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Doping dependence of thermodynamic properties in cuprate superconductors

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ABSTRACT

The doping and temperature dependence of the thermodynamic properties in cuprate superconductors is studied based on the kinetic energy driven superconducting mechanism. By considering the interplay between the superconducting gap and normal-state pseudogap, the some main features of the doping and temperature dependence of the specific-heat, the condensation energy, and the upper critical field are well reproduced. In particular, it is shown that in analogy to the domelike shape of the doping dependence of the superconducting transition temperature, the maximal upper critical field occurs around the optimal doping, and then decreases in both underdoped and overdoped regimes. Our results also show that the humplike anomaly of the specific-heat near superconducting transition temperature in the underdoped regime can be attributed to the emergence of the normal-state pseudogap in cuprate superconductors.

1. Introduction

The doping and temperature dependence of the thermodynamic properties for cuprate superconductors has been the subject of much experimental and theoretical investigation [1]. In the conventional superconductors [2], the absence of the low-energy electron excitations is reflected in the thermodynamic properties, such as the specific heat C_v. Although small deviations from exponential behavior have been observed in some conventional superconductors at the low-temperatures, the specific heat of the most conventional superconductors is experimentally found to be exponential at the low-temperatures, since the conventional superconductors are fully gaped [2]. However, the characteristic feature of cuprate superconductors is the existence of four nodes on the Fermi surface [3], where the d-wave superconducting (SC) gap vanishes $\bar{\Delta}(\mathbf{k})|_{\rm at\ nodes} = \bar{\Delta}(\cos k_x - \cos k_y)|_{\rm at\ nodes} = 0$. In this case, the thermodynamic properties for cuprate superconductors are decreased as some power of the temperature. Moreover, since cuprate superconductors are the doped Mott insulators, obtained by chemically adding charge carriers to a strongly correlated antiferromagnetic insulating state [3], the thermodynamic properties of cuprate superconductors mainly depend on the extent of dopings, and the regimes have been classified into the underdoped, optimally doped, and overdoped, respectively.

Experimentally, by virtue of systematic studies using the heat capacity measurement technique, some essential features of the evolution of the specific-heat in cuprate superconductors with doping and temperature have been established now [4–8], where the specific-heat in both the SC-state and normal-state in the underdoped regime shows anomalous properties when compared with the case in the optimally doped and overdoped regimes. The early heat capacity measurements [4–6] showed that the specific-heat of cuprate superconductors in the underdoped regime was highly anomalous and deviated strongly from a simple d-wave Bardeen–Cooper–Schrieffer (BCS) form, and the anomalies are a marked reduction in the size of the specific-heat jump near the SC transition temperature T_c and a depression in the normal state above T_c. Later, the heat capacity measurements [7] indicated that the specific-heat has a humplike anomaly near T_c and behaves as a long tail in the underdoped regime, while in the heavily overdoped regime, the anomaly ends sharply just near T_c. Moreover, it was argued these anomalous specific-heat results as evidence that in the underdoped regime the pseudogap is an intrinsic feature of the normal-state density of states that compete with the SC condensate for the low energy spectral weight [4,8]. Furthermore, by virtue of the magnetization measurement technique, the value of the upper critical field and its doping and temperature dependence have been observed for all the temperature $T \leqslant T_c$ throughout the SC dome [9–15], where at the low temperatures, the upper critical field becomes larger as one moves from the underdoped regime to the optimal doping, and then falls with increasing doping in the overdoped regime, forming a domelike shape doping dependence like T_c. However, at a given doping concentration, the temperature dependence of the upper critical field follows qualitatively the pair gap temperature dependence [9–15]. Although the doping and temperature dependence of the thermodynamic properties for cuprate superconductors are well-established experimentally [4–15] and an agreement has emerged theoretically that the specific-heat of cuprate superconductors in the underdoped regime

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is not describable within the simple d-wave BCS formalism, its full understanding is still a challenging issue. In particular, the specific-heat of cuprate superconductors has been calculated based on a phenomenological theory of the normal-state pseudogap state [16], and the results show that the strong suppression of the specific-heat jump near T_c and the corresponding reduction in condensation energy with increased underdoping can be understood as due to the emergence of a pseudogap. However, up to now, the thermodynamic properties of cuprate superconductors have not been treated starting from a microscopic SC theory, and no explicit calculations of the doping and temperature dependence of the upper critical field has been made so far.

