

Small Fermi energy, strong electron–phonon effects and anharmonicity in MgB₂

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Abstract

The investigation of the electron–phonon properties in MgB₂ has attracted a huge interest after the discovery of superconductivity with $T_c = 39$ K in this compound. Although superconductivity is often described in terms of the conventional Eliashberg theory, properly generalized in the multiband/multigap scenario, important features distinguish MgB₂ from other conventional strong-coupling superconductors. Most important it is the fact that a large part of the total electron–phonon strength seems to be concentrated here in only one phonon mode, the boron–boron E_{2g} stretching mode. Another interesting property is the small Fermi energy of the σ bands, which are strongly coupled with the E_{2g} mode. In this contribution, we discuss how the coexistence of both these features give rise to an unconventional phenomenology of the electron–phonon properties.

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1. Introduction

Since the discovery in 2001 of superconductivity in MgB₂ with $T_c = 39$ K, a large part of the research activity has been mainly devoted to investigate the multiband/multigap properties in this compound [1,2]. However, besides the multiband/multigap phenomenology, the electron–phonon coupling in MgB₂ has other peculiar features and it can be considered quite unconventional with respect to the common variety of phonon-based superconductors. A particular interesting property is that a large part of the electron–phonon coupling is concentrated in only one phonon mode, the E_{2g} one at $\mathbf{q} \approx 0$ [3], which presents an remarkably strong deformation potential $I_{E_{2g}}$ reflected in a large electron–phonon matrix element $g_{E_{2g}}$ [4,5]. On the experimental ground, most puzzling are the data from Raman spectroscopy which show an anomalously large phonon linewidth for the E_{2g} mode [6–9], often attributed to its anharmonic character. Also not yet understood are

the Raman measurements as function of Al doping, which show a transfer of spectral weight from a low- to a high-energy peaks rather than a steady hardening of the E_{2g} mode [10,11]. In this contribution, we briefly summarize our main results on the above issues. In particular, we show that (i) the anharmonic character of the E_{2g} mode can stem from a purely linear electron–phonon coupling *in the presence of a small Fermi energy*; (ii) the large E_{2g} phonon linewidth can be consistently explained within the context of the electron–phonon theory *once* damping processes in the electronic states, arising from the whole electron–phonon coupling spectrum, are properly taken into account.

In the following we introduce briefly a compact formulation of the electron–phonon problem in MgB₂ which will permit us to derive in a simple way the anharmonic character and the dynamical phonon self-energy as results of different limits. Starting point of our analysis will be the following Hamiltonian [12]:

$$H = 2 \sum_{\mathbf{k},i} [\epsilon_{\mathbf{k},i} - \mu + I_i u] c_{\mathbf{k},i}^\dagger c_{\mathbf{k},i} + \left[-\frac{\nabla_u^2}{2M} + \frac{M\omega_{E_{2g}}^2}{2} \right] u^2, \quad (1)$$

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which describes the two σ bands ($i = 1, 2$) interacting with the Jahn–Teller E_{2g} mode u at $\mathbf{q} = 0$ whose unrenormalized phonon frequency is given by $\omega_{E_{2g}}$. Here μ is the electronic chemical potential, M the effective atomic mass, and I_i the deformation potential which gives rise to a linear splitting of the two σ bands, $I_1 = -I_2 = I_{E_{2g}}$, while the π bands ($i = \pi$) at this level are totally decoupled ($I_\pi = 0$) and they act only as charge reservoir. The Hamiltonian (1) can be conveniently dealt with in the context of the path integral formalism. In particular, integrating out the fermionic Grassmann variables, we obtain an effective action in the imaginary Matsubara time for the lattice degrees of freedom:

$$S = 2 \sum_{\mathbf{k}, i} \text{Tr} \ln [G_i^{-1}(\mathbf{k}) - I_i u] - \frac{M}{2} \int_0^\beta d\tau u(\tau) \left[-\frac{\partial^2}{\partial \tau^2} + \omega_{E_{2g}}^2 \right] u(\tau), \quad (2)$$

where

$$G_i^{-1}(\mathbf{k}, \tau, \tau') = \delta(\tau - \tau') \left[-\frac{\partial}{\partial \tau'} - \epsilon_i(\mathbf{k}) + \mu \right], \quad (3)$$

and where $\text{Tr}[A] = \int_0^\beta d\tau A(\tau, \tau)$. Despite Eq. (2) looks at the first very simple, it is indeed quite hard to handle due to the fact that: (i) S is non-local in time τ ; (ii) it is higher than quadratic with respect the lattice variable u . As we are going to see, these two features are respectively related to (i) the dynamical nature of the electron–phonon interaction which gives rise to the possibility of phonon damping processes and (ii) the anharmonic character.

