Model for the variation upon doping of the isotope coefficient in high-T_c superconductors

Félix Yndurain
Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, 28049-Madrid, Spain
(Received 23 August 1994)

A model, recently developed to study the competition between conventional BCS superconductivity and spin density waves in two-dimensional systems, is extended to study the variation of the isotope effect with the hole concentration. It is found that the isotope coefficient α varies abruptly near the hole concentration where the superconducting critical temperature is maximum. The isotope coefficient α varies from 0.80 to 0.04 in a narrow hole concentration range in qualitative agreement with experimental data for La_2CuO_4-based superconductors.

One of the most intriguing experimental results concerning high-T_c superconductors is the variation of the isotope effect as a function of the hole concentration.[1] As a general result concerning high-T_c superconductors it can be said that the amplitude of the isotope effect changes substantially with the hole concentration at the vicinity of the hole concentration range where the critical temperature is highest. The isotope coefficient, defined by

$$\alpha=-\frac{\partial \ln T_c}{\partial \ln M}\ , \tag{1}$$

is in the range 0.4–0.8 in the low doping regime whereas it is almost negligible in the high doping regime. In Fig. 1, the experimental results for LaBaCuO are shown.[2] Both the variation of the superconducting critical temperature and the isotope coefficient are drawn. For other high-T_c superconductors the results are qualitatively similar although less striking as far as the variation of α with hole doping is concerned.[3,4] The fact that the isotope effect is not negligible reveals the role played by phonons (other experimental results[5,6] indicate the importance of phonons, too). However, the anomalous variation of this effect with the hole concentration cannot be simply explained considering only the electron-phonon interaction. This strongly suggests another complementary mechanism involved in the superconducting transition.

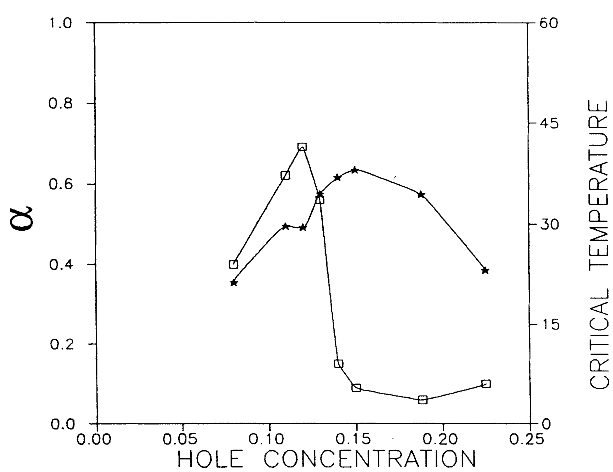

FIG. 1. Experimental results (Ref. 2) for the variation of the isotope coefficient α (open squares) and superconducting critical temperature (stars) with the hole concentration in LaBaCuO.

In this work I consider the model developed in a previous work[7] intended to study the competition between conventional BCS superconductivity and magnetic correlations and extend it to analyze the isotope effect, i.e., the variation of T_c with the atomic mass. I consider a model two-dimensional system to describe the CuO_2 planes such that the Fermi energy lies close to a saddle point of the noninteracting electronic bands (in fact at exactly the saddle-point energy for the undoped case). The details of the band dispersion are intentionally left unspecified, whereas the density of states $\rho(E)$ is approximated by $\rho(E)=(1/2W)\ln[W/|E|]$ where W is the half bandwidth. The closeness of the Fermi level to a logarithmic singularity in the density of states caused by a saddle point has been already considered[8–11] as responsible for the unusual high critical temperature in high-T_c superconductors.

It is well established that magnetic correlations play an important role in the superconducting state.[12] In order to consider them and due to the low-dimensional character of ceramic superconductors, the possibility of spin-density-wave (SDW) formation is considered. It is known[13] that in low-dimensional systems ground states displaying charge and/or spin broken symmetries are rather common giving rise to either SDW or charge-density waves (CDW). The competition between superconductivity and charge- and spin-density waves in two-dimensional systems has been analyzed in Ref. 14 and will not be considered in this work. Conventional superconductivity (i.e., BCS like) and CDW are produced by strong electron-phonon coupling. On the other hand, SDW are originated by a strong electron-electron repulsion which, in principle, tends to destroy superconductivity. It is therefore worth analyzing the competition and possible cooperation between these broken symmetries in the framework of high-T_c superconductors.

