Eur. Phys. J. B **30**, 511–517 (2002)
DOI: 10.1140/epjb/e2002-00408-2

THE EUROPEAN PHYSICAL JOURNAL B

Spin susceptibility in small Fermi energy systems: effects of nonmagnetic impurities

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Received 31 July 2002 / Received in final form 21 September 2002
Published online 31 December 2002 –

Abstract. In small Fermi energy metals, disorder can deeply modify superconducting state properties leading to a strong suppression of the critical temperature T_c. In this paper, we show that also normal state properties can be seriously influenced by disorder when the Fermi energy E_F is sufficiently small. We calculate the normal state spin susceptibility χ for a narrow band electron-phonon coupled metal as a function of the non-magnetic impurity scattering rate γ_{imp}. We find that as soon as γ_{imp} is comparable to E_F, χ is strongly reduced with respect to its value in the clean limit. The effects of the electron-phonon interaction including the nonadiabatic corrections are discussed. Our results strongly suggest that the recent finding on irradiated MgB_2 samples can be naturally explained in terms of small E_F values associated with the σ-bands of the boron plane, sustaining therefore the hypothesis that MgB_2 is a nonadiabatic metal.

PACS. 74.25.-q General properties; correlations between physical properties in normal and superconducting states – 71.28.+d Narrow-band systems; intermediate-valence solids – 74.62.Dh Effects of crystal defects, doping and substitution

1 Introduction

Scattering from weak disorder or diluted non magnetic impurities plays a marginal role on many thermodynamics quantities of conventional metals. Most peculiar is the absence of any reduction on the critical temperature T_c in conventional isotropic s-wave superconductors as stated by the Anderson's theorem and as confirmed by several experimental measurements [1].

This insensitivity stands out in particular in comparison with d-wave superconductors where the strong anisotropy of the order parameter leads to a suppression of T_c [2]. In that case for instance the reduction on T_c upon disorder can give qualitative information of the microscopic characteristic on the pairing (d- *vs.* s- wave symmetry, local *vs.* long-ranged interaction, etc.) [3].

A conventional role of nonmagnetic impurities is recently questioned in some high-T_c superconductors, as MgB_2 and fullerene compounds. In these materials a notable reduction of T_c upon disorder has been reported in spite of the s-wave symmetry of both of them [4,5]. Quite remarkable is also the reduction of the density of states (DOS) inferred by NMR measurements of the nuclear spin-lattice relaxation rate T_1 [$1/T_1T \propto N_0^2$ where N_0 is the electronic density of states at the Fermi level and T is the temperature]. In reference [6] a reduction of 62% of $1/T_1T$ upon disorder was reported by ^{11}B NMR measurements in contrast with the conventional theory of non magnetic impurity scattering which would predict no effect of the magnetic susceptibility. An additional puzzling feature is the discrepancy between spin-lattice relaxation rate measurements performed on ^{11}B NMR and on ^{25}Mg. No reduction of $1/T_1T$ was indeed observed on magnesium atoms. The authors of reference [6] speculate this difference could be related to the different nature of the electronic states: magnesium atoms would mainly probe the π bands of MgB_2 through the hybridization of B($2p_z$) orbitals with Mg(s) states, while the spin-lattice relaxation rate on the boron is expected to be very sensitive to the two dimensional σ bands formed by B($2p_x 2p_y$).

The evidences of anomalous effects of disorder and non magnetic impurities in these systems prompt thus some intriguing open questions: i) which is the origin of the suppression of T_c in s-wave systems as MgB_2 and fullerenes? ii) which is the origin of the reduction of the density of states as probed by spin-lattice relaxation rate $1/T_1T$ measurements? iii) which is the origin of the different behaviour of Mg and B NMR measurements?

The point (i) was previously addressed in reference [7] in the context of a nonadiabatic theory of superconductivity [8] where impurity effects in the nonadiabatic channels were shown to suppress T_c even for purely isotropic s-wave superconductors. In this paper we extent our analysis to the spin susceptibility. In particular we show that a

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possible unifying explanation of all this complex anomalous scenario could come from taking into account in a coherent way the small Fermi energy nature of these materials. This is clearly unavoidable in C_{60} compounds where the narrow bandwidth of the t_{1u} bands (but also the h_u bands for hole doped C_{60}) results in a Fermi energy $E_F \sim 0.25$ eV [9]. This is also true in MgB_2 where the low hole filling of the 2D σ bands leads to $E_F^\sigma \sim 0.4 - 0.6$ eV [10, 11]. These values of E_F are at least one order of magnitude less than in common metals and in conventional superconductors. The discrepancy between Mg and B NMR measurements can be thus related to the probing of different bands (π on Mg, σ on B), and, in the last analysis, to the different magnitude of the Fermi energies ($E_F^\pi \sim 5$ eV $\gg E_F^\sigma$).

