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Nodal effects on the electronic specific heat of anisotropic superconductors

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Abstract

Based on the BCS formalism, the electronic specific heat of d-symmetry superconducting states is studied. 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. Instead of the exponential temperature dependence for the s-channel, the results show second and higher power-law behaviors for d-wave superconducting specific heat, depending on the angular dependence of the single-excitation energy gap occurred at different carrier concentrations. The results of this study could help to understand a variety of power-law behaviors observed in $La_{2-x}Sr_xCuO_4$ superconductors.

Keywords: Superconducting gap symmetry; Hubbard model; Electronic specific heat

The energy spectrum of elementary excitations in solids determines the temperature dependence of their specific heat. In particular, for a superconductor it gives information regarding to the symmetry of its superconducting state. An s-wave superconductor has an exponentially temperature-dependent electronic specific heat (C), while an anisotropic nodal superconducting gap leads to a power-law C, as occur 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 second neighbor hoppings [3,4]. In this work, we study C of d-wave superconducting states on a square lattice with a lattice parameter a and a single-band generalized Hubbard Hamiltonian [5]:

$$\hat{H} = t\sum_{\langle i,j\rangle,\sigma} c^{+}_{i\sigma}c_{j\sigma} + t'\sum_{\langle\langle i,j\rangle\rangle,\sigma} c^{+}_{i\sigma}c_{j\sigma} + U\sum_{i} n_{i\uparrow}n_{i\downarrow} + \frac{V}{2}\sum_{\langle i,j\rangle} n_i n_j + \Delta t\sum_{\langle i,j\rangle,\sigma} c^{+}_{i\sigma}c_{j\sigma}(n_{i-\sigma}+n_{j-\sigma}) + \Delta t_3\sum_{\substack{\langle\langle i,j\rangle\rangle,\sigma\\ \langle i,j\rangle,\langle j,l\rangle}} c^{+}_{i\sigma}c_{j\sigma}n_{l-\sigma}, \quad (1)$$

where $c^{+}_{i\sigma}$ ($c_{i\sigma}$) is the creation (annihilation) operator with spin $\sigma = \downarrow$ or $\uparrow$ at site i, $n_{i,\sigma} = c^{+}_{i\sigma}c_{i\sigma}$, $n_i = n_{i,\uparrow} + n_{i,\downarrow}$, $\langle i,j\rangle$ and $\langle\langle i,j\rangle\rangle$ denote first- and second-neighbor sites, Δt and Δt_3 are first- and second-neighbor correlated hopping integrals, respectively. Applying the BCS formalism to Eq. (1), two coupled integral equations are obtained [5]. They determine the superconducting gap (Δ_d) and the chemical potential (μ) for a given temperature (T) and electronic density (n). The critical temperature (T_c) is obtained when $\Delta_d = 0$. The C of superconducting states is given by [6]

$$C = \frac{2k_B\beta^2}{4\pi^2}\iint_{1BZ} d^2k f(E_{\mathbf{k}})[1-f(E_{\mathbf{k}})] \times\left[(E_{\mathbf{k}})^2 + \beta E_{\mathbf{k}}\frac{dE_{\mathbf{k}}}{d\beta}\right],$$

where $\beta = 1/k_BT$, $f(E)$ is the Fermi–Dirac distribution, $E_{\mathbf{k}} = \sqrt{[\varepsilon(\mathbf{k})-\mu]^2 + \Delta_d^2(\mathbf{k})}$ is the single-excitation energy, $\varepsilon(\mathbf{k})$ is the mean-field dispersion relation, μ is the chemical potential

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and $\Delta_d(\mathbf{k}) = \Delta_d[\cos(k_x a) - \cos(k_y a)]$ [5]. The electronic specific heat of the normal state can be obtained by taking Δ_d equal to zero.

Fig. 1 shows T_c as a function of n for $t' = -0.45|t|$, $\Delta t = 0.5|t|$, $\Delta t_3 = 0.1|t|$, $V = 0$ and arbitrary U. Observe that the maximum T_c is located at the optimal $n = 1.73$, similar to that observed in cuprate superconductors since the doping concentration x is related to $2-n$ in this model.

In Fig. 2, two electronic densities (a) $n = 1.2$ and (b) $n = 1.94$ are chosen from Fig. 1 to calculate their C and compared with experimental data obtained from $La_{2-x}Sr_xCuO_4$ for $x = 0.22$ and 0.1, respectively [7]. Insets of Fig. 2 show the corresponding theoretical angular dependences of the single-excitation energy gap (Δ) defined as the minimum value of $E_{\mathbf{k}}$ in $\mathbf{k}$ direction [8]. The polar angle is given by $\theta = \tan^{-1}(k_y/k_x)$. Notice that for the overdoped regime, $n < 1.73$, Δ has a $d_{x^2-y^2}$ symmetry and in consequence C is proportional to T^2 as obtained in Ref. [9]. However, for the underdoped regime, $n > 1.73$, $C \propto T^{\nu}$ with $\nu > 2$ since Δ has a d_{xy}-like symmetry without real nodes. For low-energy single-particle excitations, the lack of real nodes has a similar effect as in an s-wave superconductor. In consequence, for $T \ll T_c$, C has an almost exponential behavior. The residual C/T value at $T = 0$ in experimental data could be due to the chemical or electronic inhomogeneity of the sample [10], and this fact is not considered in the theory.

