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Correlation between critical temperature, pressure and hopping ratio in anisotropic low-dimensional superconductors

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Abstract

High pressure can strongly influence the electronic properties of a metal, by modifying either the shape or the topology of its Fermi surface (FS). In the case of low-dimensional anisotropic superconductors, typified by high-T_c cuprates, some quasi-2D organic salts and heavy-fermion compounds, we show that the occurrence of an electronic topological transition is generic to a non-monotonic pressure dependence of the critical temperature T_c. On the other hand, a change in shape of the FS can be correlated with the steady increase of T_c as a function of the ratio between next-nearest- and nearest-neighbour hopping, as is observed in the high-T_c cuprates.

The electronic properties of a metal can be modified to a large extent by hydrostatic pressure, anisotropic stress and chemical doping, i.e. by the introduction of isovalent impurities. If we neglect any intervening pressure-induced structural phase transition, then the possible band modifications are restricted to those compatible with a given symmetry of the underlying lattice. In other words, the lattice parameters are allowed to vary, but the overall symmetry of the lattice is conserved. This enables one to describe the electronic band structure, within the tight-binding approximation, using a 'rigid-band' scheme, with hopping parameters t_{ij} for between lattice sites i, j and chemical potential μ separately depending on pressure. In most cases, a pressure-induced variation of μ at $T = 0$ can then be associated with a change of the topology of the Fermi surface (FS), i.e. to a so-called electronic topological transition (ETT) [1], while a change of t_{ij} usually corresponds to a change in shape of the FS, without a change of its connectivity number [2]. An ETT is associated with an anomalous behaviour of several transport properties of the metallic state, as a function of the critical parameter $z = \mu - \varepsilon_c$, measuring the distance of μ from the value ε_c corresponding to the ETT [3, 4]. In 3D, such anomalies come usually

in the shape of kinks or steps, without altering the monotonic z-dependence of such normal-state properties. Concerning the superconducting state, Makarov and Bar'yakhtar accordingly derived a monotonic, step-like z-dependence for the gap at $T = 0$ and the critical temperature T_c of a bulk three-dimensional (3D) superconductor near an ETT [5].

In the following, we shall review our recent results concerning some superconducting properties of a low-dimensional superconductor [6]. At variance with the 3D case, the proximity to an ETT induces a non-monotonic dependence on z (i.e., pressure) of the superconducting properties of a quasi-2D superconductor, almost regardless of the pairing symmetry of the order parameter. This is in agreement with the phenomenology of several low-dimensional classes of superconducting materials under pressure or doping, including the high-T_c cuprates [7], the heavy-fermion compounds [8] and possibly some organic salts [9]. This is also in accord with an attempt at a material-wise classification of low-dimensional superconductors according to the orbital character of their anisotropic order parameter [10]. In addition, we confirm the correlation between T_c and some material-specific properties in the high-T_c cuprates [11]. While a maximum in the pressure dependence of T_c in some quasi-2D organic superconductors can be inferred from the present analysis, no clear evidence has been reported thus far for BEDT-TTF-based salts, for uniaxial strains below $\sim$10 kbar [9], thus suggesting that higher pressures or strains are required in order to establish such a non-monotonic behaviour.

An ETT is an almost common feature to several quasi-2D strongly correlated electronic systems, such as the high-T_c cuprates, the κ-(BEDT-TTF)$_2$–X organic salts (where X = Cu(NCS)$_2$, Cu[N(CN)$_2$]Br or Cu[N(CN)$_2$]Cl), and some heavy-fermion compounds. Evidence for a FS topology change as a function of doping has been recently reported for LSCO [12], and as a function of pressure in heavy-fermion compounds [13]. Model calculations of the dispersion relation for quasi-2D organic salts also indicate that *two* ETTs may be traversed in such compounds, as a function of the chemical potential [14, 15]. In the case of most high-T_c cuprates, a realistic tight-binding approximation for their dispersion relation has to include at least nearest- and next-nearest-neighbour hoppings:

$$\xi_{\boldsymbol{k}} = -2t(\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y - \mu. \tag{1}$$

Here, t and t' are related to hopping between nearest-or next-nearest-neighbouring d orbitals sitting on planar Cu atoms [11]. The in-plane anisotropy arising from the different orientations of the BEDT-TTF dimers in the quasi-2D organic salts leads to a similar expression for $\xi_{\boldsymbol{k}}$, but with next-nearest-neighbour hopping restricted to along the (110) direction [14, 15]. In both cases, a non-zero value of the hopping ratio $r = t'/t$ slightly modulates the shape of the Fermi line (figure 1, inset).