On microscopic grounds, small Fermi energy effects are operative as soon as E_F becomes of the same order of the other relevant energy scales. For an electron-phonon system in the presence of non magnetic impurities as we consider here, E_F should be thus compared with the characteristic phonon energy scale ω_{ph} and with the impurity scattering rate γ_{imp}. The breakdown of the adiabatic hypothesis ($E_F \gg \omega_{ph}$) in a small Fermi energy system implies the onset of new channels of electron-phonon interaction which need to be taken into account. On the other hand the finiteness of the ratio γ_{imp}/E_F gives rise to anomalous impurity effects which have to be analyzed in the presence of the same electron-phonon interaction since electron, phonon and impurity energy scales could be all of the same magnitude: $E_F \sim \omega_{ph} \sim \gamma_{imp}$.

2 The model

In this section, we derive the electron spin susceptibility by employing the Baym-Kadanoff technique which permits to derive, within a conserving theory, higher order response functions as functional derivatives of the single particle Green's function in the presence of an external field [12]. This approach is thus an appropriate starting point to study small Fermi energy systems where the violation of the Migdal's theorem valid for $E_{ph} \gg \omega_{ph}$ requires a generalization of the conventional theory in the nonadiabatic regime.

Objects of our investigation is the non magnetic impurity effects on the spin susceptibility in small Fermi energy systems in the presence of a sizable electron-phonon interaction. NMR techniques can probe the electron density of states by means of different ways. Most direct is the evaluation of the static uniform limit χ of the generalized electron spin susceptibility $\chi(\mathbf{q}, \omega)$:

$$\chi = \lim_{\mathbf{q}\to 0} \lim_{\omega \to 0} \chi(\mathbf{q}, \omega) \tag{1}$$

which, for a non interacting system with large Fermi energy, is simply $\chi \propto N_0$. Electron-electron exchange interaction gives rise however to the so called Stoner enhancement: $\chi \propto N_0/(1 - I)$ (I being the Stoner factor). Experimentally the static uniform limit χ of electron spin susceptibility can be measured by a proper analysis of the Knight shift after the orbital contribution is subtracted.

Similar information are obtained by spin-lattice relaxation rate T_1 which can be also mainly related, after subtraction of orbital terms, to the electron spin susceptibility through the relation:

$$\frac{1}{T_1 T} \propto \lim_{\omega \to 0} \sum_{\mathbf{q}} A^2(\mathbf{q}) \frac{\chi(\mathbf{q}, \omega)}{\omega}, \tag{2}$$

where $A(\mathbf{q})$ is the form factor relative to the particular nucleus. As pointed out in the introduction, $1/T_1 T \propto N_0^2$ in large Fermi energy systems.

In the following we focus on the static uniform spin susceptibility χ which permits a more direct comparison with the density of states and which is only slightly affected by different form factors $A(\mathbf{q})$. As it will be clear in the following the anomalous effects of non magnetic impurities are essentially related to the similar energy scales of γ_{imp}, E_F and ω_{ph}. In this situation impurity scattering leads to an effective renormalization of the generalized spin susceptibility which is expected to appear in similar way both in the static uniform limit χ and in the spin-lattice relaxation rate. In this perspective the reduction of the magnetic susceptibility upon disorder pointed out by NMR technique should be read more as an anomalous renormalization effect appearing in small Fermi energy system than as a real reduction of the density of states.

In Quantum Field Theory the electron spin susceptibility is usually related to the one particle Green's function G through the relation [13]:

$$\chi(T) = -2\mu_B^2 T \sum_n \sum_{\mathbf{k}} G(\mathbf{k}, n)^2 \Gamma(\mathbf{k}, n), \tag{3}$$

where $G(\mathbf{k}, n)$ is the electron propagator at finite temperature expressed in Matsubara frequencies

$$G^{-1}(\mathbf{k}, n) = \mathrm{i}\omega_n - \epsilon(\mathbf{k}) + \mu - \Sigma(\mathbf{k}, n), \tag{4}$$

and $\Gamma(\mathbf{k}, n)$ is the spin vertex function. The Baym-Kadanoff formalism provides a powerful technique to related the spin vertex function $\Gamma(\mathbf{k}, n)$ to $G(\mathbf{k}, n)$. Following the standard procedure we generalize the Green's function in equation (4) in the presence of an external magnetic field h:

$$G_\sigma^{-1}(\mathbf{k}, n) = \mathrm{i}\omega_n - \epsilon(\mathbf{k}) + \mu + h\sigma - \Sigma_\sigma(\mathbf{k}, n). \tag{5}$$

The spin vertex function is thus obtained as functional derivative of the Green's function G_σ in the presence of the external magnetic field for $h \to 0$ [14]:

$$\begin{aligned} \Gamma(\mathbf{k}, n) &= \frac{1}{2} \sum_\sigma \sigma \left[\frac{\mathrm{d} G_\sigma^{-1}(\mathbf{k}, n)}{\mathrm{d}h} \right]_{h=0} \\ &= 1 - \frac{1}{2} \sum_\sigma \sigma \left[\frac{\mathrm{d}\Sigma_\sigma(\mathbf{k}, n)}{\mathrm{d}h} \right]_{h=0}. \end{aligned} \tag{6}$$

