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A possible second-order phase transition at the temperature at which a gap opens in superconductors

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Abstract

This paper shows that there should be a second-order phase transition at the temperature T^* at which a gap opens in superconductors, and points out the best way to verify this prediction, and that the phase transition might have been discovered more than ten years ago.

1. Introduction

Bardeen, Cooper, and Schrieffer showed that the gap equation for superconductors is [1]

$$1 = \sum_{\boldsymbol{k}} \frac{V}{2\sqrt{[\epsilon(\boldsymbol{k}) - E_F]^2 + |\Delta'(T)|^2}} \tanh \frac{\sqrt{[\epsilon(\boldsymbol{k}) - E_F]^2 + |\Delta'(T)|^2}}{2T} \tag{1}$$

where $-V$ represents the purely attractive potential between two electrons, $\Delta'(T)$ the gap. Just by applying the zero-gap condition to equation (1), Bardeen, Cooper, and Schrieffer obtained a formula for determining the superconducting transition temperature T_c, which is [1]

$$T_c = 1.14\hbar\omega_D e^{1/(N(0)V)} \tag{2}$$

where ω_D is the Debye frequency. Bardeen, Cooper, and Schrieffer showed that the transition at T_c is a second-order phase transition, and that the electronic specific heat jump at T_c is [1]

$$\left.\frac{C_{es}(T) - C_{en}(T)}{C_{en}(T)}\right|_{T=T_c} = 1.43. \tag{3}$$

C_{es} and C_{en} are the electronic specific heats in the superconducting and normal states, respectively.

This paper shows, in section 2, that when one just applies the zero-gap condition to equation (1) the temperature obtained is actually T^* rather than T_c, the phase transition at T^* is

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a second-order phase transition, and the specific heat jump in equation (3) occurs at T^* rather than T_c. In section 3 we point out the best way to find the second-order phase transition at T^*. In section 4 we point out that the second-order phase transition at T^* might have been discovered more than ten years ago.

2. The second-order phase transition at T^*

As is well known, superconductivity at T_c requires long-range phase coherence between Cooper-bound pairs. However, the zero-gap condition in BCS theory does not include the condition for long-range phase coherence. Doniach and Inui showed that for superconductivity at T_c, the Ginzburg–Landau phase-stiffness parameter $J_{\text{stiffness}}$ should satisfy [2]

$$J_{\text{stiffness}}(T) \geqslant \frac{2e^2}{\epsilon_\infty a_0(T)} \tag{4}$$

where ϵ_∞ is the high-frequency dielectric constant, e the charge of a free electron, $a_0(T)$ the mean pair spacing at T. If condition (4) is satisfied, then the system has long-range phase coherence, i.e. remains a superconductor. The formula for $J_{\text{stiffness}}$ is [2]

$$J_{\text{stiffness}}(T) = |\Psi(T)|^2 \lim_{q\to 0} \frac{1}{a_0^2(T)} \frac{\partial}{\partial q^2}[L(q)]^{-1} \tag{5}$$

where

$$L(q) = \sum_{k} \left[\frac{1}{2E_k} - \frac{E_k E_{k+q} + \xi_k \xi_{k+q}}{E_k E_{k+q}(E_k + E_{k+q})} \right] \tag{6}$$

where q is the wavenumber, $E_k = \sqrt{(\xi_k)^2 + (\Delta(\boldsymbol{k}, 0))^2}$, $\xi_k = \epsilon(\boldsymbol{k}) - E_F$, $\Delta(\boldsymbol{k}, T) = \Delta(T)G(\boldsymbol{k})$, $\Delta(\boldsymbol{k}, 0)$ is the gap at 0 K, and $\Psi(T)$ is the order parameter. We assume that the maximum value of $G(\boldsymbol{k})$ is one. The formula for determining T_c is thus

$$|\Psi(T_c)|^2 \lim_{q\to 0} \frac{1}{a_0^2(T_c)} \frac{\partial}{\partial q^2}[L(q)]^{-1} = \frac{2e^2}{\epsilon_\infty a_0(T_c)}. \tag{7}$$

Generally, T_c determined from equation (7) is not equal to T^* determined by applying the zero-gap condition to equation (1).