In our recent study [17], the interplay between the SC gap and normal-state pseudogap in cuprate superconductors is studied based on the kinetic energy driven SC mechanism [18], where we show that the interaction between charge carriers and spins directly from the kinetic energy by exchanging spin excitations in the higher power of the doping concentration induces the normal-state pseudogap state in the particle-hole channel and the SC-state in the particle–particle channel, then there is a coexistence of the SC gap and normal-state pseudogap in the whole SC dome. In particular, this normal-state pseudogap is closely related to the quasiparticle coherent weight, and therefore it is a necessary ingredient for superconductivity in cuprate superconductors. Moreover, both the normal-state pseudogap and SC gap are dominated by one energy scale, and they are the result of the strong electron correlation. In this paper, we start from this theoretical framework [17], and then provide a natural explanation to the doping and temperature dependence of the thermodynamic properties in cuprate superconductors. We evaluate explicitly the specific-heat and upper critical field, and qualitatively reproduced some main features of the heat capacity and magnetization measurements on cuprate superconductors [4–15]. In particular, we show that in analogy to the domelike shape of the doping dependence of the SC transition temperature, the upper critical field increases with increasing doping in the underdoped regime, and reaches a maximum in the optimal doping, then decreases with increasing doping in the overdoped regime.

The rest of this paper is organized as follows. We present the basic formalism in Section 2, and then the quantitative characteristics of the doping and temperature dependence of the thermodynamic properties are discussed in Section 3, where we show that the humplike anomaly of the specific-heat near T_c in the underdoped regime can be attributed to the emergence of the normal-state pseudogap in cuprate superconductors. Finally, we give a summary in Section 4.

2. Theoretical framework

In cuprate superconductors, the characteristic feature is the presence of the CuO_2 plane [3]. In this case, it is commonly accepted that the essential physics of the doped CuO_2 plane [19] is captured by the $t-J$ model on a square lattice,

$$H=-t\sum_{l\hat{\eta}\sigma}C^{\dagger}_{l\sigma}C_{l+\hat{\eta}\sigma}+t'\sum_{l\hat{\eta}'\sigma}C^{\dagger}_{l\sigma}C_{l+\hat{\eta}'\sigma}+\mu\sum_{l\sigma}C^{\dagger}_{l\sigma}C_{l\sigma}+J\sum_{l\hat{\eta}}\mathbf{S}_l\cdot\mathbf{S}_{l+\hat{\eta}},\qquad(1)$$

where $\hat{\eta}=\pm\hat{x},\pm\hat{y}$, $\hat{\eta}'=\pm\hat{x}\pm\hat{y}$, $C^{\dagger}_{l\sigma}$ $(C_{l\sigma})$ is the electron creation (annihilation) operator, $\mathbf{S}_l=(S^x_l,S^y_l,S^y_l)$ are spin operators, and μ is the chemical potential. This $t-J$ model (1) is in the Hilbert subspace with no doubly occupied electron states on the same site, i.e., $\sum_{\sigma}C^{\dagger}_{l\sigma}C_{l\sigma}\leqslant 1$. To incorporate this electron single occupancy local constraint, the charge-spin separation (CSS) fermion-spin theory [20,21] has been proposed, where the physics of no double occupancy is taken into account by representing the electron as a composite object created by $C_{l\uparrow}=h^{\dagger}_{l\uparrow}S^-_l$ and $C_{l\downarrow}=h^{\dagger}_{l\downarrow}S^+_l$, with the spinful fermion operator $h_{l\sigma}=e^{-i\Phi_{l\sigma}}h_l$ that describes the charge degree of freedom of the electron together with some effects of spin configuration rearrangements due to the presence of the doped hole itself (charge carrier), while the spin operator S_l represents the spin degree of freedom of the electron, then the electron single occupancy local constraint is satisfied in analytical calculations. In this CSS fermion-spin representation, the $t-J$ model (1) can be expressed as,

$$\begin{aligned}H=&\,t\sum_{l\hat{\eta}}\left(h^{\dagger}_{l+\hat{\eta}\uparrow}h_{l\uparrow}S^+_lS^-_{l+\hat{\eta}}+h^{\dagger}_{l+\hat{\eta}\downarrow}h_{l\downarrow}S^-_lS^+_{l+\hat{\eta}}\right)\\&-t'\sum_{l\hat{\eta}'}\left(h^{\dagger}_{l+\hat{\eta}'\uparrow}h_{l\uparrow}S^+_lS^-_{l+\hat{\eta}'}+h^{\dagger}_{l+\hat{\eta}'\downarrow}h_{l\downarrow}S^-_lS^+_{l+\hat{\eta}'}\right)-\mu\sum_{l\sigma}h^{\dagger}_{l\sigma}h_{l\sigma}\\&+J_{\rm eff}\sum_{l\hat{\eta}}\mathbf{S}_l\cdot\mathbf{S}_{l+\hat{\eta}},\end{aligned}\qquad(2)$$

where $J_{\rm eff}=(1-\delta)^2J$, and $\delta=\langle h^{\dagger}_{l\sigma}h_{l\sigma}\rangle=\langle h^{\dagger}_lh_l\rangle$ is the charge carrier doping concentration.