In conclusion, the low-temperature behavior of C is very sensitive to the deepness of nodes in Δ, which symmetry depends on n, as found in scanning tunneling experiments [11]. It is worth mentioning that d_{xy}-like gaps without real nodes have been observed in cuprate superconductors [12]. These results could help to understand the different $C(T)$ behaviors observed in d-wave superconductors.

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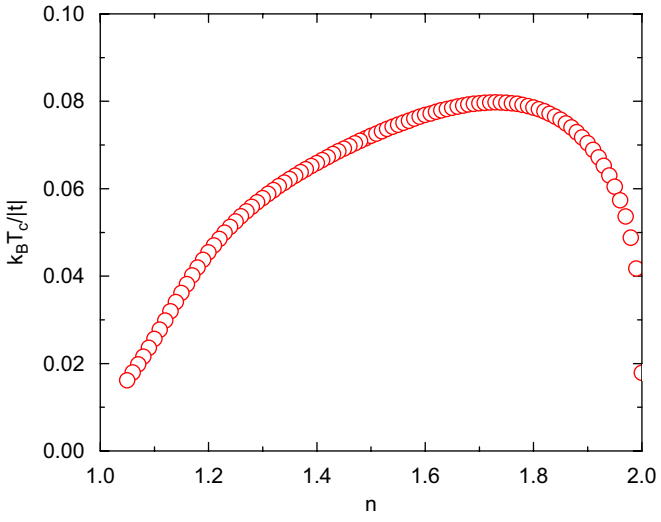

Fig. 1. Critical temperature (T_c) as a function of the electron density (n) for $t' = -0.45|t|$, $\Delta t = 0.5|t|$, $\Delta t_3 = 0.1|t|$, $V = 0$ and arbitrary U.

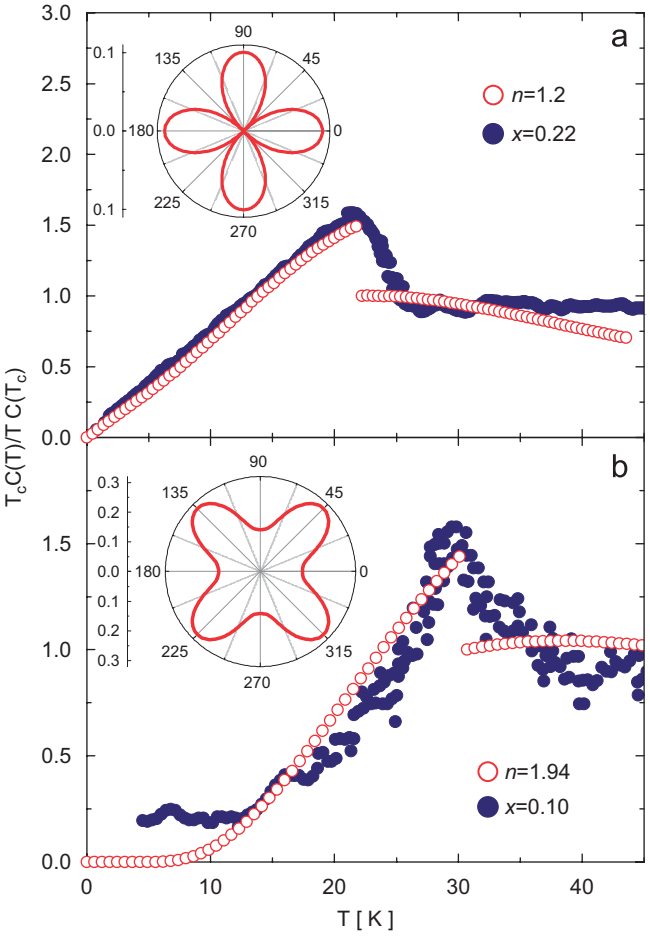

Fig. 2. Theoretical (open circles) d-wave electronic specific heat (C) versus temperature (T) for systems with the same parameters as in Fig. 1 in comparison with experimental data (solid circles) obtained from $La_{2-x}Sr_xCuO_4$ [7]. Insets: corresponding single-excitation energy gaps ($\Delta/|t|$) as a function of the polar angle (θ).

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