Bose-Einstein to BCS Crossover Picture for High-$T_c$ Cuprates

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Combining (1) the universal correlations between $T_c$ and $n_s/m^*$ (superconducting carrier density / effective mass) and (2) the pseudo-gap behavior in the underdoped region, we obtain a picture to describe superconductivity in cuprate systems in evolution from Bose-Einstein to BCS condensation. Overdoped and Zn-substituted cuprate systems show signatures of reduced superfluid density in a microscopic phase separation. Scaling of $T_c$ to the superfluid volume density $n_s$ in all these cases indicate importance of Bose condensation.

The magnetic field penetration depth $\lambda$ reflects the spectral density of superfluid as $1/\lambda^2 \propto n_s/m^*$ (the superconducting carrier density / effective mass). The absolute values of $\lambda$ can be determined accurately by Muon Spin Relaxation ($\mu$SR) measurements where the relaxation rate $\sigma \propto 1/\lambda^2 \propto n_s/m^*$ if $H_{\lambda} \ll H_{\text{ext}} \ll H_c2$. Figure 1 shows our $\mu$SR results in various cuprate and other superconductors in a plot of $T_c$ versus $\sigma(T \rightarrow 0)$ [1-3]. This figure demonstrates that: (A) $T_c$ is proportional to $n_s/m^*$ ($m^*$ predominantly reflects the in-plane value $m^*_{ab}$ in cuprates) in the underdoped region with the slope common to many different cuprates (123, 214, 2223 systems etc.) – universal correlations [1]; (B) $T_c$ shows saturation in the “optimum doping” region [1]; (C) $n_s/m^*$ decreases with increasing carrier doping in the overdoped region (Tl2201) [3,4]; and (D) not only the cuprates but also organic BEDT, doped C$_60$ and some other superconductors have ratios between $T_c$ and $n_s/m^*$ [2] comparable to those of the cuprates.

Implications of Fig. 1 become clearer if we convert the horizontal axis into an “effective” Fermi energy $\epsilon_F$ [2], with $\epsilon_F$ in 2-d systems obtained as $\epsilon_F \propto n^{1/3}d/m^* \propto \sigma \times c_{\text{int}}$ where $n_{2d}$ stands for the areal 2-d carrier density on each CuO$_2$ plane and $c_{\text{int}}$ the average interplanar distance between the CuO$_2$ planes. For 3-d systems, $\sigma$ can be combined with the Sommerfelt constant $\gamma \propto n^{1/3}d/m^*$ to obtain $\epsilon_F \propto \sigma^{3/4} \gamma^{-1/4}$. Figure 2 shows the resulting plot, together with the broken line which corresponds to the Bose-condensation temperature $T_B$ for 3-dimensional non-interacting bosons of boson density $n_s/2$ and mass $2m^*$.

This figure demonstrates that: (E) cuprates, organic BEDT, and some other “exotic” superconductors have $kT_c/\epsilon_F$ as high as 0.01-0.1, much higher than those of conventional BCS superconductors; (F) the linear relationship $T_c \propto n_s/m^*$ may originate from that of Bose-Condensation, as the points lie parallel to the broken line; (G) $T_c$ of cuprates is about 4-5 times smaller than $T_B$. The feature (G) can be attributed partly to the overlap of bosons, as several pairs exist per $\xi_{ab}$ ($\xi_{ab}$ is the in-plane coherence length) on the conducting planes in the cuprates. Even for liquid $^4$He, finite size of bosons and their interactions make the
Figure 2. A plot of $T_c$ versus the effective Fermi energy $\epsilon_F$ calculated from $\sigma$ [2]. $T_B$ denotes BE condensation temperature for non-interacting bosons with density $n_s/2$ and mass $2m^*$. The * symbol shows $T_{\theta mac}$ of ref. [14] for K$_3$C$_60$.

Lambda transition at $T_\lambda = 2.2$ K significantly reduced from $T_B \sim 3.2$ K. The 2-dimensional character of the cuprates would further reduce $T_c$, as we discuss later. Figure 2 provides a phenomenological method to classify superconductors in evolution from Bose-Einstein (BE) condensation (in real space with non-retarded strong interaction: close to the broken line) and BCS condensation (in momentum space with retarded weak interaction: at large $\epsilon_F$ and moderate $T_c$).