Now let us discuss the thermodynamic functions at $T_c < T \leqslant T^*$. When $T_c < T \leqslant T^*$, the system is in a pair state with a gap and without long-range phase coherence. Let F_{pair}, S_{pair}, and C_{pair} represent the free energy, entropy, and specific heat of a pair state, respectively. Let F_N, S_N, and C_N represent the free energy, entropy, and specific heat of a normal state without a pair and long-range phase coherence, respectively. Using the same procedures as in section 36 of reference [3], we obtain for $T \approx T^*$

$$F_{\text{pair}} - F_N = -\frac{2mp_F(T^*)^2}{7\zeta(3)}\left(1 - \frac{T}{T^*}\right)^2 \tag{8}$$

$$S_{\text{pair}} - S_N = -\frac{4mp_F T^*}{7\zeta(3)}\left(1 - \frac{T}{T^*}\right). \tag{9}$$

At $T = T^*$ the differences in free energy and entropy of the two phases, i.e. the pair and the normal states, are continuous. However, the specific heat at T^* is not continuous. From equation (9) we obtain that the specific heat jump is

$$\left.\frac{C_{\text{pair}}(T) - C_N(T)}{C_N(T)}\right|_{T=T^*} = 1.43. \tag{10}$$

Therefore, the phase transition from the normal state to the pair state is a second-order phase transition. In our theory the second-order phase transitions at T^* and T_c relate to the appearance of the gap and the phase coherence, respectively.

For many conventional superconductors the mean free path of electrons in the normal state falls below the distance ξ_0 ($\approx 10^{-4}$ cm), known as the BCS coherence length. Thus, the mean pair spacing a_0 is nearly zero. Noting that $J_{\rm stiffness}$ is proportional to $1/a_0^2$, one sees that the inequality of equation (4) is easily satisfied. In this case, T_c is only slightly smaller than T^* or approaches T^* infinitely closely. One cannot clearly distinguish the second-order phase transition at T^* from that at T_c for conventional superconductors.

In our picture, the disappearance of superconductivity above T_c does not involve Cooper-pair breaking as it would for conventional superconductors where the BCS coherence length is generally longer than the mean free path of the carriers, but is instead associated with the loss of long-range phase coherence as the Coulomb energy suppressing charge fluctuations overcomes the tendency to long-range phase coherence maintained by the Ginzburg–Landau phase-stiffness parameter.

3. The way to find the second-order phase transition at T^*

We will deal with equation (7) analytically and numerically, and show that for the high-T_c cuprates, $T^* > T_c$. Equation (6) can be simplified by making the following two approximations: adopting the effective-mass approximation for $\epsilon(\boldsymbol{k})$; and using $\Delta(0)/2$ as the mean value of $\Delta(\boldsymbol{k}, 0)$. Hence for the CuO_2 plane,

$$\lim_{q\to 0} \frac{\partial}{\partial q^2}[L(q)]^{-1} = \frac{4\pi k_{\rm F}^2}{9(m^*)^3(\Delta(0)/2)^2(a_{\rm Cu})^2} \tag{11}$$

where m^* is the effective mass of the $O_{p\sigma}$ hole, $a_{\rm Cu}$ the nearest-neighbour distance between two Cu^{2+} ions, and

$$a_0^2(T_c) = \frac{2a_{\rm Cu}^2}{x|\Psi(T_c)|^2} \tag{12}$$

where x is the number of $O_{p\sigma}$ holes in the CuO_2 plane. $|\Psi(T)|$ was given by reference [3]:

$$|\Psi(T)| = \sqrt{\pi T \Delta^2(T) \sum_{n=-\infty}^{+\infty} \frac{1}{\{[(2n+1)\pi T]^2 + \Delta^2(T)\}^{3/2}}}. \tag{13}$$

Substituting equations (11) and (12) into equation (7) yields for the CuO_2 plane

$$|\Psi(T_c)|^3 = \frac{\Delta(0)^2}{\sqrt{x}k_{\rm F}^2} \frac{9\sqrt{2}a_{\rm Cu}^3 e^2 (m^*)^3}{8\pi\epsilon_\infty}. \tag{14}$$

