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Small Fermi energy effects in MgB_2 and related compounds

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Abstract

Superconductivity at $T_c \simeq 40$ K in MgB_2 is thought to origin from the strong electron–phonon (el–ph) coupling of the σ-bands, whereas the residual interband scattering gives rise to the multigap phenomenology. The extremely low charge density of the σ-bands is reflected in the small Fermi energy E_F^σ, a fraction of eV, a common feature which is shared also by cuprates and fullerides. In our contribution we discuss the anomalous effects arising from the small Fermi energy phenomenology, when E_F^σ becomes comparable with the other energy scales of the systems. In particular we analyze the nonadiabatic effects arising from the finite adiabatic ratio ω_{ph}/E_F^σ; the anharmonic character of the E_{2g} phonon mode, which is shown to be related to the smallness of the Fermi energy with respect to the electron–phonon coupling $g_{E_{2g}}$: $E_F^\sigma \sim g_{E_{2g}}$; the anomalous effects of disorder when impurity scattering rate γ_{imp} is compared with E_F^σ. We discuss also the possibility of an enhancement of the nonadiabatic character due to zero point quantum fluctuations.

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In spite of the large amount of theoretical and experimental work in recent years, many anomalous superconducting features in MgB_2 are sill unclear. For instance, while a multiband-multigap approach seems sufficient to understand some of these aspects [1,2], the origin of a so high value of $T_c \simeq 39$ K remains an object of debate. The weak interband scattering indeed can account for an increase of T_c just of few kelvins. In addition, the significant dependence of the physical properties on the small amount of electron doping [3,4] and on the induced disorder by neutron irradiation suggests [5,6] a high sensibility on small energy scales.

An interesting peculiarity of MgB_2, which it is shared also by cuprates and fullerides, is the low density of charge carriers (holes in σ bands) involved in the superconducting pairing (holes in σ bands), reflected in a small value of the Fermi energy E_F. First principle calculations estimate $E_F \simeq 0.4$–0.6 eV [7], while experimental measurements of de Haas–van Alphen effect and of the penetration depth point towards half of this value [8,9].

The smallness of the electronic dynamics scale, parametrized by the Fermi energy, when compared to the other energy scales of the system opens the way to new physics which goes beyond the conventional Migdal–Eliashberg theory. In Table 1 we briefly summarize some of these anomalous features.

Most interesting are the consequences of the violation of the adiabatic assumption ($E_F \gg \omega_{ph}$) which is at the basis of Migdal's theorem and of the conventional

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Table 1
Comparison between Fermi energy E_F and other energy scales (phonon frequency ω_{ph}, impurity scattering rate γ_{imp}, el–ph matrix element g) and corresponding effects triggered by the finiteness of E_F with the other energy scales

$E_F \sim \omega_{ph}$	Nonadiabaticity
$E_F \sim \gamma_{imp}$	Anomalous disorder dependences (T_c, χ)
$E_F \sim g$	Anharmonicity, nonadiabatic fluctuations

theory of the electron–phonon scattering [10]. The breakdown of Migdals' theorem calls for a generalization of the el–ph quantum field theory to include vertex processes which are neglected in the adiabatic regime [11]. The evaluation of the nonadiabatic effects in MgB_2 differs from cuprates and fullerides since the smallness of the Fermi energy in MgB_2 stems from a low density of hole carriers in the highly dispersive σ bands [12] whereas in cuprates and fullerides it is more related to the bandwidth narrowness. The strong two-dimensional character of the σ bands gives thus rise to a finite nonadiabatic ratio ω_{ph}/E_F in the presence of a sizable density of states. Interesting, this situation implies an intrinsic selection of the positive sign of the vertex diagrams, reflected in an increase of the effective el–ph pairing [12–14]. The magnitude of these nonadiabatic effects however does not seems sufficient by alone to account for drastic enhancements of the critical temperature value.

A more compelling evidence of nonadiabatic effects is provided by the identification of qualitatively new phenomena which are expected to be absent in the conventional adiabatic theory. One of them could be the experimentally observed high sensibility of T_c and of the NMR spin-lattice relaxation rate $1/T_1$ on the induced disorder [5,6]. The electronic scattering with the induced disorder or nonmagnetic impurities is commonly parametrized in terms of the impurity scattering rate γ_{imp}. In the adiabatic limit $E_F \gg \omega_{ph}, \gamma_{imp}$ Anderson's theorem assures the critical temperature to be unaffected by the presence of disorder or nonmagnetic impurities [15]. Similar considerations hold true for the spin susceptibility and hence for $1/T_1$. Things however can be drastically different in small Fermi energy systems when the Fermi energy gets comparable to the impurity scattering rate $E_F \sim \gamma_{imp}$. In this regime indeed the spin susceptibility acquires a strong dependence on the amount of disorder parametrized by γ_{imp} (and on the el–ph quantities λ and ω_{ph} if electron–phonon scattering is also considered) [16]. This analysis suggests that the experimental reduction of T_c and of ^{11}B NMR $1/T_1$ can be related to the smallness of the σ band Fermi energy. Note the absence of reduction of ^{25}Mg NMR $1/T_1$ can be naturally explained at the same level as related to the high Fermi energy of the π bands, which are mainly probed by NMR on the magnesium atoms.

As a final object of investigation we consider the remarkable anharmonicity of the E_{2g} phonon mode, which has been claimed to play an important role with respect to the superconducting properties [17]. An interesting insight about the microscopic origin of the anharmonicity itself comes from noting that anharmonic contributions arise when the electronic structure is deeply modified upon phonon lattice distortions u_{2g}. More precisely first principle calculations identify two regimes [18]. In the first one the σ band degeneracy at the Γ point is split, but a Fermi surface exists for both the σ bands; frozen phonon potential $V(u_{2g})$ is essentially harmonic in this regime. The second one corresponds to a large u_{2g} regime $u_{2g} > u_c$ where lattice distortion is strong enough to shift one of the σ below the Fermi level and gives rise to anharmonic terms. It is clear that this latter regime, strictly related to the phonon anharmonicity, is physically observable only if the Fermi energy of the σ band E_F^σ is small enough to be comparable with electronic shift associated with lattice distortions, parametrized by the energy-dimension el–ph matrix element g ($E_F \sim g$). It should be noted that the condition $E_F \sim g$ implies that some nonadiabatic effects are present at the level of *quantum fluctuations* even if the adiabatic ratio E_F/ω_{ph} is relatively small. The evaluation of these nonadiabatic effects induced by lattice fluctuations will be object of future research work.

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