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Electronic specific heat of anisotropic superconductors and its doping dependence

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Abstract

The specific heat of electrons in *p*- and *d*-symmetry superconducting states (C_S) is comparatively studied within the BCS framework. This study is performed on a square lattice described by a generalized Hubbard model, in which correlated-hopping interactions are included in addition to the repulsive Coulomb ones. The temperature dependences of C_S show a power law behavior, instead of the exponential behavior found in the *s* channel, and for a given gap amplitude the number of nodes in the gap enhances C_S in the low temperature regime. Moreover, the normalized discontinuity of C_S at the critical temperature (T_c) is smaller than the BCS analytical result of 1.43 for a wide range of electron densities. Finally, the results show that the single-particle van Hove singularity determines the location of the maximum gap, and then the position of the maximum discontinuity of the specific heat at T_c.

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The low-temperature electronic specific heat is highly sensitive to the low-energy excitations of the system; hence it gives information about the symmetry of superconducting states. A superconductor with an isotropic gap has an electronic specific heat (C_S) that depends exponentially on temperature while an anisotropic gap leads to an electronic specific heat following a power law of the temperature, as occurred in the cuprate superconductors [1] and in Sr_2RuO_4 [2]. For these materials, three-band Hubbard models have been proposed to describe the dynamics of the carriers on the CuO_2 and RuO_2 planes, and the electronic states close to the Fermi energy can be reasonably well described by a single-band square-lattice tight-binding model with next-nearest neighbor hoppings [3,4]. Recently, we have found that the second-neighbor correlated-hopping interaction (Δt_3) is essential in the $d_{x^2-y^2}$ wave superconductivity [5] and a further small distortion of the right angles in the square lattice leads to *p*-wave superconductivity [6]. It is worth mentioning that a similar distortion has been observed at the surface of Sr_2RuO_4 [7]. In this work, we study C_S of *p* and *d* anisotropic superconducting states by means of the previously used generalized Hubbard model [5,6] with nearest (t) and next-nearest neighbor (t') hoppings. In addition, correlated-hopping interactions between first (Δt) and second (Δt_3) neighbors are considered along with on-site (U) and nearest-neighbor (V) Coulomb interactions [5]. If we further consider a small distortion of the right angles in the square lattice, the second-neighbor interactions change and their new values are $t'_{\pm} \equiv t' \pm \delta$ and $\Delta t_3^{\pm} \equiv \Delta t_3 \pm \delta_3$, where $\pm$ refers to the $\hat{x} \pm \hat{y}$ direction. Applying the BCS formalism to our generalized Hubbard model, we obtain two coupled integral equations [6], which determine the superconducting gap (Δ_α) and the chemical potential (μ_α) for a given temperature (T) and electronic density (n), where $\alpha = p$ or d indicates the superconducting gap symmetry. Hence, the electronic specific heat of

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superconducting states (C_S^α) is given by [8]

$$C_S^\alpha = \frac{2k_B\beta^2}{4\pi^2}\int\int_{1BZ} f(E_k^\alpha)[1-f(E_k^\alpha)]\times \left[(E_k^\alpha)^2+\beta E_k^\alpha\frac{dE_k^\alpha}{d\beta}\right],$$

where $\beta = 1/(k_B T)$, $f(E)$ is the Fermi–Dirac distribution, $E_k^\alpha = \sqrt{[\varepsilon(k)-\mu_\alpha]^2+\Delta_\alpha^2(k)}$ is the single-particle excitation energy, $\varepsilon(k)$ is the mean-field dispersion relation and μ_α is the chemical potential [6]. The electronic specific heat of the normal state (C_N) can be obtained by taking Δ_α equal to zero.

In Fig. 1, the electronic specific heat (C) of p- (open circles) and d-wave (open squares) superconducting states is plotted as a function of temperature (T), for arbitrary U, $V=\delta=0$, $t=-1$, $t'=0.45|t|$, $\Delta t=0.5|t|$, $\Delta t_3=0.15|t|$, $\delta_3=0.1|t|$, with electron densities (a) $n=0.5$, (b) $n=0.56$, and (c) $n=0.7$. Notice that T_c of p and d superconducting states, shown by the discontinuities of C, strongly depends on n. For $n=0.56$, the T_c of both channels have almost the same value, but C_S of d-channel is larger than that of the p-channel in the low-temperature regime, due to their different numbers of nodes in the superconducting gap. However, this fact does not occur when Δ_p is significantly smaller that Δ_d, as shown in Fig. 1(a).

