducting gap of
Figure 1. Tunneling spectra for Bi2212 at three different doping levels indicated in the figure at low temperatures and just above $T_c$ obtained by tunneling spectroscopy using IJJs.

Bi2212 in the underdoped region [7, 8], implying that the pseudogap may exist in a topologically heterogeneous form in the wavevector space ($k$-space) or in real space.

It is seen that when the doping level is varied from an optimal to an underdoped level, the Josephson critical current density $J_c$ decreases almost exponentially [9, 10], implying that it becomes increasingly likely that some kind of heterogeneity of superfluid density plays an important role in high-$T_c$ superconductivity [10].

From these phenomenological insights into the relationship between the pseudogap and the superconducting gap, we have come to propose a model in which the superconducting gap exists in a limited range in $k$-space and the pseudogap in the other range. Based on this preliminary phenomenological model, the tunneling characteristics are calculated for a tunnel junction between an ordinary metal and a superconductor having such gap structures. The result demonstrates that the tunneling spectrum systematically evolves with doping and the pseudogap manifest itself as a broad gap structure above $T_c$.

2. Experimental background

2.1. Intrinsic Josephson junctions

Intrinsic Josephson junctions (IJJs) in Bi2212 [11, 12] are naturally formed in the layered crystal structure of Bi2212 and are crystal structure itself so that the tunneling characteristics reflect predominantly the bulk properties. For the same reason, the interfaces of the IJJs are clean and flat on an atomic scale, and the tunneling characteristics observed are almost ideal. These facts strongly tempt us to conduct research into uncommon physical properties of high-$T_c$ superconductors through IJJs [7, 8, 5].

2.2. Intrinsic Tunneling spectra

Intrinsic tunneling spectroscopy [7, 8, 5] usually employs a small mesa structure containing less than 10 IJJJs with a size of 10 $\mu$m or less in order to suppress Joule heating due to self-injection of quasiparticle current. Figure 1 show tunneling characteristics for three samples with different
2.3. Doping dependence
Associated with these changes in the tunneling spectra of IJJs, $J_c$ is also subjected to significant change with doping. Figure 2 shows the doping dependence of $J_c$, showing an almost exponential decrease with the doping parameter $p$. It also indicates that the experimental results for $J_c$ are orders of magnitude smaller than the theoretical estimate in which a homogeneous superconducting order parameter is assumed in $k$-space as well as in real space. This implies that the superconducting order parameter is no longer homogeneous at all even in $k$-space [10].

3. Superfluid density and wavevector space heterogeneity
A model to explain these experimental results is schematically shown in Fig. 3, in which the $k$ vectors of mobile carriers are confined within the Fermi arcs and the range of the rest requires an extra energy for carriers to be mobile. The energy for the latter correspond to a semiconductor energy gap, if viewed in a fixed $k$ vector, with its range being limited in the present case. In the superconducting state, the order parameter establishes in the region of the Fermi arc. When the doping level decreases, the range of the Fermi arc is reduced, which causes a significant decreases in the superconducting fluid density, as would become clear when we work on Fig. 3 [10]. It is interesting to know that this kind of specific configuration for the superconducting order parameter and the pseudogap gives rise to the tunneling spectra as observed in experiments.
4. A model for spectrum calculation

Let $\theta$ be the angle in $k$-space with respect to $k_x$ axis. Here, we only consider the range in the $k$-space from 0 to $\pi/4$ and the rest is symmetrically defined. In order to calculate the tunneling characteristics, we assume that the range of $\theta$ for the mobile carriers spans from $\theta_0$ to $\pi/4$. Likewise, the pseudogap manifests itself in the range of 0 to $\theta_0$ with a semiconductive gap, which is assumed to obey the $d$-wave symmetry [13]. When $\theta_0 = 0$, the superconductor is pure $d$-wave, and as $\theta_0$ increases the pseudogap evolves gradually and finally the superconductor changes to a semiconductor near $\theta_0 = \pi/4$. The superconducting order parameter $\Delta_S(\theta)$ is defined by the following equation.

$$\Delta_S(\theta) = \Delta_S^0 \cos 2\theta \quad (\theta_0 < \theta < \pi/4). \quad (1)$$

The pseudogap $\Delta_P(\theta)$ is also defined similarly as follows.

$$\Delta_P(\theta) = \Delta_P^0 (\cos 2\theta - \cos 2\theta_0) \quad (0 < \theta < \theta_0). \quad (2)$$

Outside the $\theta$ range indicated in both equations, each function is set to zero. Figure 4 depicts the $\theta$ dependence of $\Delta_S$ and $\Delta_P$. In the superconducting range the density of state (DOS) above $T_c$ is assumed to be independent of $\theta$ and set to unity in the present calculation. The DOS, $N_S$ and $N_P$, is defined for each range as follows.

$$N_S(E) = \text{Re} \frac{E - i\Gamma}{\sqrt{(E - i\Gamma)^2 - \Delta_S^2}}, \quad (3)$$

where $\hbar/\Gamma$ is the life time of a quasiparticle.