In order to make clear this point it is useful to disentangle the two issues. In particular the second issue can be promptly pointed out by assuming a static *classical* approximation for the variable $u(\tau)$: $u(\tau) \rightarrow \bar{u} = \langle u \rangle$ (and hence also $\partial u(\tau)/\partial \tau = 0$). It is easy to see that in this case Eq. (2) defines a static lattice potential [$S = \beta V_{\text{eff}}(\bar{u})$] equivalent to the frozen-phonon one in the first-principle calculations, properly generalized to finite temperature

$$V_{\text{eff}}(\bar{u}) = -\frac{M\omega_{E_{2g}}^2}{2} \bar{u}^2 + 2 \sum_{\mathbf{k}, i} T \ln \{ 1 + \exp[\beta(\mu - \epsilon_i(\mathbf{k}) - I_i \bar{u})] \}. \quad (4)$$

Eq. (4) can be easily evaluated in the zero temperature limit and, for the simple model with constant densities of states described in Ref. [12], we obtain

$$V_{\text{eff}}(\bar{u}) = \frac{M\omega_{E_{2g}}^2}{2} \bar{u}^2 - 2N_\sigma I_{E_{2g}}^2 \bar{u}^2 + \frac{2N_\sigma + N_\pi}{1 + N_\pi/N_\sigma} (I_{E_{2g}} |\bar{u}| - E_F^\sigma)^2 \theta[I_{E_{2g}} |\bar{u}| - E_F^\sigma], \quad (5)$$

where E_F^σ is the Fermi energy of the σ bands and N_σ , N_π are respectively the σ - and π -density of states. The static lattice potential $V_{\text{eff}}(u)$ so obtained, using realistic values for N_σ , N_π , E_F^σ , $\omega_{E_{2g}}$, $I_{E_{2g}}$ [12] is shown in Fig. 1, as compared with the harmonic one extrapolated by the small- u curvature. It

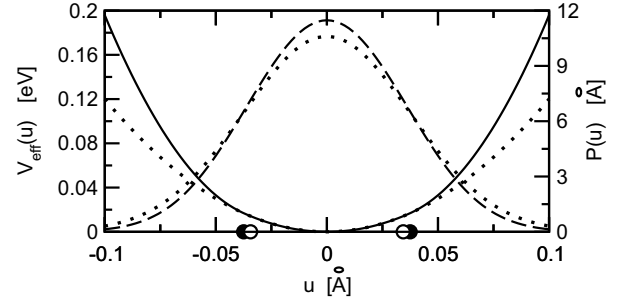


Fig. 1. Effective lattice potential $V_{\text{eff}}(u)$ (solid line) [12] and probability distribution function $P(u)$ (dashed line) [15] as evaluated respectively by Eqs. (5) and (7) using realistic values for the microscopical parameters. Dotted lines represents the same quantities by assuming a purely harmonic behavior $V_{\text{eff}}(u) \approx a_2 u^2$ extrapolated by the small- u dependence. The filled symbols mark $u = \pm u_c = E_F^\sigma / I_{E_{2g}}$, while the empty symbols denote $u = \pm \sqrt{u^2}$.

