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A model Hamiltonian for MgB_2 which takes into account its unusual phononic features

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Abstract. Taking as a starting point the results of LDA calculations, which show that in MgB_2 the phonons have a strong quartic anharmonicity and that the bond-stretching electron-phonon interaction (EPI) has both a linear and a large quadratic component, we propose a model Hamiltonian which successfully matches a number of experimental evidences. We relate the single critical temperature for both superconducting gaps to a phonon-induced inter-band coupling whose amplitude increases with temperature. We also obtain phonon frequencies and linewidths depending on the band filling, as well as band energies and hybridization amplitudes depending on the phonon number.

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1 Introduction

The electronic structure of the 40 K superconductor MgB_2 is characterized by the presence at the Fermi level of two hybrid bands (σ and π) of very different character [1]. This feature reflects itself in the experimental evidence of two different gaps [2–6], which however, in the absence of magnetic fields, have a common critical temperature [7]. The observation of a large Boron isotope effect [8] rules out the applicability of theories of Coulomb-interaction-driven two-band superconductivity [9], suggesting instead that the electron-phonon-interaction(EPI) is the key factor.

According to the standard theory of the EPI-driven two-band superconductivity [10], a single critical temperature for both gaps implies an interaction between the bands contributing to the Fermi surface. The microscopic origin of this interaction for the σ and π bands in MgB_2 is not yet clarified. Impurity scattering can be ruled out [11,12] and, to the best of our knowledge, no other precise suggestion has been advanced for the EPI scenario. An estimate of the interband coupling strength has been given in reference [13], based on the band structure calculation of reference [14], yielding a small, but decidedly non-negligible value. The strong temperature dependence of the anisotropy of the critical field [13] indicates that the interband coupling increases with temperature. The present work suggests that such coupling might be due to the unusual phononic structure of MgB_2. There is a general consensus that the dominant electron-phonon interaction is due to a modulation of the inter-site hopping amplitudes due to the bond-stretching vibration of the Boron ions [14–19]. By working out the corresponding Eliashberg's λ, reference [15] shows that there is a good agreement with the results following the LDA data, and with the experiments. In one-dimensional materials, this type of interaction is usually termed the Su-Schrieffer-Heeger (SSH) interaction, and we shall use this terminology also in the present context for convenience.

The unusual phononic features (first revealed by *ab initio* calculations of the electron and phonon band structures [14,16–18,20]) are the presence of anharmonic contributions (up to fourth order in the displacements) to the phononic Hamiltonian, and of both a linear and a quadratic term in the SSH interaction. Experimental evidence of anharmonicity comes from neutron [16] and Raman scattering [21] data. More specifically, the first-principle calculations in reference [20] find that the E_{2g} branch has, along the $\Gamma-$ A line in the Brillouin zone, an energy around 120 meV in the harmonic compound AlB_2 and of only 70 meV in MgB_2, in good quantitative agreement with the neutron scattering data [16]. Additionally, reference [21] presents first-principle calculations of the evolution of the phonon spectra when Al substitutes Mg agreeing with Raman data, which confirm the frequency softening on passing from harmonic AlB_2 to anharmonic MgB_2. One important aspect of such measurements is that, as Al substitution changes the occupancy of the bands at the Fermi surface, the phonon frequency and lifetime both depend on the band filling. So, in relating those data to the change in phononic properties, one should be able to

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disentangle the effects of anharmonicity from those of band-filling variations. However, one must also mention that Raman and infrared data of reference [19] for $Mg_{1-x}Al_xB_2$ when $0 \leq x \leq 0.50$, on the contrary, find the frequency of the E_{2g} mode almost insensitive to the Al content.

Another theoretically predicted effect of the anharmonicity is the reduction of the averaged electron-phonon coupling, as expressed by Eliashberg's λ. For that, the experimental evidence is not so clear. Indeed, the first-principle calculation of the phonon spectra of reference [18] are in excellent agreement with the experimental data, and they yield at the same time that the strength of λ is reduced in the anharmonic case. However, if one takes the phonon linewidth as roughly expressing the combined intensity of the electron-phonon interactions, both references [19] and [21] show that it strongly decreases with x. As Eliashberg's λ for a bond-stretching interaction [22] depends on structure, band-filling and frequencies, it is difficult to precisely identify the cause(s) of the observed effects.