The set of equations (3–6) defines a self-consistent method to obtain the spin susceptibility from the knowledge of the

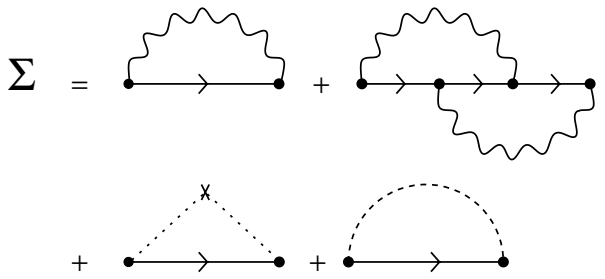

Fig. 1. Diagrammatic picture of the electron self-energy. Legend of the pictorial elements: electrons (solid line), phonons (wavy lines), elastic scattering (dotted lines) with dilute non magnetic impurities (cross), electron-electron repulsion (dashed line).

self-energy. The complex nature of the interactions in the systems is thus hidden in the specific form of the self-energy which needs to be explicitly provided.

In order to investigate the interplay between non magnetic impurities and the electron-phonon interaction in small Fermi energy systems an appropriate approach is the nonadiabatic theory which accounts for the additional interaction channels arising when $E_{\rm F} \sim \omega_{\rm ph}$. The formal derivation of the nonadiabatic theory has been already presented in several papers where we refer for more details [7,8,14]. Here we focus on the role of non magnetic impurities. In the spirit of the Baym-Kadanoff theory our starting point will be the self-energy which is diagrammatically depicted in Figure 1. The first two diagrams represent the electron-phonon interaction in nonadiabatic regime ($E_{\rm F} \sim \omega_{\rm ph}$) including the first order vertex processes; the third diagram is the self-energy in Born approximation for impurities of density $n_{\rm imp}$ interacting with electrons *via* a scattering potential $v_{\rm imp}$. The last diagram is the exchange electron-electron interaction: this term is just a constant and does not play any role in the self-energy, but it gives rise to the Stoner factor in the spin susceptibility.

Figure 1 defines in an unambiguous way the self-energy and the one particle properties of the system. Standard procedure in isotropic materials is to replace the self-energy $\Sigma(\mathbf{k}, n)$ with its Fermi surface average: $\Sigma(\mathbf{k}, n) \rightarrow \Sigma(n) \equiv \langle\langle \Sigma(\mathbf{k}, n)\rangle\rangle_{\rm FS}$. It is convenient to take into account self-energy effects in the electronic Green's function is to introduce the renormalized Matsubara frequencies defined as $\mathrm{i}W_n = \mathrm{i}\omega_n - \Sigma(n)$. In addition, for sake of simplicity we consider a half-filled band with bandwidth E and constant density of states $N(\epsilon) = N_0$ $[-E/2 \leq \epsilon \leq E/2]$. The parameter $E/2$ represents thus the Fermi energy $E_{\rm F} = E/2$. Within these assumptions the analytic expression of the renormalized Matsubara frequencies W_n involving the self-energy depicted in Figure 1 reads:

$$W_n = \omega_n - 2T\sum_M V(n,m)\arctan\left(\frac{E_{\rm F}}{W_m}\right) + 2\gamma_{\rm imp}\arctan\left(\frac{E_{\rm F}}{W_n}\right), \quad (7)$$

where

$$V(n,m) = \lambda D(n-m)[1 + \lambda P(Qc; n, m)] \quad (8)$$

is the nonadiabatic electron-phonon kernel appearing in the self-energy equation and where we have neglected the electron-electron exchange interaction which leads just to a constant term. In equation (8), $D(n-m)$ is the phonon propagator which for a single Einstein mode $\omega_{\rm ph} = \omega_0$ reduces simply to $D(n-m) = -\omega_0^2/[(\omega_n - \omega_m)^2 + \omega_0^2]$ and $P(Q_c; n, m)$ is the vertex function [7,14]:

$$P(Q_c; n, m) = -T\sum_l D(n-l)\Bigg\{ B(n,m,l) + \frac{A(n,m,l) - B(n,m,l)(W_l - W_{l-n+m})^2}{(2E_F Q_c^2)^2} \times \left[R(Qc; n, m, l) - 1 - \log\left(\frac{1 + R(Q_c; n, m, l)}{2}\right)\right]\Bigg\}, \quad (9)$$

where

$$A(n,m,l) = (W_l - W_{l-n+m})\left[\arctan\left(\frac{E_F}{W_l}\right) - \arctan\left(\frac{E_F}{W_{l-n+m}}\right)\right], \quad (10)$$

$$B(n,m,l) = (W_l - W_{l-n+m})\frac{E_F W_{l-n+m}}{[E_F^2 + W_{l-n+m}^2]^2} - \frac{E_F}{E_F^2 + W_{l-n+m}^2}, \quad (11)$$

$$R(Q_c; n, m, l) = \sqrt{1 + \left(\frac{4E_F Q_c^2}{W_l - W_{l-n+m}}\right)^2}. \quad (12)$$

