Temperature Dependence of the Superconducting Gap in High-T_c Cuprates

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It is proposed that the temperature dependence of the superconducting gap $\Delta(T)$ in high-T_c cuprates can be predicted just from the knowledge of $\Delta(0)$ and the critical temperature T_c, and, in particular, $\Delta(0)/T_c > 4$ implies that $\Delta(T_c) \neq 0$, while $\Delta(0)/T_c \leq 4$ corresponds to $\Delta(T_c) = 0$. A number of tunneling experiments appear to support the above proposition, and, furthermore, show reasonable quantitative agreement with a model based on the two-dimensional stripe hypothesis.

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In conventional superconductors, the phenomenology of the superconducting (SC) energy gap closely follows that of the model of Bardeen, Cooper, and Schrieffer (BCS) [1]: (i) Below the SC transition temperature (T_c), there are no one particle excitations within the SC gap $\Delta(T)$, where T is the temperature. (ii) At the gap boundaries $\pm\Delta(T)$, there are symmetric SC peaks. (iii) The ratio $\Delta(0)/T_c$ is close to 1.76. (iv) $\Delta(T_c) = 0$. In contrast, the tunneling studies of high-T_c cuprates show that: (i) the density of states within the SC gap is not zero, (ii) the SC peaks are frequently asymmetric, (iii) the ratio $\Delta(0)/T_c$ is significantly larger than 1.76 and not universal, and (iv) in some high-T_c compounds, $\Delta(T_c) \neq 0$. The above nonuniversality implies that any BCS-like one-parameter description of the tunneling spectra cannot be adequate for high-T_c cuprates. The complexity of these materials further suggests that their proper microscopic description should contain many parameters. In this Letter, however, I report a surprising finding that the phenomenology of the SC gap in high-T_c cuprates may be describable by only two parameters.

The present study was originally undertaken to test a simple model proposed in Ref. [2]. The calculations of the tunneling characteristics based on that model require only two input parameters, $\Delta(0)$ and T_c. The reasonable success of this test, of course, lends credibility to the model, but, also, irrespectively of the model, it suggests that, even though the ratio $\Delta(0)/T_c$ may exhibit a nonuniversal doping dependence, and, moreover, may be different for different samples of the same material, the measured values of $\Delta(0)$ and T_c are sufficient to predict the entire evolution of $\Delta(T)$. Of particular interest is the following model-based rule:

$$\begin{aligned} \Delta(0)/\mathrm{T_c} > 4 &\Leftrightarrow \Delta(\mathrm{T_c}) \neq 0/\text{asymmetric SC peaks;} \\ \Delta(0)/\mathrm{T_c} \leq 4 &\Leftrightarrow \Delta(\mathrm{T_c}) = 0/\text{symmetric SC peaks.} \end{aligned} \tag{1}$$

It was the surprisingly good agreement between the symmetry/asymmetry part of this rule and many experiments [2], that prompted me to test the model predictions for the shape of the $\Delta(T)$ curve.

The model of Ref. [2] is based on the hypothesis that a two-dimensional (2D) arrangement of stripes shown in Fig. 1 exists in the CuO_2 planes of high-T_c cuprates. In such a superstructure there exist hole states localized either inside the stripes (b states) or in the antiferromagnetic (AFM) domains between the stripes (a states). Because of the small size of the AFM domains and stripe elements (20–30 Å), the energy levels within each unit should be broadly spaced (estimated [2] 40 meV). The model proceeds by assuming the existence of only one low-energy a state per AFM domain and two low-energy b states per stripe element. As argued in Ref. [2], a promising choice for the model Hamiltonian is

$$\mathcal{H} = \varepsilon_a \sum_i a_i^+ a_i + \varepsilon_b \sum_{i,j(i),\sigma}^{\eta_i=1} b_{ij,\sigma}^+ b_{ij,\sigma} + g \sum_{i,j(i)}^{\eta_i=1} (b_{ij,+}^+ b_{ij,-}^+ a_i a_j + \text{H.c.}), \tag{2}$$

where the index i or j labels AFM domains; $j(i)$ implies that the jth AFM domain is the nearest neighbor of the ith domain; a_i is the annihilation operator of a hole inside the ith AFM domain; $b_{ij,\sigma}$ is the annihilation operator of a hole