I start with the model Hamiltonian

$$H = H_0 + H_{e\text{-ph}} + H_{e\text{-}e} \ . \tag{2}$$

The one-electron Hamitonian H_0 reads

$$H_0 = \sum_{k,\sigma} E(k) C^*_{k\sigma} C_{k\sigma} \ , \tag{3}$$

where $E(k)$ is the one-electron band dispersion at the CuO_2 planes and $C^*_{k\sigma}$ ($C_{k\sigma}$) stands for the creation (annihilation) operator of electrons with momentum k and spin σ. The electron-phonon interaction has the usual form

$$H_{e\text{-ph}} = \sum_{k,q,\sigma} V(k,q) C^*_{(k+q)\bar\sigma} C^*_{(-k-q)\sigma} C_{-k\sigma} C_{k\bar\sigma} \ , \tag{4}$$

such that it is approximated by the BCS expression

$$V(k,q) = \begin{cases} -V_0 & \text{if } |E(k)-E_F| < \hbar\omega_D \text{ and } |E(k+q)-E_F| < \hbar\omega_D \\ 0 & \text{otherwise} \ , \end{cases} \tag{5}$$

where E_F is the Fermi energy and ω_D stands for the Debye phonon frequency. The electron-electron part $H_{e\text{-}e}$ is assumed to take the following Hubbard-like form:

$$H_{e\text{-}e} = U/2 \sum_{k,k',\sigma} C^*_{k\sigma} C^*_{k'\bar\sigma} C_{k'\sigma} C_{k\bar\sigma} \ . \tag{6}$$

As in previous work[7] the Hamiltonian (2) can be approximated by

$$H = H_0 + H_{\mathrm{SC}} + H_{\mathrm{SDW}} \ , \tag{7}$$

where H_{SC} is similar to the BCS Hamiltonian H_{BCS} of the form

$$H_{\mathrm{BCS}} = -\Delta \sum_k{}' (C^*_{k\sigma} C^*_{-k\bar\sigma} + C_{-k\bar\sigma} C_{k\sigma}) + \Delta^2/V_0 \ , \tag{8}$$

the prime indicates that the summation is restricted to the states k such that $|E(k)-E_F| < \hbar\omega_D$. The superconducting order parameter Δ is, in this case, energy dependent through the following form:

$$\Delta[E(k)] = \begin{cases} \Delta_2 - \Delta_1 & \text{if } |E(k)-E_F| < \hbar\omega_D \\ -\Delta_1 & \text{otherwise} \ , \end{cases} \tag{9}$$

where

$$\Delta_2 = V_0 \sum_k{}' \langle C^*_{k\sigma} C^*_{-k\bar\sigma} \rangle \ , \tag{10}$$

$$\Delta_1 = U \sum_k \langle C^*_{k\sigma} C^*_{-k\bar\sigma} \rangle \ . \tag{11}$$

The SDW part of the Hamiltonian H_{SDW} has the form

$$H_{\mathrm{SDW}} = -\gamma \sum_{k\sigma} C^*_{k\sigma} C_{k+Q\bar\sigma} + \gamma^2/U \ , \tag{12}$$

where the SDW order parameter is

$$\gamma = U \sum_{k\sigma} \langle C^*_{k\sigma} C_{k+Q\bar\sigma} \rangle \ . \tag{13}$$

The Hamiltonian (7) is solved by performing a unitary transformation and the order parameters calculated self-consistently in the manner described in Refs. 7 and 15. It is important to mention that, due to the two-dimensional character of the CuO_2 planes, there is a saddle point in the one-electron bands, thus the unperturbed electron states are such that $E(k) = E(k+Q)$ if the energy origin is taken at the saddle-point energy. Therefore, contrary to what happens in a one-dimensional-like case where $E(k) = -E(k+Q)$, the existence of a SDW produces no gap in the density of states but rather a shift in the nonperturbed bands. The existence of the saddle point in the one-electron bands induces a logarithmic singularity in the density of states which relevance for the high-T_c superconductors phenomenology has been extensively discussed in the literature.[8–11] It must be stressed that the model is intended to describe the superconducting region and therefore it is unappropriated to describe the insulating antiferromagnetic phase.

In Fig. 2, the calculated (at $T=0$ and $x=0.1$) phase diagram for the possible different ground states depending on the values of the electron-electron and electron-phonon interaction parameter is shown (the values of $\hbar\omega_D = 300$ K and $W = 2000$ K are used throughout this work). We first notice in this figure that large U parameter favors the formation of SDW and tends to suppress superconductivity. On the other side, large V_0 favors superconductivity and destroys SDW. For small values of both parameters both possible broken symmetries destroy each other giving rise to a paramagnetic phase (denoted P