The dimensionless parameter $Q_c = q_c/2k_{\rm F}$, where $k_{\rm F}$ is the Fermi momentum, takes into account the upper cutoff q_c for the momentum transfer in the electron-phonon interaction. This cutoff has been introduced to simulate a momentum dependent renormalization due to possible strong electronic correlations [15]. For weak correlated metals $Q_c \simeq 1$, while $Q_c \ll 1$ when correlation is strong. As we are going to see, the parameter Q_c plays only a marginal on the static spin susceptibility, whereas it strongly affects the superconducting critical temperature [8].

In the formula for W_n, equation (7), $\gamma_{\rm imp}$ is the impurity scattering rate which in the Born approximation reduces to $\gamma_{\rm imp} = \pi n_{\rm imp} N_0 v_{\rm imp}^2$ [16]. This expression holds true for low values $n_{\rm imp}$ of impurity concentrations and weak scattering potential $v_{\rm imp}$. An expression of $\gamma_{\rm imp}$ valid also for strong, but diluted, impurity interactions is provided by the T-matrix approximation: $\gamma_{\rm imp} = \pi n_{\rm imp} N_0 v_{\rm imp}^2/[1 + (\pi N_0 v_{\rm imp})^2]$.

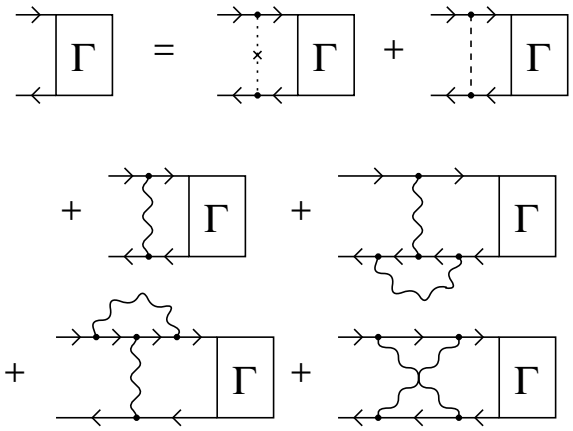

Fig. 2. Diagrammatic picture of spin vertex function Γ. See caption of Figure 1 for a legend of the pictorial elements.

Using the Baym-Kadanoff formalism we are able to obtain also an analytic expression for the spin vertex function $\Gamma(\mathbf{k}, n)$. The diagrammatic expression of $\Gamma(\mathbf{k}, n)$ corresponding to the self-energy depicted in Figure 1 is shown in Figure 2. In the isotropic case we have considered here we can replace also the spin vertex function $\Gamma(\mathbf{k}, n)$ with its Fermi surface average $\Gamma(n)$. The momentum average of the spin vertex implies that the momentum correlations between spin up electrons and spin down holes are taken into account only at a mean level through the parameter Q_c. This will be a poor approximation when the dispersion of collective modes is investigated, while it is expected to not affect in a qualitative way the static uniform spin susceptibility. Disregarding the momentum dependence of $\Gamma(\mathbf{k}, n)$ and we get thus:

$$\Gamma(n) = 1 + T\sum_m \left[I + V_\Gamma(n,m)\right] \frac{2E_F}{W_m^2 + E_F^2}\Gamma(m) - \gamma_{\rm imp}\frac{2E_F}{W_n^2 + E_F^2}\Gamma(n), \quad (13)$$

where the quantity $I = N_0 U$ is the Stoner factor arising from the electron-electron exchange interaction and the last term comes from the impurity scattering processes. Moreover

$$V_\Gamma(n,m) = \lambda D(n-m)\left[1 + 2\lambda P(Q_c; n, m)\right] + \lambda^2 C(Q_c; n, m) \quad (14)$$

describes the electron-phonon processes in nonadiabatic regime which include electron-phonon vertex $P(Q_c; n, m)$ given by equations (9–12) the and cross diagrams:

$$C(Q_c; n, m) = T\sum_l D(n-l)D(l-m) \times \left\{ 2B(n,m,l) + \arctan\left(\frac{4E_F Q_c^2}{|W_l - W_{n+m-l}|}\right) \times \frac{A(n,m,l) - B(n,m,l)(W_l - W_{n+m-l})^2}{2E_F Q_c^2 |W_l - W_{n+m-l}|} \right\}, \quad (15)$$

where $A(n, m, l)$ and $B(n, m, l)$ are given by equations (10) and (11), respectively. Note that $V_\Gamma(n, m)$ is deeply different from $V(n, m)$ since the first describes electron-phonon scattering in the spin electron-hole channel, and the second one the electron-phonon interaction in the single particle propagator.