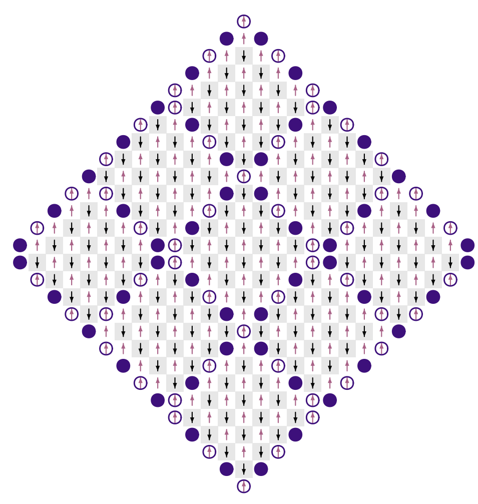

FIG. 1 (color online). 2D configuration of diagonal stripes (a cartoon).

inside the stripe element separating the ith and the jth AFM domains; σ is the spin index, which can have two values "+" or "−"; ε_a and ε_b are position-independent on-site energies for a and b states, respectively, counted from the chemical potential; and, finally, g is the coupling constant. The spins of a states are tracked by index η_i, which alternates between 1 or -1, thus tracing the sign of the AFM order parameter in the AFM domains. The sum superscript "$\eta_i = 1$" indicates that the summation extends only over the supercells having $\eta_i = 1$.

The total energy of such a system as a function of the chemical potential μ has at least two minima [2]: $\mu = \varepsilon_a$ and $\mu = \varepsilon_b$, which implies two most promising regimes: Case I, $\varepsilon_b = 0$; Case II, $\varepsilon_a = 0$. The mean-field solution then leads to the density of states described by the following system of equations [2]: in Case I,

$$\varepsilon_A(\mathbf{k}) = \sqrt{\varepsilon_a^2 + \frac{1}{4} g^2 (2n_B - 1)^2 |V(\mathbf{k})|^2}, \tag{3}$$

$$\varepsilon_B = -\frac{g^2(2n_B - 1)}{64\pi^2} \times \int_{-\pi}^{\pi} dk_x \int_{-\pi}^{\pi} dk_y \frac{[1 - 2n_A(\mathbf{k})]|V(\mathbf{k})|^2}{\varepsilon_A(\mathbf{k})}, \tag{4}$$

and, in Case II,

$$\varepsilon_A(\mathbf{k}) = -\frac{g^2 |V(\mathbf{k})| C_a (1 - 2n_B)}{8\varepsilon_B}, \tag{5}$$

$$\varepsilon_B = \sqrt{\varepsilon_b^2 + \frac{1}{16} g^2 C_a^2}, \tag{6}$$

where subscripts A and B indicate the Bogoliubov quasiparticles associated with a and b states, respectively; $\varepsilon_{A/B}$ and $n_{A/B}$ are the quasiparticle energies and the occupation numbers, respectively. A quasiparticles are characterized by well defined wave vectors $\mathbf{k}$. All B quasiparticles have the same ε_B. The expressions for $n_A(\mathbf{k})$ and n_B, and for the auxiliary quantities C_a and $V(\mathbf{k})$, are

$$n_A(\mathbf{k}) = \frac{1}{\exp\left(\frac{\varepsilon_A(\mathbf{k})}{T}\right) + 1}, \tag{7}$$

$$n_B = \frac{1}{\exp(\frac{\varepsilon_B}{T}) + 1}, \tag{8}$$

$$V(\mathbf{k}) = 2\left[\cos\left(\frac{k_x + k_y}{2}\right) - i\cos\left(\frac{k_x - k_y}{2}\right)\right], \tag{9}$$

$$C_a = \frac{1}{8\pi^2} \int_{-\pi}^{\pi} dk_x \int_{-\pi}^{\pi} dk_y [2n_A(\mathbf{k}) - 1]|V(\mathbf{k})|. \tag{10}$$