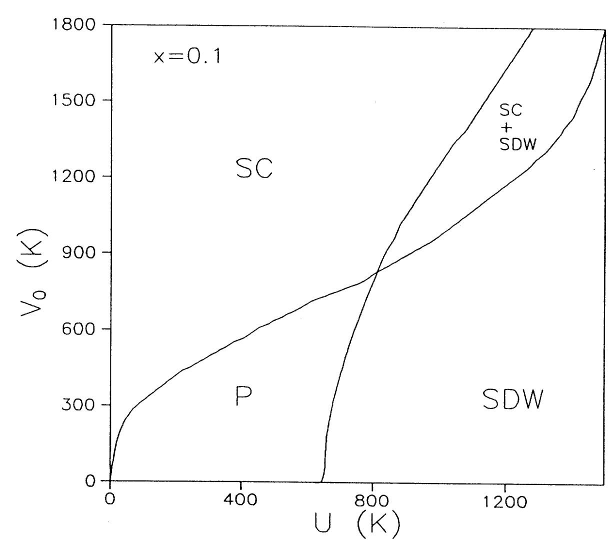

FIG. 2. Phase diagram in terms of the electron-electron and electron-phonon interaction parameters at $T=0$ and hole occupation $x=0.1$. The diagram shows coexistence and annihilation of superconductivity (SC) and SDW. The phase P is the paramagnetic phase produced by the annihilation of superconductivity by the electron-electron interaction.

in the figure). However, for large values of both U and V_0 both superconductivity and SDW coexist in a large portion of the phase space. As indicated in Ref. 14 part of the pure superconductivity phase region is destroyed when the possibility of CDW is considered, nevertheless, a detailed phase boundary has not been determined yet due to numerical uncertainty in the calculation.

In order to understand how the order parameters vary in the case of coexistence of superconductivity and SDW in Fig. 3 the variation of the superconducting order parameters Δ_2 and Δ_1 and the SDW γ as a function of temperature are shown for $V_0=1750$ K and $U=1400$ K. The superconducting gap $\Delta_2-\Delta_1$ decays near T_c faster than in a pure BCS case. This is a result of the competing superconductivity and SDW (in the case of CDW is similar) order parameters. The SDW order parameter being largest at the superconductivity critical temperature. It is worth mentioning that, in the case of coexistence of superconductivity and SDW, the electrons are, at the same time, superconducting and display magnetic correlations. Magnetic ordering does exist above the superconducting T_c which could be related to the anomalous behavior of the so-called normal state.[12,16]

To study the isotope effect I consider the variation of the superconducting transition temperature when varying the Debye cutoff phonon frequency. It is therefore considered that ω_D varies like $M^{-1/2}$, whether the oxygen or the copper mass is involved is beyond the capability of the model. The isotope coefficient α is then calculated numerically according to Eq. (1). Results of the calculation for the set of parameters used throughout this work (for other parameters the results are qualitatively similar) are shown in Fig. 4. We first notice the variation of the isotope coefficient near the hole concentration where the superconducting critical temperature is maximum. The qualitative behavior of α is very similar to the experimental result for LaBaCuO of Fig. 1. The origin of this behavior of the isotope coefficient is intimately related to the coexistence of the SDW and superconductivity which in turn is responsible for the existence of a maximum in T_c. In order to qualitatively understand this anomalous behavior of the isotope effect I have plotted in Fig. 5 the electronic density of states for different hole concentrations at the temperature just above T_c. Therefore the variations of the density of states curves is due solely to the presence of the SDW, the separation between the two peaks being proportional to the SDW order parameter γ. When the SDW is large ($x=0.15$, say) the density of

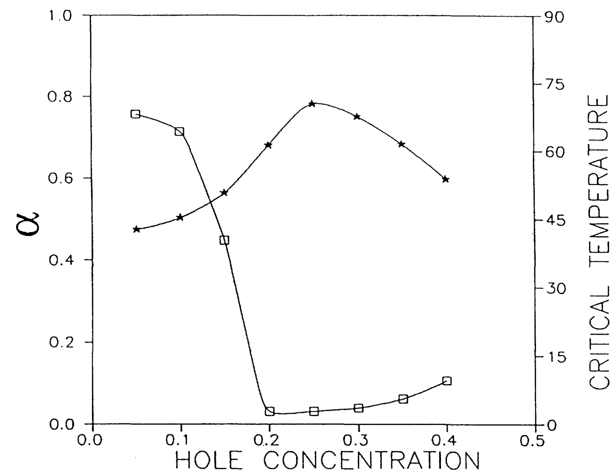

FIG. 4. Results for the variation of the isotope coefficient α (open squares) and superconducting critical temperature (stars) with the hole concentration for the set of parameters used throughout the work.