Fig. 2(a) shows T_c (open symbols) and Δ_α (solid symbols) for $\alpha = p$ (circles) and d (squares) as a function of n. Observe that there are two maxima for the p-channel and only one for the d-channel. We have verified that these maximums occur when μ is located near a single-particle van Hove singularity (VHS). Within the mean-field theory,

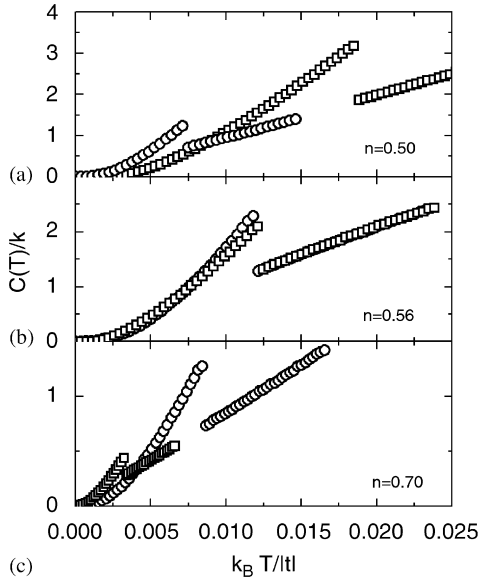

Fig. 1. Temperature dependence of the electronic specific heat (C) of p- (open circles) and d-wave (open squares) superconducting and normal states separated by a discontinuity located at T_c, for electron densities (a) $n=0.5$, (b) $n=0.56$ and (c) $n=0.7$.

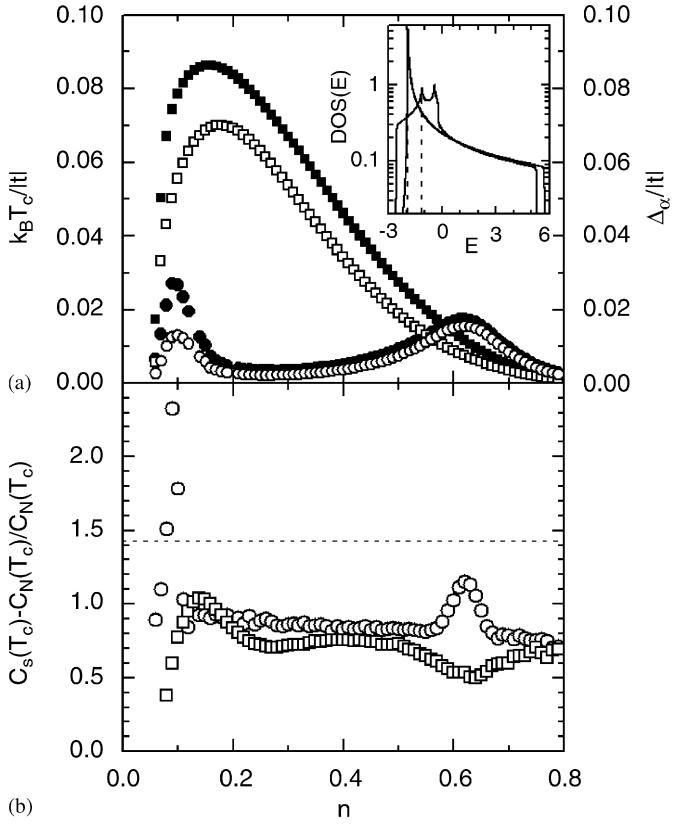

Fig. 2. (a) Critical temperature (T_c, open symbols) and superconducting gap (Δ_α, solid symbols), for $\alpha = p$ (circles) and d (squares), versus electron density (n). Inset: single-particle density of states (DOS) vs. energy (E) for $n=0.091$ (grey line) and $n=0.62$ (black line), where the dashed lines indicate the corresponding chemical potentials. (b) Normalized p- (open circles) and d-wave (open squares) electronic specific heat discontinuity as a function of n. The dashed line indicates the BCS result [8].

the effective hopping strengths are $t_{MF} = t + n\Delta t$ and $t'_{MF\pm} = t'_\pm + 2n(\Delta t_3 \pm \delta_3)$, hence, the location of VHS depends on n. For a system with the mentioned parameters and $n=0.091$ (grey line in inset) or $n=0.62$ (black line in inset), the mean-field single-particle density of states (DOS), evaluated at the corresponding μ indicated by the dashed lines in the inset, take very high values, where the integration up to μ lead to the respective n. On the other hand, according to the BCS theory, the T_c is maximum when $W\cdot \mathrm{DOS}(\mu)$ takes its highest value, where W is the average attractive interaction [9]. Therefore, the location of the maximum T_c is shifted by the smooth dependence of W with n [9]. For the second maximum, d-channel superconductivity is disfavored for high n, since the anisotropy in the second neighbor interactions is proportional to n, i.e., $t'_{MF+} - t'_{MF-} = 4n\delta_3$.

Fig. 2(b) shows the normalized discontinuities in the electronic specific heat at the critical temperature (T_c) for p- and d-wave superconducting states as a function of n. Observe that these discontinuities are smaller than the BCS analytical value of 1.43 for a wide range of n.

In summary, the presence of nodes in the superconducting gap significantly modifies the electronic absorption of

the thermal energy at low temperatures. We observe a power law behavior and a smaller specific heat discontinuity at T_c in a wide range of n for p- and d-wave superconductors, in comparison with the s-channel behavior. Finally, the optimal n for T_c and Δ_α is found when μ is located close to a VHS.

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