The tunneling spectra of A states have van Hove singularities, which, in Case I, are located at

$$\varepsilon_{A0} = \pm\sqrt{\varepsilon_a^2 + g^2(2n_B - 1)^2}. \tag{11}$$

and, in Case II, at

$$\varepsilon_{A0} = \pm \frac{g^2 C_a (1 - 2n_B)}{4\varepsilon_B} \tag{12}$$

Three representative zero-temperature tunneling spectra of both A and B states can be found in Fig. 7 of Ref. [2].

In both Cases I and II, the mean-field T_c can be obtained [2] numerically from the following equation:

$$T_c = \frac{g^2\left[\exp\left(\frac{|\varepsilon_a - \varepsilon_b|}{T_c}\right) - 1\right]}{8|\varepsilon_a - \varepsilon_b|\left[\exp\left(\frac{|\varepsilon_a - \varepsilon_b|}{T_c}\right) + 1\right]}. \tag{13}$$

Given the above picture, the basic features of the tunneling phenomenology can be interpreted as follows: (1) The SC peaks at $\pm\Delta$, are identified with the van Hove singularities at $\pm\varepsilon_{A0}$ in the density of A states. (2) The density of B states is assumed to be more difficult to detect due to, perhaps, smaller tunneling elements.

The knowledge of $\Delta(0)$ and T_c is thus sufficient to obtain the model parameters $|\varepsilon_a|$ and g in Case I [Eqs. (11) and (13), with $n_B = 1$], and $|\varepsilon_b|$ and g in Case II [Eqs. (6), (9), (10), (12), and (13), with $n_A(\mathbf{k}) = 1; n_B = 0$]. After that, $\Delta(T)$ can be calculated numerically using Eqs. (3)–(12) without additional adjustable parameters. Importantly, Cases I and II do not overlap in terms of the ratio $\Delta(0)/T_c$: in Case I, $\Delta(0)/T_c > 4$, while, in Case II, $\Delta(0)/T_c < 4$. The entire family of the $\Delta(T)$ curves is presented in Fig. 2.

In both Cases I and II, $|\varepsilon_a - \varepsilon_b|$ is a measure of the pseudogap (see Sec. V of Ref. [2]). This pseudogap is a real

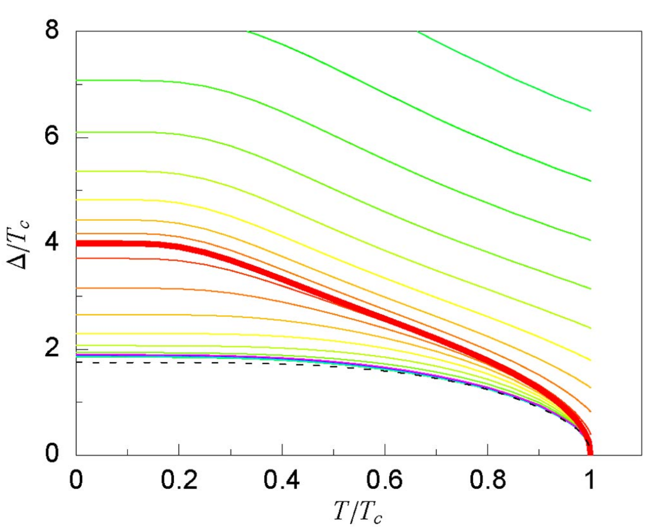

FIG. 2 (color online). Family of theoretical curves for the temperature dependence of the superconducting gap. Thick line corresponds to the critical ratio $\Delta(0)/T_c = 4$. Solid lines above the thick line describe Case I, and below the thick line Case II. The dashed line represents the BCS result.