The *ab initio* numerical calculations [14,16–18,20] have yielded valuable insights about the electronic and phononic structure of MgB_2, which we take as the input information for the work presented here. Our aim in this paper is to propose a model Hamiltonian which represents the physics implied by the results of the first-principle calculations as far as the phononic features are concerned. We have no ambition of giving detailed quantitative results. However, our model is quantitatively consistent with the numerical results of references [14,16,18]. While suggesting a plausible mechanism for the inter-band coupling, and therefore justifying [10] the presence of a single critical temperature for both superconducting gaps [2–6], at the same time it also qualitatively allows for other experimentally observed features: the increase with temperature of the inter-band coupling [13] and the fact that the phonon frequency and linewidth both depend on band-filling [19,21]. In particular, we find indications that the frequency hardening on Al substitution can not be accounted for by the anharmonic-to-harmonic change only.

Detailed quantitative estimates based on the proposed model are left for future work.

2 The electronic Hamiltonian

Our model of the electronic structure of MgB_2 by a Hamiltonian has two bands, labeled c and d, which hybridize through an inter-site hopping term. Then, in the real space representation, the bare electronic Hamiltonian reads:

$$H_{el} = \varepsilon^c \sum_{l\sigma} n^c_{l\sigma} + \varepsilon^d \sum_{l\sigma} n^d_{l\sigma} + \sum_{l\langle j\rangle\sigma} \left[t^{cc}_{lj} c^\dagger_{l\sigma} c_{j\sigma} + t^{dd}_{lj} d^\dagger_{l\sigma} d_{j\sigma} \right] + \sum_{l\langle j\rangle\sigma} t^{cd}_{lj} \left(c^\dagger_{l\sigma} d_{j\sigma} + d^\dagger_{j\sigma} c_{l\sigma} \right) \quad (1)$$

where $\sum_{l\langle j\rangle}$ means summing on the z nearest neighbors j of a given site l, and then on l. In MgB_2 one expects that $t^{cc}_{lj}, t^{dd}_{lj} \gg t^{cd}_{lj}$ [1,13,15]. The electron-phonon coupling parameters in the SSH scenario are derivatives of the hopping amplitudes with respect to the inter-site distance. By using $c^\dagger_{l\sigma} = N^{-1/2} \sum_k c^\dagger_{k\sigma} \exp(ikR_l)$ we pass to the reciprocal space representation, yielding :

$$H_{el} = \sum_{k\sigma} \left(\varepsilon^c + z t^{cc}_k \right) n^c_{k\sigma} + \sum_{k\sigma} \left(\varepsilon^d + z t^{dd}_k \right) n^d_{k\sigma} + \sum_{k\sigma} z t^{cd}_k \left(c^\dagger_{k\sigma} d_{k\sigma} + d^\dagger_{k\sigma} c_{k\sigma} \right) \quad (2)$$

where $t^{\mu\nu}_k = z^{-1} \sum_{\langle j\rangle} t^{\mu\nu}_{lj} \exp\left[ik \left(R_l - R_j \right) \right]$ with $\mu, \nu = c, d$. To diagonalize H_{el} we express the bare operators $c^\dagger_{k\sigma}, d^\dagger_{k\sigma}$ through the hybridized operators $\alpha^\dagger_{k\sigma}, \beta^\dagger_{k\sigma}$ according to:

$$c^\dagger_{k\sigma} = \alpha^\dagger_{k\sigma} \cos\varphi_k + \beta^\dagger_{k\sigma} \sin\varphi_k$$

$$d^\dagger_{k\sigma} = -\alpha^\dagger_{k\sigma} \sin\varphi_k + \beta^\dagger_{k\sigma} \cos\varphi_k. \quad (3)$$

