OXYGEN-DISPLACIVE INTERACTION IN HIGH-TEMPERATURE SUPERCONDUCTORS

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The two-dimensional motion of the charge carriers (holes) in the Cu-oxygen layers of the high-temperature superconductors is assumed to be governed by a Hubbard-type hamiltonian whereof Coulomb repulsion is greatly diminished by the low-site occupancy. The charge carriers experience a strong interaction with the oxygen lattice which may, in its simplest form, be written as [1]

$$- g_0 \sum_{i\sigma} Q_i n_{i\sigma} - g_1 \sum_{<ij>\sigma} Q_i n_{j\sigma} \quad , \qquad (1)$$

where Q_i is the harmonic-oscillator coordinate of the i-th Cu-oxygen aggregate, $n_{i\sigma}$ is the occupation number of the electronic state with spin σ localized on the i-th site and the summation $<ij>$ extends over the nearest-neighbours. This interaction shifts the lattice coordinates to new equilibrium positions (as observed experimentally) and induces an attraction among the charge carriers which, under certain conditions, may lead to a superconductivity of classical Cooper-pairing type. The most notable feature of this pairing interaction is the fact that it affects all the available electronic states in the conduction band, what explains the high values of the critical temperature.

For a model disc-like Fermi sea and assuming a gap at the half-filling of the Brillouin zone (arising probably from antiferromagnetic ordering) the critical temperature [2]

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$$T_c = 2.28\sqrt{3}\pi\ t\ x\ \exp[\alpha/(x-2/\pi)]\ ,\quad \alpha = t/2(J-t)\ , \qquad (2)$$

is obtained, where t is the (renormalized) bandwidth parameter, $J = g_0 g_1/M\omega^2$ is the strength of the attractive interaction, M is the oxygen mass, ω is the characteristic frequency of the lattice and x is the hole concentration. The latter parameter is given by the charge neutrality of the chemical formula; for example $La_{2-x}M_xCuO_4$ for La-based compounds (M being here an alkaline earth), $RM_2Cu_3O_{6.5+1.5x}$ for the 123-class of superconductors (with R = Y, Sc or lanthanide rare-earth element), $R_2Ca_nM_2Cu_{n+1}O_{6+2n+(n+1)x/2}$ for the 2n2(n+1)-class of superconductors n = 0, 1, 2 (where R = Bi for M = Sr and R = Tl for M = Ba), etc. It is remarkably in this context [3] that the 124-class of compounds with fixed stoichiometry $RM_2Cu_4O_8$ (x = 0.25) displays an impressively narrow range of critical temperatures around $T_c \sim 77K$. A non-monotonous (increasing-then-decreasing) x-dependence of T_c is predicted by (2) with a maximum T_c reached for a certain optimum concentration, in agreement with the experimental data [4].

An isotope shift

$$-\partial(\ln T_c)/\partial(\ln M) = (1-3\eta)\left[\frac{\alpha(2\alpha+1)}{2/\pi - x} - 1\right]\ln(t_o/t) + (1-2\eta)\frac{\alpha(2\alpha+1)}{2/\pi - x} \qquad (3)$$

is also predicted by this theory [5], where $\eta = -\partial(\ln\omega)/\partial(\ln M)$ and t_o is the bare bandwidth parameter. This isotope shift is very sensitive to η and can acquire both positive and negative values; the experimental values of the isotope shift lead (for α and t obtained from fitting (2) to the experimental x-dependence of T_c and t_o taken from band calculations) to $0.3 \lesssim \eta \lesssim 0.57$ in agreement with the experimental data. Vanishing values of the isotope shift (3) are also possible for certain η values and hole concentrations, what might explain some earlier reported data.

The ratio $2\Delta/T_c$ of twice the superconducting gap to the critical temperature can also be estimated as

$$2\Delta/T_c = 3.53(1 - \pi x/2)^{-1} \quad , \qquad (4)$$

being always greater than the classical value 3.53, in agreement with the infrared spectroscopy and tunneling experiments.

The presumable effect of the lattice modulation on the superconducting critical temperature in the Bi(Tl)-based compounds can also be accounted for within the present theory [6,7] by estimating the filling factor of the Brillouin zones newly created by the lattice modulation. A characteristic sawtoothed behaviour is obtained versus the hole concentration x, as a consequence of the filling factor crossing gradually and successively the middles and edges of the Brillouin zones. An averall reduction in the critical temperature follows as an effect of the lattice modulation. Providing that the effect is real (i.e., the lattice modulation does affect the band structure of the charge carriers) one obtains for a five-fold periodicity (as for the Bi-based compounds) a reduction of about 0.75 in the critical temperature for a modulation along one crystalline direction and about 0.2 for a modulation along both crystalline directions. Assuming that the Bi-2223 phase is not affected by lattice modulation and using the critical temperature $T_c \sim 85K$ for the modulated Bi-2122 phase (which seems to have $x \tilde{=} 0.15$) one gets $T_c \sim 113K$ for the former, in agreement with the experimental evidence. However, one should stress upon the point that it is not yet clear whether the lattice modulation does or does not affect the superconductivity in these compounds.

A comparative study of the x-dependence of the critical temperature for the La-, Y- and Bi(Tl)-based superconductors shows that the parameter α in (2) is almost constant, $\alpha \tilde{=} 0.98$, for all these

families of compounds; on the other hand the bandwidth parameter t depends on $f = (1/2r + 2r)^{-1}$, $r = g_1/g_o$, which can acquire a maximum value $f = 1/2$ for $r = 1/2$. Both these α and f parameters signify the flexibility of the Cu-oxygen aggregates and the degree of screening of the Cu-oxygen layers. For the aforementioned values of α and f one may infer [6,7] from (2) a maximum critical temperature $T_c^{max} \sim 160K$, which may be viewed as the highest critical temperature attainable in this class of superconductors; corresponding, probably, to well-screened layers of Cu-oxygen rhomboedra (like in the 2223-phases) unaffected by various structural defects such as ion disorder, crystal imperfections, lattice modulation, etc.

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