feature in the normal density of states (as, e.g., in the proposal of Ref. [3]), i.e., it is not associated with the SC fluctuations above T_c. This feature is a generic consequence of the nanoscale phase separation: two different kinds of real space regions (stripes and AFM domains) imply two different energies associated with them. The model pseudogap equals zero only in the critical case, $\varepsilon_a = \varepsilon_b$, which, as argued in Ref. [2], may correspond to the doping concentration 0.19. The model has two different SC energy gaps: ε_{A0} for A states and ε_B for B states. In Case I, ε_B turns to zero at $T = T_c$, while ε_{A0} becomes equal to the pseudogap $|\varepsilon_a - \varepsilon_b|$. In Case II, the situation at $T = T_c$ is opposite: $\varepsilon_{A0} = 0$, while $\varepsilon_B = |\varepsilon_a - \varepsilon_b|$. Thus the difference between the two model regimes is not qualitative but only quantitative. However, since, by assumption, the observable SC peaks represent only A states, the phenomenology of the SC gap appears to be qualitatively different in the two regimes.

In Fig. 3, I compare the theoretical predictions with the results of the break junction (BJ) [4–6] and the interlayer tunneling (ILT) [7–12] experiments. The ILT technique gives better energy resolution and comes closer to measuring the true intrinsic density of states in the bulk of cuprates, but, at the same time, it generates significant overheating of the sample. In order to avoid this problem, the authors of Refs. [7,8,12] have used a short-pulse method, which, however, comes at a cost of somewhat lower energy resolution [Fig. 3 (c)-(g) and (q)-(r)].