is important to underline that Eq. (5) presents a non-analytical behavior as function of u and it *cannot* be correctly represented as a power-law expansion $V_{\text{eff}}(u) \simeq a_2 u^2 + a_4 u^4$. This means that we cannot model the anharmonic effects in term of an effective quartic phonon–phonon interaction $H^{\text{anharmonic}} \propto (a + a^\dagger)^4$ [13] which would give rise, in a phonon self-energy treatment, to a finite phonon lifetime. In addition Eq. (5) shows in the most striking way how the onset of anharmonic effects is related to the smallness of the σ band Fermi energy E_F^σ . As a matter of fact its non-analytical dependence can be split in two different regimes [12]: a small- u one, for $|\bar{u}| \leq u_c = E_F^\sigma / I_{E_{2g}}$, where the lattice potential can be still described by a quadratic shape; and a large- u one, for $|\bar{u}| \geq u_c = E_F^\sigma / I_{E_{2g}}$, which is anharmonic. The σ band Fermi energy E_F^σ plays thus the role of a tuning parameter for the anharmonic effects. Interesting enough, the harmonic behavior is recovered in both the opposite extreme cases, $E_F^\sigma \rightarrow \infty$ and $E_F^\sigma \rightarrow 0$. The highest anharmonic character in this simple model is thus associated with finite lattice distortions u , where $u \simeq E_F^\sigma / I_{E_{2g}}$. How much physically relevant are the anharmonic effects is thus matter of how large is the physical range of u effectively sampled by to the quantum (and thermal) fluctuations.

In order to establish the physical range of u , we have thus to explicitly introduce the dynamics of the lattice fluctuations. A controlled way to do that is provided by the time gradient expansion [14] where the logarithmic term in Eq. (2) is formally expanded in powers of u :

$$2 \sum_{\mathbf{k}, i} \text{Tr} \ln [G_i^{-1}(\mathbf{k}) - g_i u] = 2 \sum_{\mathbf{k}, i} \text{Tr} \ln [G_i^{-1}(\mathbf{k})] - 2 \sum_{\mathbf{k}, i} \sum_{n=1}^{\infty} \frac{1}{n} \text{Tr} [(G_i(\mathbf{k}) g_i u)^n]. \quad (6)$$

At the lowest order of approximation we can assume that the lattice dynamics is much slower than the electronic one. In this case only local-time terms $u(\tau)$ are retained and the first term of (2) becomes also diagonal in time.

The expansion in Eq. (6) can be re-summed and one ends up with:

$$S = \int_0^\beta d\tau \left\{ u(\tau) \frac{M}{2} \frac{\partial^2 u(\tau)}{\partial \tau^2} - V_{\text{eff}}[u(\tau)] \right\}, \quad (7)$$

where $V_{\text{eff}}[u]$ has the same expression as in Eq. (5). This result corresponds to the semi-classical approximation as it was discussed in Ref. [15] and the phonon eigenstates can be found by solving the stationary Schrödinger equation associated with Eq. (7). In particular the ground-state wave-function $\psi_0(u)$ defines a probability distribution function $P(u) = |\psi_0(u)|^2$, shown in Fig. 1, which permits to evaluate the physical range of the lattice fluctuations as $\sqrt{\langle u^2 \rangle} = [\int du u^2 P(u)]^{1/2}$. We find $\sqrt{\langle u^2 \rangle} \simeq 0.034 \text{ \AA}$ to be compared with $u_c = E_F^c / I_{E_{2g}} \simeq 0.037 \text{ \AA}$ [15]. It is important to note that in the semiclassical approximation of Eq. (7) the whole phonon spectrum can be evaluated exactly by solving the stationary Schrödinger equation associated with Eq. (7). Due to the anharmonic effects, it will be described not by a unique peak but by a set of phonon δ -functions. Although this approach is indeed able to reveal anharmonic features, it cannot account thus for damping processes which will arise only from non-local terms in time.

The simplest way to see this issue is to disregard anharmonic effects and to expand the action (2) at the quadratic order in u : $S[u] = S_0 + \int_0^\beta d\tau \int_0^\beta d\tau' u(\tau) \Pi(\tau - \tau') u(\tau')$. The quadratic action acquires a simple diagonal form in the Matsubara frequency space

$$S = -\frac{M}{2} \sum_{\omega_m} u(-\omega_m) \left[\omega_m^2 + \omega_{E_{2g}}^2 + \frac{1}{M} \Pi(\omega_m) \right] u(\omega_m), \quad (8)$$