In the following, any operator O expressed through the hybridized operators will be denoted by a tilde $\widetilde{O}$. By choosing

$$\tan(2\varphi_k) = -\frac{2 z t^{cd}_k}{\varepsilon^c_k - \varepsilon^d_k + z\left(t^{cc}_k - t^{dd}_k \right)}. \quad (4)$$

H_{el} is brought to diagonal form $H_{el} \Longrightarrow \widetilde{H}_{el} = \sum_{k\sigma} \left(E^\alpha_k n^\alpha_{k\sigma} + E^\beta_k n^\beta_{k\sigma} \right)$, with the particle energies in the hybridized bands given by:

$$E^\alpha_k = \frac{1}{2} \left[\varepsilon^c + \varepsilon^d + z\left(t^{cc}_k + t^{dd}_k \right) \right] + \frac{1}{2} \sqrt{\left[\varepsilon^c - \varepsilon^d + z\left(t^{cc}_k - t^{dd}_k \right) \right]^2 + \left(2 z t^{cd}_k \right)^2} \quad (5)$$

$$E^\beta_k = \frac{1}{2} \left[\varepsilon^c + \varepsilon^d + z\left(t^{cc}_k + t^{dd}_k \right) \right] - \frac{1}{2} \sqrt{\left[\varepsilon^c - \varepsilon^d + z\left(t^{cc}_k - t^{dd}_k \right) \right]^2 + \left(2 z t^{cd}_k \right)^2}. \quad (6)$$

The α and β bands, at this stage completely decoupled by the transformation of equation (3), represent in our model the σ and π bands of MgB_2.

3 The phononic Hamiltonian with anharmonic terms

Following [16,18] we assume that the purely phononic Hamiltonian H_{ph} for MgB_2 has to include, apart from the

usual harmonic term, also a non-negligible quartic contribution. The anharmonicity of the MgB_2 phonon modes has been analyzed in [17], showing that two E_{2g} modes, degenerate at the Γ point, have anharmonicities differing in the presence (mode labeled a in [17]), or absence (mode b), of a third-order term. In reference [14] a cubic term was included in the development of the deformation energy. Its amplitude was found to be of the same order as the linear term, *i.e.* about five times smaller than the quartic term amplitude. It gives rise to terms non conserving the phonon numbers, analogously to the linear SSH term. We'll consider only the mode labeled $E_{2g}(b)$ in reference [17], which has no third-order anharmonicity, both for short, and because the effect of the dropped terms is similar, in amplitude and in type, to the one due to the linear SSH term, which we keep. A similar assumption of neglecting the $E_{2g}(a)$ mode has been explicitly [23] or implicitly [16,18] made in other studies.

Under such assumptions, H_{ph} takes the form [24]:

$$H_{ph} = \sum_q \frac{P_q P_{-q}}{2M} + \frac{M}{2}\sum_q \Omega_q^2 u_q u_{-q} + \frac{M^2}{4N}\sum_{qp} x_{qp}\Omega_q^2\Omega_p^2 u_q u_{-q} u_p u_{-p} \quad (7)$$

where M is the Boron mass and Ω_q is the frequency, at the wavevector q along the $\Gamma - A$ line, of the optical mode of E_{2g} symmetry. The parameter x_{qp} expresses the strength of the quartic term involving the wavevectors $\pm q$ and $\pm p$. In MgB_2, from reference [16], one can estimate $x_{qp} \approx 7.8\ \mathrm{eV}^{-1}$.

By quantizing the phonon field according to the usual relations:

$$u_q = \sqrt{\frac{\hbar}{2M\Omega_q}}\left(b_{-q}^\dagger + b_q\right)$$

$$P_q = i\sqrt{\frac{\hbar\Omega_q}{2M}}\left(b_{-q}^\dagger - b_q\right)$$

$$L_q = \sqrt{\frac{\hbar}{2M\Omega_q}} \quad (8)$$

the harmonic part becomes $\sum_q \hbar\Omega_q\left(b_q^\dagger b_q + \frac{1}{2}\right)$. When quantizing the quartic term, we neglect the terms with different numbers of creation and destruction operators and keep the remaining four-operator products only when diagonal. Namely, we approximate $b_{-q}^\dagger b_q^\dagger b_{-p} b_p \approx \left(\delta_{p,q} + \delta_{p,-q}\right)\nu_q\nu_{-q}$, where $b_q^\dagger b_q = \nu_q$. The quartic contribution then reduces to:

$$\begin{aligned}
&\sum_{qp} x_{qp}\left(\frac{\hbar\Omega_q}{4}\right)\left(\frac{\hbar\Omega_p}{4}\right)\left(b_{-q}^\dagger + b_q\right)\left(b_q^\dagger + b_{-q}\right) \\
&\qquad \times \left(b_{-p}^\dagger + b_p\right)\left(b_p^\dagger + b_{-p}\right) \approx \\
&4\sum_q \left(\frac{\hbar\Omega_q}{4}\right)\left(\frac{1}{2} + \nu_q\right)\sum_p x_{qp}\left(\frac{\hbar\Omega_p}{4}\right)\left(1 + \delta_{qp}\right) \\
&\quad + 4\sum_{qp} x_{qp}\left(\frac{\hbar\Omega_p}{4}\right)\left(\frac{\hbar\Omega_q}{4}\right)\nu_q\nu_p\left(1 + \delta_{q,-p}\right) \\
&\quad + 2\sum_q \left(\frac{\hbar\Omega_q}{4}\right)\left(b_{-q}^\dagger b_q^\dagger + b_{-q}b_q\right)\sum_p x_{qp}\left(\frac{\hbar\Omega_p}{4}\right) \\
&- 2\sum_{qp} x_{qp}\left(\frac{\hbar\Omega_q}{4}\right)\left(\frac{\hbar\Omega_p}{4}\right) + \sum_{qp} x_{qp}\left(\frac{\hbar\Omega_q}{4}\right)\left(\frac{\hbar\Omega_p}{4}\right).
\end{aligned} \quad (9)$$

The product $\nu_q\nu_p$ is approximated in the MFA fashion, *i.e.* $\nu_q\nu_p \approx \nu_q\langle\nu_p\rangle + \langle\nu_q\rangle\nu_p - \langle\nu_p\rangle\langle\nu_q\rangle$. Putting together the constant terms, we can rewrite equation (9) as:

$$\begin{aligned}
&\sum_q \hbar\Omega_q\left(\frac{1}{2} + \nu_q\right)\left[\frac{1}{N}\sum_p x_{qp}\left(\frac{\hbar\Omega_p}{2}\right)\left(\frac{1}{2} + \langle\nu_p\rangle\right)\right. \\
&\qquad \left.\times\left(1 + \delta_{q,-p}\right)\right] + \sum_q \hbar\Omega_q\left(b_{-q}^\dagger b_q^\dagger + b_{-q}b_q\right) \\
&\qquad \times\left[\frac{1}{N}\sum_p x_{qp}\left(\frac{\hbar\Omega_p}{8}\right)\right] + \text{const.}
\end{aligned} \quad (10)$$

Adding the harmonic contribution and defining

$$X_q \equiv 1 + \frac{1}{N}\sum_p x_{qp}\left(\frac{\hbar\Omega_p}{2}\right)\left(\frac{1}{2} + \langle\nu_p\rangle\right)\left(1 + \delta_{q,-p}\right) \quad (11)$$

we obtain the purely phononic Hamiltonian as:

$$\begin{aligned}
H_{ph} &= \sum_q \hbar\Omega_q X_q\left(\frac{1}{2} + \nu_q\right) \\
&+ \sum_q \hbar\Omega_q\left(b_{-q}^\dagger b_q^\dagger + b_{-q}b_q\right)\left[\frac{1}{N}\sum_p x_{qp}\left(\frac{\hbar\Omega_p}{8}\right)\right] + \text{const.}
\end{aligned} \quad (12)$$

This form can be diagonalized by a "squeezing" transformation [25] $e^S \equiv \exp\left[-\sum_q \eta_q\left(b_{-q}^\dagger b_q^\dagger - b_{-q}b_q\right)\right]$ under the condition that

$$\tanh\left(2\eta_q\right) = -\frac{1}{X_q}\left(\frac{1}{N}\right)\sum_p x_{qp}\left(\frac{\hbar\Omega_p}{4}\right). \quad (13)$$