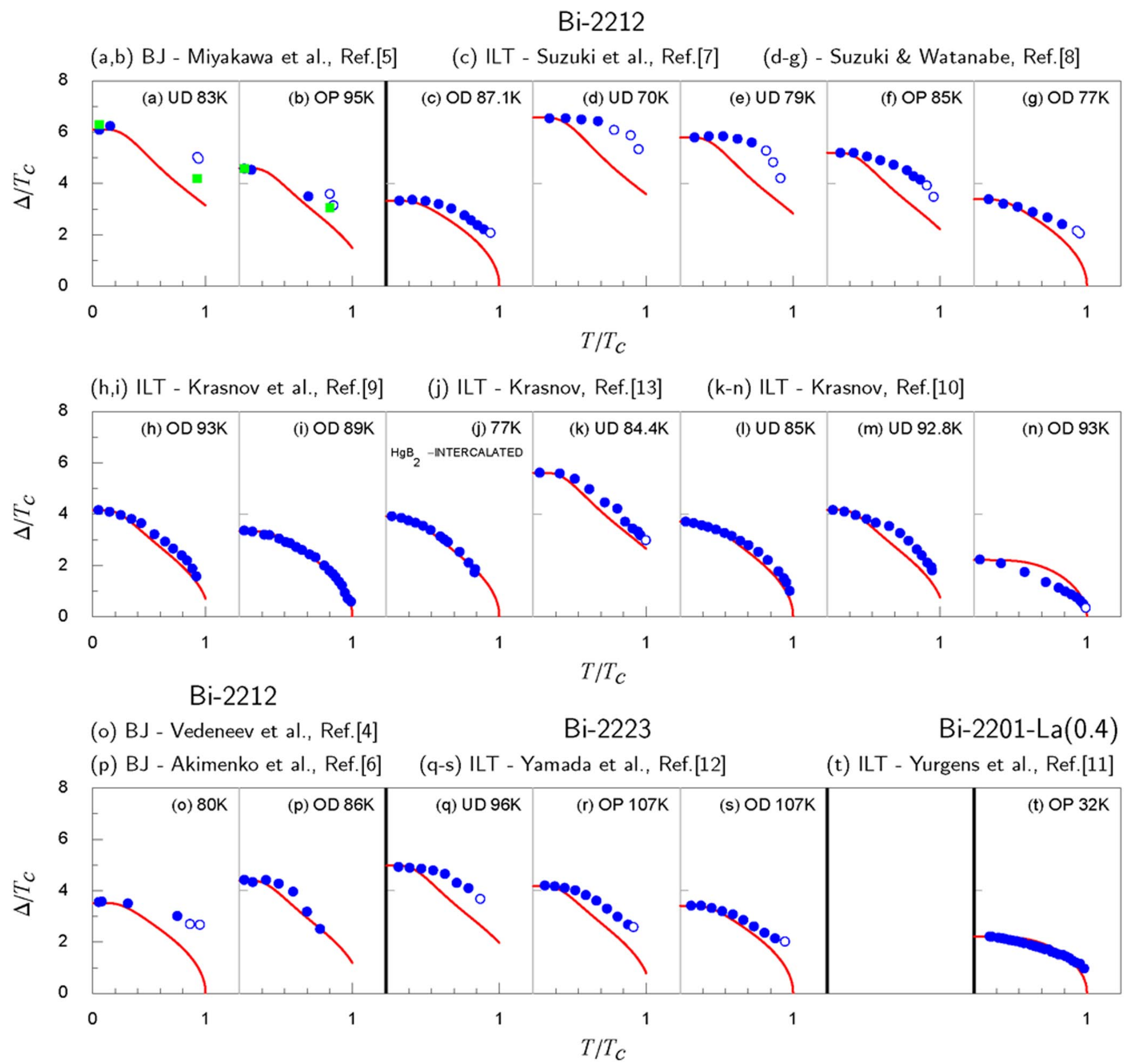

FIG. 3 (color online). Temperature evolution of the SC gap. Solid lines, theory; circles, experiments; BJ, break junction; ILT, interlayer tunneling. Horizontal marks in each frame indicate $\Delta/T_c = 4$. Whenever the original tunneling spectra were reported (a)-(h), (k), (n)-(t), filled circles indicate reasonably well-pronounced SC peaks, while open circles indicate very broad *and* small SC peaks. Filled circles in frames (i), (j), (l), (m) imply no additional information about the SC peaks. Squares in frames (a),(b) represent the bare values of Δ estimated in Ref. [5].

Alternatively, the authors of Refs. [9–11,13] [Fig. 3 (h)-(n) and 3(t)] have perfected the "conventional" ILT technique by manufacturing sufficiently small *mesas* and thus reducing the overheating. In the latter case, the experimental data points reflect the ambient temperature of experiment. The question, however, remains concerning the true value of the temperature of the *mesas* [14,15]. Theoretical and experimental estimates made in Refs. [13,16,17], have indicated possible significant overheating, but there is still a chance that, at least in the underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi-2212), the temperature was not too much distorted at the voltage biases probing the SC peaks.

Most of the theoretical curves shown in Fig. 3 agree with the experimental data within the limits of (sometimes, large) uncertainty associated with the broadening of the SC peaks (see the original references). The data points in Fig. 3 are obtained from the peak-to-peak separation in the experimental tunneling spectra. Usually, the peak broadening shifts the peak maximum towards higher energies. If this effect is undone by extracting the "bare" values of Δ, then the experimental points in Figs. 3 (a)-(g),(o), (q)-(s), would appear significantly closer to the theoretical curves. This is a consequence of the fact that the SC peaks are broader at higher temperatures. The magnitude of the above correction can be judged on the basis of the estimates of bare Δ made in Ref. [5] and presented in Figs. 3(a) and 3(b). [Note: the widths of the SC peaks corresponding to Figs. 3(a) and 3(b) are comparable or smaller than those corresponding to Figs. 3 (d)-(g), and (o)-(s).]

The agreement between the theory and the experiment is typically better, whenever the SC peaks are sharper. This is, particularly, true for the "pulsed" ILT experiments [Fig. 3 (c)-(g) and (q)-(s)]: up to $T/T_c \sim 0.7$ the data points from the overdoped samples [Figs. 3(c), 3(g), and 3(s)] correspond to sharper SC peaks and better agree with the theory. Figure 3(n) constitutes an exception from the above trend, but, in this case, a stronger degree of overheating is suspected. The best agreement between the theory and the experiment can be observed in Figs. 3 (h)-(m), in which case the data points were generated by the conventional ILT technique (expected to give the best energy resolution). If these data also stand the test of time with respect to the true temperature of the samples, then such an agreement would amount to a striking success of the present model.