$$N_P(E) = \left( a \tanh \alpha E' + \frac{b E'}{E'^2 + \beta} \right) K(E'), \quad E' = E - \Delta_P(\theta), \quad (4)$$

where $K(E)$ is a step function of $E$. The reason for expressing $N_P(E)$ as Eq. (4) is as follows. In the pseudogap range for $\theta$, carriers in the $k_\theta$ direction are confined by the superconducting gap below $T_c$ when $E$ is small. In this case, the DOS is one-dimension-like, in which there is a singular peak just above the gap. When $E$ is large or above $T_c$, carriers are not confined and the DOS is two-dimension-like. The expression in Eq. (4) is devised to reflect qualitatively such behavior of the DOS as above. Figure 5 depicts the DOS for two typical cases of below and above $T_c$.

5. Tunneling spectra calculated

Tunneling spectra were calculated for a tunnel junction between a superconductor with the gap structure described above and an ordinary metal in which the $k$ space is isotropic and the DOS for the metal is constant for the energy range calculated. Figures 6 and 7 show the calculated...
Figure 5. The DOS for the superconducting region and the pseudogap region. Their functional forms are described in Eq. 4 below and above $T_c$. (a) $a = 1$, $b = 0.5$, $\alpha = 4$, and $\beta = 0.125$. (b) $a = 1$, $b = 0$, and $\alpha = 4$.

Figure 6. Tunneling spectra at 10 K representing evolving superconducting peak and pseudogap calculated at various $\theta_0$ values with values of $\Delta_{S0} = 30$ meV, $\Delta_{P0} = 100$ meV, $\Gamma = 1$ meV, $a = 1$, $b = 0.5$, $\alpha = 4$, and $\beta = 0.125$

tunneling spectra ($dI/dV-V$) at various $\theta_0$ values from $0.2\pi/4$ to $0.9\pi/4$ at two temperatures of 10 K and 90 K, i.e., below and above $T_c$. It is clearly demonstrated in Fig 6 that the superconducting peak gradually diminishes as $\theta_0$ increases, that is, equivalently as the doping level decreases. It even appears that the superconducting peak smoothly shifts toward higher energies with increasing $\theta_0$. This is compared with the scanning tunneling spectroscopy (STS) experiments, where a similar behavior was observed [14]. For $\theta_0$ from $0.125\pi$ to $0.175\pi$, there is a cusp at the shoulder of the main peak, which was also observed in STS experiments [14]. If we choose the magnitude of $\Delta_{P0}$, which is to be compared with the zero temperature pseudogap, we can reproduce a double peak structure, which implies the distinctness of the superconducting gap and the pseudogap, like one shown in Fig. 1(b).

At 90 K, just above $T_c$, we set $\Delta_{S0} = 0$ and $b = 0$ and obtained the results shown in Fig. 7. It is seen that the pseudogap of a typical type usually observed in tunneling spectroscopy is reproduced, showing a tendency of increasing gap magnitude with the decrease in the doping level. Thus the model explains reasonably well the evolution of peak structures with the varying doping level. This may indicate that the heterogeneity in the $k$-space plays an imperative role in the occurrence of high-$T_c$ superconductivity.
6. Discussion
In the present model, there are two important points that are essential for the results presented. One is the orientation dependent semiconductive gap with $d$-wave symmetry. This behavior is observed experimentally by Ding et al. [13] and probably in materials which undergo a composition-induced metal-insulator transition. The other point is that the possibility whether the superconducting order parameter can vary as shown in Fig 4. There is no straightforward answer to this question at present and we have to rely on a microscopic theoretical work in which the magnitude of angular dependent order parameter is determined self-consistently. However, since the magnitude of the order parameter can vary depending on the DOS in the normal state, it is not totally hopeless to obtain an order parameter like one in Fig. 4, though the shape might change to a certain degree.

In Fig. 6, there is apparently no so-called dip and hump structure [15]. If we increase $\Delta P_0$ to a value larger than the value in Fig. 6, or if we take nearly $\theta$-independent $\Delta P_0$ with a magnitude larger than the $\Delta S_0$ value, a dip structure [15, 16] is possible to produce. The transfer of the DOS and its conservation is explicable if we subtract the contribution coming from $N_P$ from the tunneling conductance. The negative conductance at the dip bottom [15, 17] is difficult to reproduce by the present model. However, such selections of $\Delta P(E)$ are too arbitrary at the present stage. The present result is not meant to rule out the possibility of the dip structure caused by the strong interaction with bosons [16, 18].

7. Conclusions
We have proposed a model in which the superconducting gap and the pseudogap both with $d$-wave symmetry coexist in the $k$-space. The calculation of the tunneling spectra based on this model has demonstrated that the evolution of the superconducting gap and the pseudogap with the doping level is explained reasonably well in terms of this model. It has been found that the calculation result is basically successful in qualitatively explaining the tunneling experiments in their essential aspects.

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