In the case of the cuprates, equation (1), as μ increases from the bottom to the top of the band, the Fermi line evolves from an electron-like contour, centred around the Γ point in the first Brillouin zone (1BZ), to a hole-like contour, centred around the corner point $M = (\pi, \pi)$ (figure 1, inset). Such a behaviour has been recently confirmed by ARPES experiments on $La_{2-x}Sr_xCuO_4$, where an ETT takes place at $x \simeq 0.15$ [12]. In the case of BEDT-TTF-based salts, as μ is increased, the Fermi line actually changes topology twice: once from electron-like to hole-like contours; and the second time from a singly connected hole-like contour to a doubly connected one, still retaining its hole-like character [6, 14].

The first and foremost effect of an ETT in the spectrum of a 2D pure electronic system is that of producing a logarithmic Van Hove singularity in the density of states (DOS) each time the Fermi level traverses a saddle point in the dispersion relation $\varepsilon_{\boldsymbol{k}}$ [16]. Due to the effect of impurities, however, such a singularity is usually smeared into a pronounced maximum with finite height. Moreover, two close singularities, as is the case for the BEDT-TTF-based organic

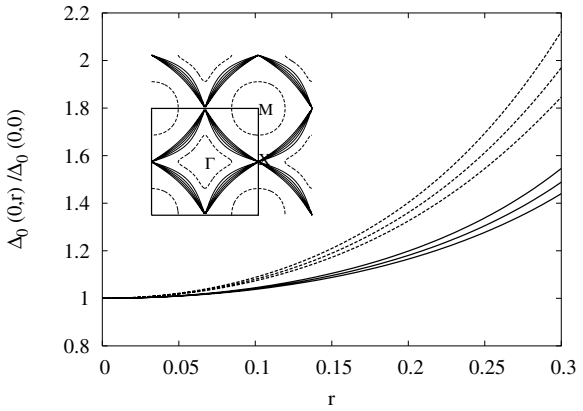

Figure 1. Normalized gap amplitude at $T = 0$, as a function of the hopping ratio r, for different couplings. Dashed curves refer to the s-wave case, while solid curves refer to the d-wave case. One can recognize the direct correlation between $T_c^{\max} \propto \Delta_0(z = 0)$ and r, as argued by Pavarini *et al* [11]. Inset: typical Fermi lines corresponding to equation (1) at the ETT, with $r = 0.20$–0.40 (solid curves), and away from the ETT, with $r = 0.45$ (dashed curves), in the first and adjacent Brillouin zones ($-\pi \leqslant k_x, k_y < 2\pi$).

salts, or those resulting from splitting the singularity associated with equation (1), e.g. due to a tetragonal-to-orthorhombic distortion of the lattice [17], are expected to merge into a single, broader maximum.

In order to study the z-dependence of the superconducting properties near an ETT in 2D, we solved the BCS gap equation at $T = 0$ for an s-wave or a d-wave order parameter Δ_k, assuming the dispersion relation equation (1) [6]. As a consequence of the presence of an ETT in the electronic spectrum, the gap magnitude Δ_0 at $T = 0$ is characterized by a non-monotonic dependence on the critical parameter z, both in the s- and in the d-wave case. In view of the fact that $T_c \propto \Delta_0$, as in any mean-field theory, such a finding is in agreement with the phenomenology of high-T_c cuprates under pressure [7]. By isolating the singular contribution to the DOS coming from the ETT, it is possible to derive the asymptotic dependence of the gap amplitude Δ_0 at $z = 0$ on the dimensionless coupling constant. Figure 1 shows the r-dependence of our (analytic) results for Δ_0, in the weak-coupling limit [6]. Our plot confirms a direct correlation between the critical temperature $T_c^{\max} \propto \Delta_0(z = 0)$ and such a material-dependent property, as argued by Pavarini *et al* [11] for several high-T_c cuprate compounds. We point out that a variation of the hopping ratio t'/t can be obtained not only by considering different materials, but also by applying in-plane anisotropic strain to the same material.

Summarizing, we have discussed the relevance of the proximity to an ETT for the superconducting properties of low-dimensional materials, such as the high-T_c cuprates, some organic salts and possibly some heavy-fermion compounds. Varying the chemical potential, as an effect of applied pressure, a FS topology change in 2D is accompanied by a non-monotonic behaviour of $T_c \propto \Delta_0(T = 0)$. A maximum in T_c can be correlated with material-specific properties, such as the ratio of the next-nearest- to nearest-neighbour hopping parameters in tight-binding band models, as well as with pressure for the high-T_c superconductors, as observed experimentally. Such a result applies to both s- and d-wave superconductivity, thus confirming that the non-monotonic pressure and doping dependence of T_c in the high-T_c cuprates is mainly due to their reduced dimensionality, rather than to their unconventional superconductivity. On the other hand, evidence for a non-monotonic dependence of T_c on

uniaxial strain in κ-(BEDT-TTF)$_2$-X is still lacking, below $\sim$10 kbar, thus suggesting that higher pressures or anisotropic strains are required, in order to demonstrate the relevance of ETTs in such quasi-2D organic salts.

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