For discussions of the doping and temperature dependence of the thermodynamic properties in cuprate superconductors, we need to evaluate the internal energy of the system, which can be separated into two parts in the CSS fermion-spin representation as,

$$U_{\rm total}(T,\delta)=U_{\rm charge}(T,\delta)+U_{\rm spin}(T,\delta),\qquad(3)$$

with $U_{\rm charge}(T,\delta)$ and $U_{\rm spin}(T,\delta)$ are the corresponding contributions from the charge carriers and spins, respectively, and can be expressed as,

$$U_{\rm charge}(T,\delta)=2\int_{-\infty}^{\infty}\frac{{\rm d}\omega}{2\pi}\omega\rho_{\rm charge}(\omega,T,\delta)n_F(\omega),\qquad(4a)$$

$$U_{\rm spin}(T,\delta)=\int_{-\infty}^{\infty}\frac{{\rm d}\omega}{2\pi}\omega\rho_{\rm spin}(\omega,T,\delta)n_B(\omega),\qquad(4b)$$

where $\rho_{\rm charge}(\omega,T,\delta)$ is the charge carrier density of states, $\rho_{\rm spin}(\omega,T,\delta)$ is the spin density of states, and the two in the charge carrier part of the internal energy is for spin degeneracy, while $n_F(\omega)$ and $n_B(\omega)$ are the fermion and boson distribution functions, respectively.

As in the conventional superconductors, the key phenomenon occurring in cuprate superconductors in the SC state is the pairing of charge carriers [3]. The system of charge carriers forms pairs of bound charge carriers in the SC state, while the pairing means that there is an attraction between charge carriers. For a microscopic description of the SC-state of cuprate superconductors, the kinetic energy driven SC mechanism [18] has been developed based on the CSS fermion-spin theory [20,21], where the attraction between charge carriers mediated by the spin excitations occurs directly through the kinetic energy, then the electron Cooper pairs originating from the charge carrier pairing state are due to the charge-spin recombination, and their condensation reveals the SC ground-state. In particular, the SC transition temperature is identical to the charge carrier pair transition temperature. Within this kinetic energy driven SC mechanism, we have discussed the interplay between the SC-state and normal-state pseudogap state in cuprate superconductors [17], and the obtained phase diagram with the two-gap feature is consistent qualitatively with the experimental data observed on different families of cuprate superconductors [22]. Following these previous discussions [17,18], the full charge carrier diagonal and off-diagonal Green's functions and the mean-field (MF) spin Green's functions can be obtained explicitly as,

$$g(\mathbf{k},\omega)=\frac{U^2_{1{\rm h}\mathbf{k}}}{\omega-E_{1{\rm h}\mathbf{k}}}+\frac{V^2_{1{\rm h}\mathbf{k}}}{\omega+E_{1{\rm h}\mathbf{k}}}+\frac{U^2_{2{\rm h}\mathbf{k}}}{\omega-E_{2{\rm h}\mathbf{k}}}+\frac{V^2_{2{\rm h}\mathbf{k}}}{\omega+E_{2{\rm h}\mathbf{k}}},\qquad(5a)$$

$$\begin{aligned}\Gamma^{\dagger}(\mathbf{k},\omega)=&-\frac{\alpha_{1\mathbf{k}}\bar{\Delta}_{\rm h}(\mathbf{k})}{2E_{1{\rm h}\mathbf{k}}}\left(\frac{1}{\omega-E_{1{\rm h}\mathbf{k}}}-\frac{1}{\omega+E_{1{\rm h}\mathbf{k}}}\right)\\&+\frac{\alpha_{2\mathbf{k}}\bar{\Delta}_{\rm h}(\mathbf{k})}{2E_{2{\rm h}\mathbf{k}}}\left(\frac{1}{\omega-E_{2{\rm h}\mathbf{k}}}-\frac{1}{\omega+E_{2{\rm h}\mathbf{k}}}\right),\end{aligned}\qquad(5b)$$