Equation (14) is a general theoretical formula for T_c versus x. To obtain the values of T_c from equations (14) and (13), the gap $\Delta(T)$ would have to be known first. For two high-T_c cuprates (Bi2212 and Y123), reference [4] gave the curves for $\Delta(T)$ versus x and T^* versus x (these were shown in figures 1 and 2 of reference [4]). Substituting the known $\Delta(T)$ from reference [4] into equations [14] and [13], we can obtain the curve for T_c versus x, which is shown in figure 1 of this paper. Figure 1 demonstrates clearly that $T^* > T_c$. The gap at $T_c < T < T^*$ is often called the pseudogap [5]. However, references [4, 6] and this paper show that all of the gaps in the regions $T_c < T < T^*$ and $T < T_c$ relate to the same Cooper-bound pairs. The only difference between the states in the regions $T_c < T < T^*$ and $T < T_c$ is that there is not long-range phase coherence between Cooper-bound pairs for the former, while there is for the latter.

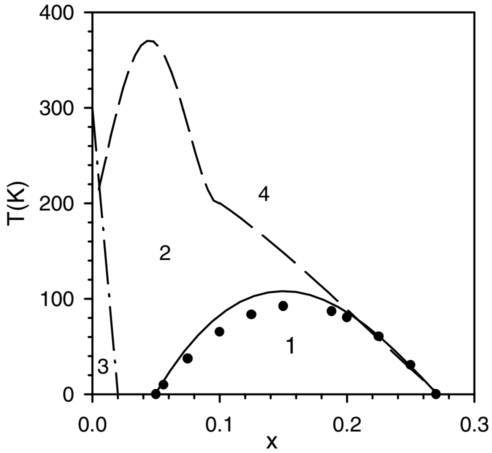

Figure 1. The phase diagram. The solid line is our theoretical curve for T_c versus x. Here x is the hole number in one unit cell in the CuO_2 plane. The solid circles are given by the formula $T_c = 93[1 - 82.6(x - 0.16)^2]$ [9]. The dashed line is from reference [4]. The dotted–dashed line is from reference [10]. The state in range 1 is superconducting. The states in ranges 2, 3, and 4 are normal with a gap, antiferromagnetically insulating [10], and normal without a gap, respectively.

Making electronic specific heat measurements is very difficult since, at high temperature where T^* can be found, the specific heats of typical high-T_c superconductors are dominated by phonons [5]. Reference [6] pointed out that for the n-type cuprate $Nd_{2-x}Ce_xCuO_4$ with $x = 0.12$, $T^* = 43$ K and $T_c = 0$ K. We feel that $Nd_{2-x}Ce_xCuO_4$ is the best candidate for verifying the specific heat jump at T^*.

4. Possible existing verifications for the specific heat jump at T^*

Up to now, it has been thought that it was the case that the specific heat jump given by equation (10) takes place just at T_c, with no specific heat jump, related to the Cooper-bound-pair formulation, at $T > T_c$. So, even when people discovered the specific heat jump at $T > T_c$, they always attributed it to some cause other than that related to the Cooper-bound-pair formulation, or just simply neglected it.

Inderhees *et al* said that they found a specific heat jump at 89 K for their overdoped $T_c = 89$ K Y123 sample [7]. However, we notice that in their data for specific heat versus temperature there is clearly another specific heat jump at 93 K. Figure 1 indicates that if $T_c = 89$ K, then $T^* = 95$ K. Considering the errors in experiment and theory, our theory suggests that the jump observed at 93 K in reference [7] is the jump at T^*.

Dunlap *et al* found a specific heat jump at 31 K for their underdoped $T_c = 31$ K LSCO sample [8]. Dunlap *et al* also noticed that there is a phase transition at $\approx$80 K, which is not transformed in a single heating cycle. Figure 2 of reference [6] indicates that if $T_c = 31$ K for LSCO, then $T^* = 83$ K. Considering the errors in experiment and theory, our theory suggests that the observed jump at $\approx$80 K in reference [7] is the jump at T^*.

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