3 Results and discussion

Equations (7–15) can be solved in a self-consistent iterative way to obtain W_n and $\Gamma(n)$. Equation (3), in its isotropic form:

$$\chi(T) = \chi_{\rm P} T \sum_n \frac{2E_{\rm F}}{W_n^2 + E_{\rm F}^2}\Gamma(n), \quad (16)$$

provides finally the spin susceptibility as function of generic impurity scattering rate $\gamma_{\rm imp}$, electron-phonon coupling constant λ, adiabatic ratio $\omega_0/E_{\rm F}$ and momentum cut-off Q_c. Here $\chi_{\rm P}$ is the free electron Pauli spin susceptibility $\chi_{\rm P} = 2\mu_{\rm B}^2 N_0$.

In order to point out the role of small Fermi energy in the impurity scattering effects on the spin susceptibility, we consider for the moment the simple case of no electron-phonon interaction ($\lambda = 0$). In this case the only energy scales in the system are $\gamma_{\rm imp}$ and $E_{\rm F}$. From equation (16), equation (13) has thus the simple self-consistent solution as function of the spin susceptibility itself:

$$\Gamma(n) = \frac{1 + I(\chi/\chi_{\rm P})}{1 + \gamma_{\rm imp}\dfrac{2E_F}{W_n^2 + E_F^2}}, \quad (17)$$

and the spin susceptibility χ recovers the usual Stoner-like expression:

$$\chi = \frac{\chi_0}{1 - I(\chi_0/\chi_{\rm P})}, \quad (18)$$

where the bare spin susceptibility χ_0 is now affected by the non magnetic impurity scattering:

$$\chi_0 = \chi_{\rm P} T \sum_m \frac{2E_F}{W_m^2 + E_F^2 + \gamma_{\rm imp} 2E_F}\,. \quad (19)$$

For large Fermi energy systems, $E_{\rm F} \gg \gamma_{\rm imp}$, equation (19) reduces to the Pauli spin susceptibility $\chi_0 = \chi_{\rm P}$. It is thus clear the non magnetic impurity effects can appear only if the Fermi energy is small enough to be comparable with $\gamma_{\rm imp}$. Note that in the presence of electron-phonon interaction an additional energy scale is provided by $\omega_{\rm ph}$, so that additional anomalous impurity effects are ruled by the additional parameter $\gamma_{\rm imp}/\omega_{\rm ph}$.

In Figure 3 we plot the behaviour of the static spin susceptibility χ in a small Fermi energy system ($\omega_0/E_{\rm F} = 0.7$) as function of the impurity scattering rate $\gamma_{\rm imp}$. The data are normalized with respect to the "pure" limit $\gamma_{\rm imp} \to 0$. Left panel refer to a weak coupling electron-phonon case ($\lambda = 0.4$), right panel to strong

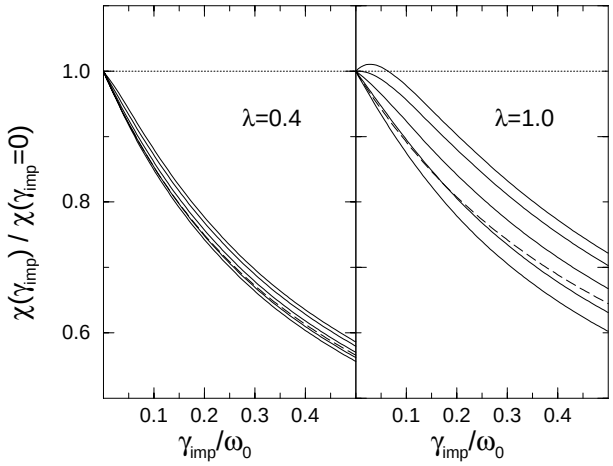

Fig. 3. Spin susceptibility χ as function of the impurity scattering rate $\gamma_{\rm imp}$ in the presence of electron-phonon interaction($\lambda = 0.4$, left panel; $\lambda = 1.0$, right panel, $\omega_0/E_{\rm F} = 0.7$ and electron-electron exchange repulsion $I = 0.4$. Solid lines: nonadiabatic vertex corrected theory with different values of Q_c (from the top to the bottom: $Q_c = 0.1, 0.3, 0.5, 0.7, 0.9$); dashed line: non crossing approximation.