where $\Pi(\omega_m) = T \sum_{\mathbf{k}, \nu, i} I_i^2 G_i(\mathbf{k}, \nu + \omega_m) G_i(\mathbf{k}, \nu)$ defines the lowest order phonon self-energy. It is interesting to compare this result with the lowest order (local time) of the time gradient expansion, $\tilde{\Pi} = T \sum_{\mathbf{k}, \nu, i} I_i^2 G_i^2(\mathbf{k}, \nu)$ which is nothing else than the static limit $\tilde{\Pi} = \lim_{\omega_m \rightarrow 0} \Pi(\omega_m)$ of the retarded self-energy (8). This is by definition real so that damping processes, associated with the imaginary part (on the real frequency axis), are neglected. These effects are however fully retained in the dynamical self-energy in Eq. (8) whose imaginary part on the real axis ($i\omega_m \rightarrow \omega + i0^+$) reads

$$\begin{aligned} \Pi''(\omega) &= \pi \sum_{\mathbf{k}, i} |I_i|^2 \int d\omega' A_i(\mathbf{k}, \omega' + \omega) A_i(\mathbf{k}, \omega') \\ &\times [f(\omega' + \omega) - f(\omega')]. \end{aligned} \quad (9)$$

It is clear that for $\omega \rightarrow 0$ $\Pi''(\omega) \rightarrow 0$, recovering then the result of the local-time approximation. It is also clear on the other hand that damping processes will be *in principle* relevant for any phonon at finite frequency for which the renormalized phonon frequency $\Omega_{E_{2g}}$ and the phonon linewidth $\gamma_{E_{2g}}$ will be given by

$$\Omega_{E_{2g}}^2 = \omega_{E_{2g}}^2 + (1/M) \Pi'(\Omega_{E_{2g}}), \quad (10)$$

$$\gamma_{E_{2g}} = -(1/M \Omega_{E_{2g}}) \Pi''(\Omega_{E_{2g}}). \quad (11)$$

As a final, interesting consideration we note that for a *free* electron system $\Pi''(\omega) = 0$ for any $\omega \neq 0$ since Eq. (9) involves in this case a convolution of two non-overlapping δ -functions, $A_i(\mathbf{k}, \omega) = \delta(\omega - \epsilon_{\mathbf{k}, i})$. This observation points out that, neglecting interband scattering as in this case, the source of the damping processes for a $\mathbf{q} = 0$ phonon are intimately related to the presence of damping processes in the *electronic* states [16]. Following a similar derivation as it is done for the optical conductivity [17], one can indeed derive an approximate expression for the imaginary part of the phonon self-energy valid in the weak-coupling and for not “too small” ω

$$\Pi''(\omega) \propto \frac{\lambda_{E_{2g}}}{\omega^2} \int_0^\omega d\omega' \Sigma''(\omega'), \quad (12)$$

where $\Sigma''(\omega)$ is the imaginary part of the *electronic* self-energy. An analytic result can be derived for instance in the case of impurity scattering where $\Sigma''(\omega) = -i\Gamma$ and $\Pi''(\omega) \propto \omega_{E_{2g}} \lambda_{E_{2g}} 4\omega\Gamma / (\omega^2 + 4\Gamma^2)$. This relation should be compared with the Allen’s formula $\gamma_{\mathbf{q}} = \pi N(0) \omega_{\mathbf{q}}^2 \lambda_{\mathbf{q}}$ [18] (where $N(0)$ is the electronic density of states) which relates the phonon linewidth of a mode \mathbf{q} only to the electron–phonon properties of *this* particular mode, namely the phonon frequency $\omega_{\mathbf{q}}$ and its electron–phonon coupling $\lambda_{\mathbf{q}}$ [19]. On the other hand, Eq. (12) shows that a strong electron–phonon coupling $\lambda_{E_{2g}}$ is a necessary but not sufficient condition to account for a large phonon linewidth whereas significant electronic damping processes are also needed [16]. In addition Eq. (12) is also interesting because it relates the linewidth of the E_{2g} phonon to the electronic damping processes with energy ω *smaller* than $\Omega_{E_{2g}}$. In other words it implies that the strongly coupled E_{2g} phonon cannot be responsible for the own finite linewidth but other sources of electronic damping at energy $\omega < \Omega_{E_{2g}}$ are required. This is indeed the case of MgB₂ where, although a large part of the total electron–phonon coupling is associated with the E_{2g} phonon modes, a significant contribution is also spread over other different modes with typical energies $\omega < \Omega_{E_{2g}}$ [1–3]. We can analyze this situation by inserting in Eq. (9) the interacting spectral function for the σ band, $A_i(\mathbf{k}, \omega') = -(1/\pi) \text{Im}\{1/[\omega - \epsilon_{\mathbf{k}} - \Sigma(\mathbf{k}, \omega)]\}$ [16], where the electronic self-energy $\Sigma(\mathbf{k}, \omega)$ is evaluated by employing the full Eliashberg spectral function for the σ bands $\alpha_\sigma^2 F(\omega)$ obtained by first-principle calculations and an unrenormalized phonon frequency $\omega_{E_{2g}} = 100 \text{ MeV}$ [20]. The real part of the phonon self-energy can also be easily calculated by means of the Kramer–Krönig relations. In addition, we consider also the possible presence of impurity/disorder scattering.