The experimental data in Figs. 3 are also fairly consistent with the first line of the rule (1). As far as the second line of that rule is concerned, then Figs. 3(i) and 3(n) can be cited as supporting the rule. The data points in Figs. 3(c), 3(g), 3(o), and 3(s) , while corresponding to $\Delta(0)/T_c < 4$, show trends toward $\Delta(T_c) \neq 0$. However this trend is due to the highest temperature points, which originate from poorly characterized SC peaks. The conclusive verification of rule (1) should thus await further experiments. It should also be noted in this context that the scanning tunneling spectroscopy studies of Bi-2212 [18] and Bi-2201 [19], which indicated that $\Delta(T_c) \neq 0$, were all performed on the samples exhibiting $\Delta(0)/T_c > 4$.

In a future study, I plan to test the model predictions for the specific heat experiments, which should be equally sensitive to the densities of both A and B states.

In conclusion, I express cautious optimism that (i) there exists a two-parametric description of the $\Delta(T)$ curves in high-T_c cuprates, (ii) there exists a critical ratio $\Delta(0)/T_c$, which signifies a transition between two different kinds of SC states, and (iii) the above critical ratio is approximately equal to 4. The quantitative agreement between the experimental data reproduced in Fig. 3 (h)-(m) and the model calculations also appears quite promising.

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[1] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).
[2] B. V. Fine, Phys. Rev. B **70**, 224508 (2004).
[3] J. W. Loram, K. A. Mirza, J. R. Cooper, W. Y. Liang, and J. M. Wade, J. Supercond. **7**, 243 (1994).
[4] S. I. Vedeneev, A. G. M. Jansen, P. Samuely, V. A. Stepanov, A. A. Tsvetkov, and P. Wyder, Phys. Rev. B **49**, 9823 (1994).
[5] N. Miyakawa, P. Guptasarma, J. F. Zasadzinski, D. G. Hinks, and K. E. Gray, Phys. Rev. Lett. **80**, 157 (1998).
[6] A. I. Akimenko, R. Aoki, H. Murakami, and V. A. Gudimenko, Physica C (Amsterdam) **319**, 59 (1999).
[7] M. Suzuki, T. Watanabe, and A. Matsuda, Phys. Rev. Lett. **82**, 5361 (1999).
[8] M. Suzuki and T. Watanabe, Phys. Rev. Lett. **85**, 4787 (2000).
[9] V. M. Krasnov, A. Yurgens, D. Winkler, P. Delsing, and T. Claeson, Phys. Rev. Lett. **84**, 5860 (2000).
[10] V. M. Krasnov, Phys. Rev. B **65**, 140504 (2002).
[11] A. Yurgens, D. Winkler, T. Claeson, S. Ono, and Y. Ando, Phys. Rev. Lett. **90**, 147005 (2003).
[12] Y. Yamada, K. Anagawa, T. Shibauchi, T. Fujii, T. Watanabe, A. Matsuda, and M. Suzuki, Phys. Rev. B. **68**, 54 533 (2003).
[13] V. M. Krasnov, Physica C (Amsterdam) **372-376**, 103 (2002).
[14] V. N. Zavaritsky, Phys. Rev. Lett. **92**, 259701 (2004).
[15] V. N. Zavaritsky, Physica C (Amsterdam) **404**, 440 (2004).
[16] A. Yurgens, D. Winkler, T. Claeson, S. Ono, and Y. Ando, Phys. Rev. Lett. **92**, 259702 (2004).
[17] V. M. Krasnov, M. Sandberg, and I. Zogaj, Phys. Rev. Lett. **94**, 077003 (2005).
[18] Ch. Renner, B. Revaz, J.-Y. Genoud, K. Kadowaki, and Ø. Fischer, Phys. Rev. Lett. **80**, 149 (1998).
[19] M. Kugler, Ø. Fischer, Ch. Renner, S. Ono, and Y. Ando, Phys. Rev. Lett. **86**, 4911 (2001).