As an interpretation of these results, we presented a picture for the high-$T_c$ cuprates in terms of a crossover from BE to BCS condensation in 1994 [5,6]. This picture stems from the following observations and concepts [5,6]: (A) and (F) mentioned above; (H) the loss of magnetic response below the pseudo-gap temperature $T^*$ observed by NMR and neutrons [7] may infer a formation of singlet pairs (i.e. pre-formed bosons); (I) the insulating behavior observed in c-axis conductivity below $T^*$ [8] may be due to reduction of hopping/tunneling probability between CuO$_2$ planes for a 2e particle compared to that of a single fermion. Then the situation in the cuprates can be mapped to a more general phase diagram in Fig. 3 [5,6] expected for BE-BCS crossover with increasing carrier doping.

When the energy scale of attractive interaction is higher than $T_B$ in the low density region, the singlet pairs will be first formed at $T^*$ and then they undergo BE condensation at a much lower temperature. With increasing carrier doping, $T_c$ will increase as $T_c \propto T_B$ while $T^*$ would decrease. $T_c$ and $T^*$ would merge in the “crossover region”, which corresponds to the “optimum $T_c$” region of the cuprates. The higher density side is characterized by the simultaneous pair-formation and condensation at $T_c$, i.e., the most fundamental feature of BCS condensation. We further conjectured that (J) the crossover will occur where $\epsilon_F$ becomes comparable to the energy scale $\hbar\omega_B$ of the exchange bosons which mediate the pairing interaction [5,6], thus characterizing the underdoped cuprates with retarded coupling. Assuming (J), we can estimate $\hbar\omega_B/k_B$ to be comparable to $\epsilon_F/k_B \sim 2,000$ K of the “optimally doped” cuprates. We recently pointed out [9] that: (K) this energy scale matches well with that of the antiferromagnetic exchange interaction $J$. 

Figure 3. Phase diagram describing BE-BCS crossover with increasing carrier concentration $n$. This phase diagram can be mapped to that of the cuprates by assuming that the pseudo gap temperature $T^*$ corresponds to the formation of normal-state pairs. [5,6]
providing a support for pictures that spin fluctuations indeed mediate the pairing interaction; and (L) the mid infrared reflection (MIR) in optical conductivity of the cuprates, appearing with energy scales comparable to $\hbar \omega_B$, could originate from the pairing interaction, in [6] contrast to the Drude part representing the translational motion of carriers (with an energy scale $\epsilon_F$).

This picture is re-inforced by recent observation of photo-emission studies [10] that the superconducting gap in the “optimal” $T_c$ region evolves smoothly to the pseudo gap in the underdoped region with the same geometrical symmetry. General concepts of negative-U Hubbard model and BE-BCS crossover have been considered by number of authors [11,12]. In 1990, Doniach and Inui pointed out that the pseudo gap behavior may be interpreted in terms of phase fluctuations of the superconducting order parameter [13]. In 1995, Emery and Kivelson [14] discussed that the universal correlations between $T_c$ and $n_s/m^*$ (A) is expected when $T_c$ is determined by the phase fluctuations. Although they argued this as “re-interpretation” of (A), the present author believes that their phase-fluctuation picture is essentially identical to our BE-BCS crossover picture.

Emery and Kivelson calculated the kinetic energy for phase fluctuations, and estimated the maximum condensation temperature $T^\text{max}_\theta \propto n_s/m^* \times y$, where $y$ is a parameter representing distance. For 2-d systems they substituted the interplanar distance $c_{\text{int}}$, which lead to $T^\text{max}_\theta \propto T_B$. Their choice of the coherence length $\xi$ as $y$ for 3-d systems led to unrealistically high value of $T^\text{max}_\theta \gg T_B$, as shown in Fig. 2 for the example of K$_3$C$_60$. (Note that for $\xi \to \infty$, $T^\text{max}_\theta \to \infty$.) The ultimate upperlimit for condensation temperature should be given by $T_B$, since any interaction, dimensionality, and other factors would reduce actual $T_c$ from $T_B$. These considerations indicate that $y=\xi$ for 3-d systems in ref. [14], which led to an apparent difference between 2-d and 3-d systems in their Table 1, is a bad choice. Instead, if one substitutes the interparticle distance for $y$ for 3-d systems, Table 1 of ref. [14] reduces to Fig. 3 of ref. [2].