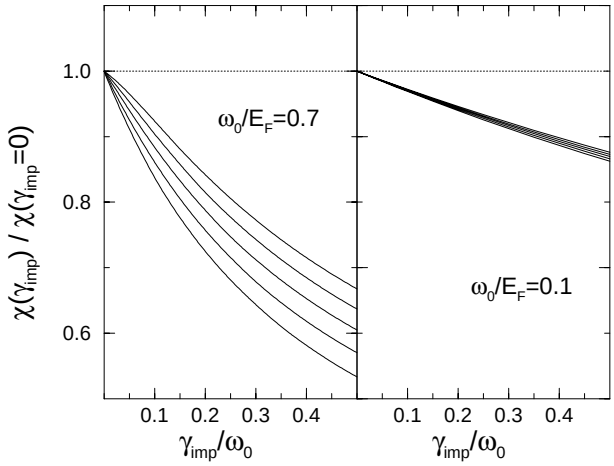

Fig. 4. Spin susceptibility χ as function of the impurity scattering rate $\gamma_{\rm imp}$ for a small Fermi energy ($\omega_0/E_{\rm F} = 0.7$, left panel) and for a large Fermi energy system ($\omega_0/E_{\rm F} = 0.1$, right panel). Solid lines correspond to different values of λ: (from bottom to the top) $\lambda = 0.2, 0.4, 0.6, 0.8, 1$. Other parameters: $Q_c = 0.4$ and $I = 0.4$. Dotted line: infinite Fermi energy case.

coupling ($\lambda = 1.0$). In both the case a Stoner factor $I = 0.4$ was considered. Solid lines represent the nonadiabatic vertex corrected theory with different values of Q_c (from the top to the bottom: $Q_c = 0.1, 0.3, 0.5, 0.7, 0.9$) and the dashed line the non crossing approximation where only finite bandwidth effects were retained ($P(Qc; n, m) = C(Q_c; n, m) = 0$ in Eqs. (8–14)). Figure 3 shows a strong reduction of χ due to the impurities scattering with respect to a large Fermi energy case ($E_{\rm F} \gg \omega_0$, dotted line). We observe only a weak dependence on the electron-phonon coupling (right panel data are slightly higher than the left panel), while the introduction of the nonadiabatic vertex and cross diagrams essentially leads to a spread of the different curves for different values of Q_c.

From this behaviour we can argue that the electron-phonon interaction λ plays a secondary role in the reduction of χ due to impurity scattering. In similar way a marginal role is recovered for the electron-electron interaction (Stoner factor I). As matter of facts, the leading effects are ruled by the comparison between the energy scales $\gamma_{\rm imp}$, ω_0 and $E_{\rm F}$. In order to highlight this point we compare in Figure 4 the dependence of the magnetic susceptibility χ on the impurity scattering rate for a small Fermi energy ($\omega_0/E_{\rm F} = 0.7$, left panel) and for a large Fermi energy system ($\omega_0/E_{\rm F} = 0.1$, right panel). Solid lines corresponds to different values of λ (from bottom to the top): $\lambda = 0.2, 0.4, 0.6, 0.8, 1$. Here we set $Q_c = 0.4$ and $I = 0.4$ but, as above discussed, different values would not change the physics. Note the remarkable difference between left and right panel. The same impurity scattering rate, which in the presence of a small Fermi energy ($\omega_0/E_{\rm F} = 0.7$) would lead to a reduction of χ of about 33–47%, gives rise only to a 12–14% reduction when Fermi energy is considerably increased ($\omega_0/E_{\rm F} = 0.1$), and to no reduction at all for the infinite Fermi energy case (dotted line).

Curiously the presence of the electron-phonon interaction decreases the sensitivity of χ to impurity scattering rate. This can be understood considering that the the electron-phonon scattering reduces by itself the magnetic susceptibility χ [14], so that further reduction by non magnetic impurity scattering is disfavored. For the same reasons a stronger Stoner factor I would enhance the reduction of χ.

4 Disorder and nonmagnetic impurities in real materials (MgB_2, fullerenes, ...)

We are now in the position to re-address the open questions arisen in the introduction, concerning namely: the origin of the reduction of the density of states as probed by NMR susceptibility measurements; the discrepancy between the different behaviour of Mg and B NMR measurements. In particular we suggest that the reduction of the spin-lattice relaxation rate $1/T_1T$ upon induced disorder could reflect the small Fermi energy nature of the electronic structure probed by the experiments. Within this context the insensitivity to disorder scattering of the spin-lattice relaxation rate $1/T_1T$ probed on ^{25}Mg in contrast to the marked reduction of ^{11}B NMR measurements acquires a natural explanation related to the different Fermi energy scales involved in the two cases. ^{25}Mg NMR measurements mainly probe the π band structures with high Fermi energy $E_{\rm F} \sim 5$ eV. Using a typical phonon frequency $\omega_0 \simeq 70$ meV [17] we estimate $\omega_0/E_{\rm F}^{\pi} \sim 0.014$ which yields a negligible dependence of the spin susceptibility on the amount of disorder. On the other hand NMR on the ^{11}B boron nucleus is strongly coupled with the in-plane σ orbitals with Fermi energy $E_{\rm F} \sim 0.4 - 0.6$ eV.