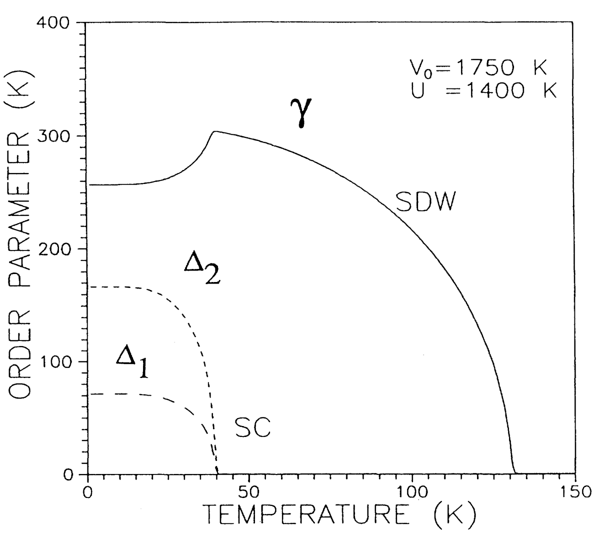

FIG. 3. Variation with temperature of the superconductivity (dashed lines) and SDW (solid lines) order parameters for $x=0.1$.

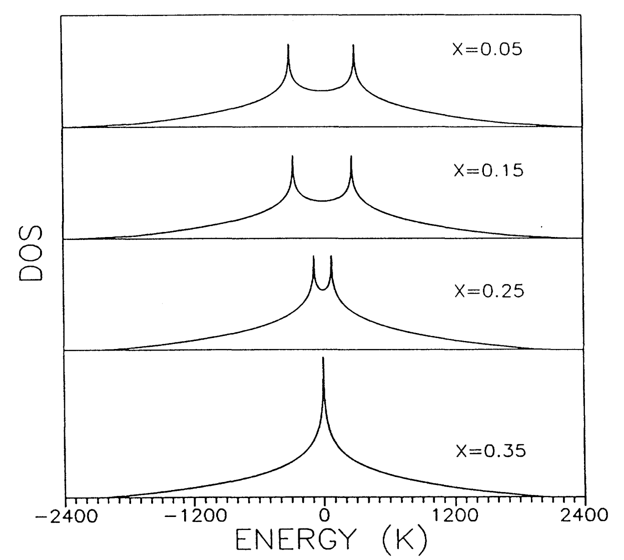

FIG. 5. One-electron densities of states for different values of the hole doping in the presence of a SDW and at a temperature just above the superconducting critical temperature T_c. The Fermi energy lies very close to 0 for the different dopings.

states varies very rapidly near the Debye frequency and therefore the isotope effect is large. However, when the SDW is small or zero, the main contribution of the density of states to the superconducting phase lies within the Debye frequency cutoff and the isotope effect is then negligible. As indicated above, the results are qualitatively similar for other set of parameters as long as there is coexistence between superconductivity and SDW. By varying, for instance, the bandwidth W, the variation with the hole concentration of the isotope coefficient can be smoother than above. In Fig. 6, the results for $W=2200$ K along with the experimental results for YBaCuO-based superconductors are drawn.

The variation of the isotope coefficient near the maximum T_c has also been recently discussed[17] in the framework of strong Coulomb correlations in the phonon-mediated strong-coupling superconductivity.

In summary, I have presented a model which qualitatively accounts for the anomalous variation of the isotope effect upon doping in high-T_c superconductors. In spite of the simplicity and the limitations of the model, the results strongly suggest that this anomalous behavior is due to the coexistence of spin-density wave and superconducting ground states. The results of the calculations are certainly only in qualitative agreement with the experimental data, a much better agreement could have been obtained by fitting the model parameters. However, the model is only intended to describe the experimental trends rather than to reproduce accurately experimental data. The competition of the particular ground state discussed in this work with charge-density waves can be very important and it is being currently considered.

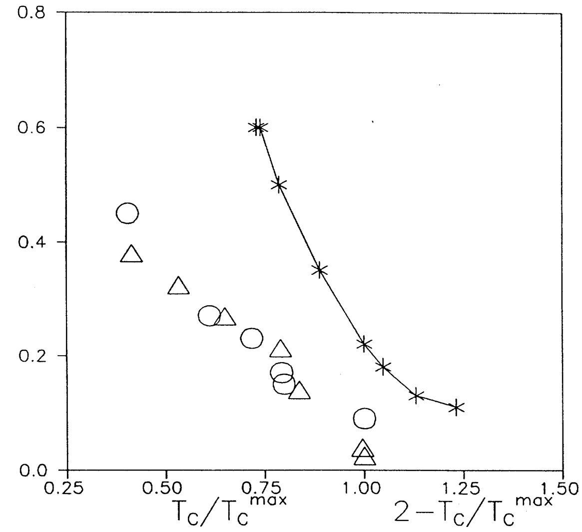

FIG. 6. Variation of the isotope coefficient α with T_c. Theoretical results for $W=2200$ K (stars). Triangles and circles stand for the experimental results for YBaCuO-based samples of Refs. 3 and 4, respectively.

Work supported partially by the Dirección General de Investigación Cinetífica y Technológica (DGIYCT) through Grant No. PB92-0169.

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