The role of the 2-dimensional nature of cuprates is an interesting issue. Figure 1 does not give much information on this, as the horizontal axis represents the 3-d carrier density $n_s$ as well as the 2-d density $n_{2d} = n_s \times c_{\text{int}}$ for the 123, 214 and 2223 systems, all having the interlayer distance $c_{\text{int}} \sim 6\AA$. Recently, we have performed $\mu$SR measurements in Hg1201 [15] systems, with $c_{\text{int}} = 9.5 \AA$. Our previous data of nearly-optimally doped TI2201 system [3] represented the case with $c_{\text{int}} = 11.5 \AA$. All these results and those of underdoped 214, 123 and 2223 systems lie approximately on the same straight line when we plot $T_c$ versus $\sigma \times c_{\text{int}} \propto n_{2d}/m^*$. However, when plotted versus $\sigma \times c_{\text{int}} \propto n_{2d}/m^*$ in Fig. 4, we find that: (M) systems with smaller $c_{\text{int}}$ have higher $T_c$ for a given $n_{2d}/m^*$, following a relation $T_c \propto 1/c_{\text{int}}$. This result is consistent with the reduction of $T_c$ for increasing thickness of PrBa$_2$Cu$_3$O$_7$ (PBCO) layer in thin films of YBa$_2$Cu$_3$O$_7$ (YBCO) having a single unit-cell stacked in the c-axis direction with non-superconducting PBCO [16] (see Fig. 4).

This feature $T_c \propto n_{2d}/c_{\text{int}} (=n_s)$ indicates: (N) a Kosterlitz-Thouless transition in its simplest form, where $n_{2d}/m^*$ is the sole factor for $T_c$, in not sufficient for predicting $T_c$; and (O) BE condensation in quasi 2-d systems gives a better

Figure 4. Plot of $T_c$ versus $\sigma \times c_{\text{int}} \propto n_{2d}/m^*$ for the underdoped region of Y123 [1], Hg1201 [15] and nearly-optimally doped TI2201 [3] systems. Inset: $T_c$ vs. $c_{\text{int}}$ in YBCO-PBCO [16].
the reduction of Zn-substituted 214 and 123 systems [18], where Tc should depend exponentially on c_int as \( T_c \propto \exp(-c_{int}) \), leading to \( T_c \propto 1/c_{int} \times n_{2d}/m^* \).

The decrease of \( n_s/m^* \) with increasing Zn in the overdoped Tl2201 systems (feature (C) in Fig. 1) can not be expected in the BCS model with retarded interaction, where the normal state carrier density \( n \) should be equal to \( n_s \). In ref. [3], we proposed (P) a spontaneous microscopic phase separation between superconducting and normal regions (\( n_s < n \)) as a possible explanation. Recently, we found a similar situation in Zn-substituted 214 and 123 systems [18], where the reduction of \( n_s/m^* \) with increasing Zn doping suggests that: (Q) carriers within the region \( \pi c_{int}^2 \) on the CuO\(_2\) planes around each Zn impurity may be excluded from the superfluid – like “swiss cheese”. Specific heat in overdoped Tl2201 and Zn-doped 123/214 systems both exhibit increasing T-linear term at \( T \to 0 \) with increasing carrier/Zn doping [19], further supporting our models (P) and (Q) with phase separation.

The short coherence length \( \xi \) in cuprates will help reduce the energy cost for creating phase boundaries, facilitating phase separation. Indeed the swiss cheese model for Zn-doped systems is reminiscent of the behavior of superfluid \(^4\)He in porous media [20]. For overdoped cuprates, we propose the following scenario: (R) if an abrupt decrease of effective attractive interaction occurs in the cuprates as the doping exceeds the “optimal” concentration, then energy gain for maintaining superconductivity might win over energy cost for phase separation: the “cheese” part composed of regions with local \( n_s \) near the “optimum concentration”, while its volume fraction decreasing as further doping.

In underdoped (M), overdoped (P) and Zn-doped (Q) cuprates, \( T_c \) is proportional to the (spatially averaged) 3-dimensional volume density \( n_s \) of superfluid. This demonstrates fundamental importance of BE condensation.

This study is supported by NSF (DMR-95-10453, 10454) and NEDO (Japan). The author is indebted to Oleg Tchernyshyov for discussions leading to the interpretations (N) and (O).

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