The same phonon frequency scale gives thus $\omega_0/E_{\rm F}^{\sigma} \sim 0.12 - 0.14$, where visible impurity scattering effects are expected. We conclude that the small Fermi energy of the σ bands is the major responsible for the reduction of the magnetic susceptibility when probed on ^{11}B nuclei compared with NMR measurements on the same quantity on ^{25}Mg.

Note that the usual two band model within the Migdal-Eliashberg framework, with different electron-phonon coupling for σ and π bands ($\lambda_\sigma \sim 1$, $\lambda_\pi \sim 0.2$), can not alone explain the discrepancy between the reduction rate probed by NMR. Indeed: a) electron-phonon interaction does not affect impurity scattering for high Fermi energy systems ($E_{\rm F} \gg \gamma_{\rm imp}, \omega_0$); b) the larger electron-phonon coupling constant in the σ bands would predict a smaller reduction rate of χ as compared with the smaller λ of the π bands.

The above discussion suggests that the reduction of χ upon disorder is a possible tool to point out nonadiabatic effects in small Fermi energy materials where $\omega_0 \sim E_{\rm F}$. In this perspective it is interesting to compare the simultaneous reduction of χ and T_c as function of the impurity scattering rate $\gamma_{\rm imp}$. In this way in principle one can trace out the effects of non magnetic impurity scattering in small Fermi energy systems as functions of physical measurable quantities as χ and T_c avoiding the use of the unaccessible parameter $\gamma_{\rm imp}$.

A conserving derivation of the superconducting equations in a fully consistent way with the evaluation of the spin susceptibility follows once again the Baym-Kadanoff theory based on Figure 1 written in Nambu notation. A formal derivation of those equations and some technicalities about the numerical calculations of T_c were discussed in reference [7] where we refer for more details. In Figure 5a we plot χ and T_c as functions of $\gamma_{\rm imp}$ for $I = 0.2$ and the couples of parameters ($\lambda = 1.0$, $\omega_0/E_{\rm F} = 0.2$), ($\lambda = 0.2$, $\omega_0/E_{\rm F} = 0.02$). These cases should be qualitatively representative of the MgB_2 σ and π bands which are respectively: strong coupled with small Fermi energy; and weak coupled with large Fermi energy. Note that a significant dependence on $\gamma_{\rm imp}$, for both T_c and χ is observed only for ($\lambda = 1.0$, $\omega_0/E_{\rm F} = 0.2$) which represents the case of σ bands. The T_c *vs.* χ plot is shown in Figure 5b for ($\lambda = 1.0$, $\omega_0/E_{\rm F} = 0.2$, $I = 0.2$). A reduction of T_c of the order of 30–80% is predicted for a reduction of χ of $\sim 20\%$, depending on the parameter Q_c. The general trend is thus in agreement with the experimental data reported in reference [6].

In MgB_2, where the electronic correlation is thought to be negligible, there is no reason to expect a significant momentum selection and Q_c is expected to be $Q_c \sim 1$. In this situation our analysis would underestimate the suppression of T_c ($\Delta T_c/T_c \sim 30\%$) and χ ($\Delta\chi/\chi \sim 20\%$) when compared with the experimental scenario, although some care should be used to extrapolate from the static magnetic susceptibility χ to $1/TT_1$.

It is clear however that additional ingredients are required to be taken into account for a quantitative analysis of the experimental data of T_c *vs.* induced disorder. In particular the discussion in terms of two separated σ and π bands is expected to be a poor description for the superconducting properties of a complex multiband system as MgB_2. On this basis we conclude that further investigation is needed to account in a fully satisfactory way for the anomalous dependence of T_c on the amount disorder. On the other hand the reduction of the spin susceptibility upon disorder and non magnetic impurities in MgB_2 could be qualitatively understood within the present analysis. In particular our results suggest that a primary role could be played by the small Fermi energy effects driven in MgB_2 by the closeness of the chemical potential to the top of the σ band. In this framework the different behaviour of B and Mg NMR data receives a natural explanation.

Interesting perspectives are also opened in regards to the fullerene based materials. The analysis is indeed simplified in these compounds as a single Fermi energy