In Fig. 2, we show the corresponding imaginary part of the phonon self-energy $\Pi''(\omega)$ (upper panel), and the phonon spectral function $B(\omega) = -(1/\pi) \text{Im}\{2\omega_{E_{2g}} / [\omega_{E_{2g}}^2 - \omega^2 + 2\omega_{E_{2g}} \Pi(\omega)]\}$ (lower panel). We see that the phonon

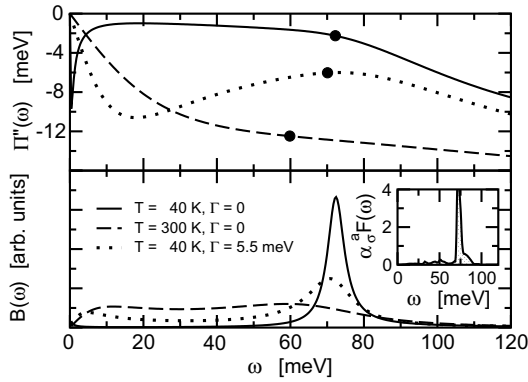


Fig. 2. Imaginary part of the phonon self-energy (upper panel) and phonon spectral function (lower panel) for three representative different cases. The marks in the upper panel denote $\Pi''(\omega)$ evaluated at the renormalized phonon frequency $\omega_{E_{2g}}$. Inset: effective Eliashberg function $\alpha_{\sigma}^2 F(\omega)$ relevant for the σ bands as evaluated in Ref. [20].

linewidth is highly sensitive to the amount of electronic damping. For instance for $T = 40$ K and in the absence of impurity scattering ($\Gamma = 0$) we predict a phonon linewidth $\gamma_{E_{2g}} \simeq 6$ MeV, which is essentially only due to the spectral weight of $\alpha_{\sigma}^2 F(\omega)$ for $\omega \leq \omega_{E_{2g}}$. The magnitude of the phonon linewidth is even more remarkable when finite temperature effects or impurity scattering are taken into account. In this case for instance we find $\gamma_{E_{2g}} \simeq 17$ MeV for $\Gamma = 5.5$ MeV at $T = 40$ K, in qualitative good agreement with the experimental value $\gamma_{E_{2g}}^{\text{exp}}(T = 40 \text{ K}) \simeq 22$ MeV, while for $T = 300$ K we find $\gamma_{E_{2g}} \simeq 36$ MeV and $\gamma_{E_{2g}} \simeq 32$ MeV, respectively for $\Gamma = 0$ and for $\Gamma = 5.5$ MeV, also in good agreement with the experimental value $\gamma_{E_{2g}}^{\text{exp}}(T = 300 \text{ K}) \simeq 34$ MeV [16].

We want to stress once more that there are *two* peculiar features of MgB_2 which cooperate to yield a large E_{2g} phonon linewidth. On one hand the E_{2g} phonon mode is indeed strongly coupled. This assures that the coupling prefactor is actually not negligible. On the other hand, a crucial role is also played by the sizable electron–phonon coupling

spread over all the other modes. These indeed give rise to significant electronic damping processes which is a compelling requirement in order to observe a finite phonon linewidth in a $\mathbf{q} = 0$ mode.

In conclusion, in this contribution we have shown as both the anharmonic character and the huge phonon linewidth of the E_{2g} mode observed in MgB_2 can be derived from a unique effective action for the E_{2g} lattice degrees of freedom employing different approximations. Aim of our future work is thus to generalize this approach to investigate the interplay between anharmonicity and damping processes.

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