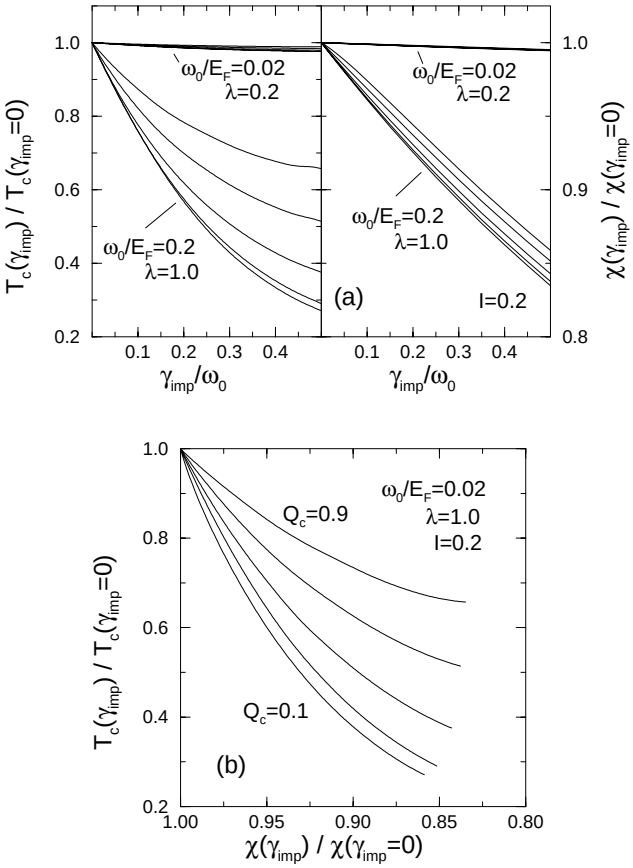

Fig. 5. (a) Reduction of T_c (left panel) and χ (right panel) as function of $\gamma_{\rm imp}$ for the cases ($\lambda = 1.0$, $\omega_0/E_{\rm F} = 0.2$, $I = 0.2$) and ($\lambda = 0.2$, $\omega_0/E_{\rm F} = 0.02$, $I = 0.2$), qualitatively representative respectively of the σ and π bands in MgB_2. Different lines corresponds to different Q_c's (from the bottom to the top in left panel, from the top to the bottom in right panel): $Q_c = 0.1, 0.3, 0.5, 0.7, 0.9$. (b) Corresponding plot of T_c *vs.* χ as varying $\gamma_{\rm imp}$ ($\gamma_{\rm imp} = 0$ at the left end, $\gamma_{\rm imp} = 0.5\omega_0$ at the right end) for ($\lambda = 1.0$, $\omega_0/E_{\rm F} = 0.2$, $I = 0.2$). Different values of Q_c are reported as in the previous captions.

is present. The extreme smallness of E_F is fullerenes ($E_F \simeq 0.25$ eV) suggests that disorder or nonmagnetic impurity effects could lead to even more marked reduction of T_c and χ than in MgB_2. A suppression of T_c upon induced disorder as previously been reported in reference [4]. At our knowledge no measurements of magnetic susceptibility as function of disorder or impurity amount as been at the present performed. Experimental work along this line is thus encouraged.

This work was partially supported by INFM Research Project PRA-UMBRA

References

1. P.W. Anderson, J. Phys. Chem. Solid **11**, 26 (1959)
2. A.B. Aleksashin *et al.*, Physica C **153-155**, 339 (1988); Gang Xiao *et al.*, Phys. Rev. B **42**, 8752 (1990); W.N. Hardy *et al.*, Phys. Rev. Lett. **70**, 3999 (1993); E.R. Ulm *et al.*, Phys. Rev. B **51**, 9193 (1995)
3. M.E. Flatté, J.M. Byers, Solid State Phys. **52**, 137 (1996)
4. S.K. Watson *et al.*, Phys. Rev. B **55**, 3866 (1997)
5. A.E. Kar'kin *et al.*, JETP Lett. **73**, 570 (2001)
6. A.P. Gerashenko *et al.*, Phys. Rev. B **65**, 132506 (2002)
7. M. Scattoni, C. Grimaldi, L. Pietronero, Europhys. Lett. **47**, 588 (1999)
8. L. Pietronero, S. Strässler, C. Grimaldi, Phys. Rev. B **52**, 10516 (1995); C. Grimaldi, L. Pietronero, S. Strässler, Phys. Rev. B **52**, 10530 (1995)
9. O. Gunnarsson, Rev. Mod. Phys. **69**, 575 (1997)
10. J.M. An, W.E. Pickett, Phys. Rev. Lett. **86**, 4366 (2001)
11. J. Kortus *et al.*, Phys. Rev. Lett. **86**, 4656 (2001)
12. G. Baym, L.P. Kadanoff, Phys. Rev. **124**, 287 (1961)
13. We neglect here non local effects appearing in the neighbouring of a single impurity. In this perspective only physical quantities averaged on the impurity configuration, which do not break translational invariance, will be in the following involved
14. E. Cappelluti, C. Grimaldi, L. Pietronero, Phys. Rev. B **64**, 125104 (2001)
15. M.L. Kulić, R. Zeyher, Phys. Rev. B **49**, 4395 (1994); R. Zeyher, M. Kulić, Phys. Rev. B **53**, 2850 (1996)
16. G. Rickayzen, *Green's Functions and Condensed Matter* (Academic Press, New York, 1980)
17. B. Renker, K.B. Bohnen, R. Heid, D. Ernst, H. Schober, M. Koza, P. Adelmann, P. Schweiss, T. Wolf, Phys. Rev. Lett. **88**, 067001 (2002)