Notice that equation (13) yields $\eta_q < 0$. The diagonalized Hamiltonian $e^S H_{ph} e^{-S}$ can now be written as:

$$e^S H_{ph} e^{-S} = \sum_q \hbar\Omega_q \left[X_q \cosh\left(2\eta_q\right) + 2\sinh\left(2\eta_q\right) \left(\frac{1}{N}\right) \sum_p x_{qp} \frac{\hbar\Omega_p}{8} \right] \times \left(b_q^\dagger b_q + \frac{1}{2} \right) + \text{const.} \quad (14)$$

By substituting η_q from equation (13) into equation (14), the renormalized frequency ω_q of the harmonic Hamiltonian for the squeezed phonons is written explicitly as:

$$\omega_q = \Omega_q X_q \left[\sqrt{1 - \tanh^2\left(2\eta_q\right)} \right] \quad (15)$$

where $\Omega_q X_q$ is the phonon frequency entering the quadratic part of the unsqueezed phononic Hamiltonian (see. Eq. (12)). It is not the true bare frequency, because, from equation (11), $X_q - 1$ yields the contribution from the diagonal part of the quartic terms treated in MFA, so that $\Omega_q X_q$ already contains some effects of anharmonicity, analogous to those taken into account, *e.g.* in reference [16]. Thus, equation (15) shows that ω_q is increased (hardened) with respect to the "harmonic frequency" Ω_q by $X_q > 1$, but the squeezing effect, taking account of the two-phonon terms terms previously [16] neglected, counteracts the hardening. According to references [14,16,18] however, the squeezing effect is not strong enough for an overall softening to result.

4 The linear electron-phonon interaction

The linear part of the SSH electron-phonon interaction is written, in the real space representation symmetrized with respect to the site indexes, as

$$H_{ep}^{(1)} = \frac{1}{2} \sum_{l\langle j\rangle\sigma} \left[g_{lj}^{cc} \left(c_{l\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{l\sigma} \right) + g_{lj}^{dd} \left(d_{l\sigma}^\dagger d_{j\sigma} + d_{j\sigma}^\dagger d_{l\sigma} \right) \right] \left(u_l - u_j\right) + \frac{1}{2} \sum_{l\langle j\rangle\sigma} g_{lj}^{cd} \left(d_{l\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger d_{l\sigma} + d_{j\sigma}^\dagger c_{l\sigma} + c_{l\sigma}^\dagger d_{j\sigma} \right) \left(u_l - u_j\right) \quad (16)$$

where $g_{lj}^{\mu\nu} = \partial t_{lj}^{\mu\nu} / \partial \left(u_l - u_j\right)|_0 = -g_{jl}^{\mu\nu}$ with $\mu, \nu = c, d$, are the coupling constants, and the $1/2$ factor avoids double counting.

The Fourier-transformed form of equation (16) is written in terms of $g_k^{\mu\nu} = (1/z) \sum_{\langle j\rangle} g_{lj}^{\mu\nu} \exp(ik \cdot \Delta_{lj})$ (where Δ_{lj} is the vector connecting the sites l and j) which we combine in the definition of the coupling strength $\gamma_{k,k-q}^{\mu\nu}$ according to:

$$\frac{z}{2} \left(g_{k-q}^{\mu\nu} + g_k^{\mu\nu} - g_{-(k-q)}^{\mu\nu} - g_{-k}^{\mu\nu} \right) = i \sum_{\langle j\rangle} g_{lj}^{\mu\nu} \left\{ \sin\left[(k-q)\cdot\Delta_{lj}\right] - \sin\left[k\cdot\Delta_{lj}\right] \right\} \equiv \gamma_{k,k-q}^{\mu\nu} / L_q. \quad (17)$$

Equation (17) is the simplest possible form of the bond-stretching electron-phonon interaction which includes the relevant physics. It is adequate for a qualitative discussion, but it is not good enough for a quantitative study.

Quantization of the phonons according to equation (8) leads to:

$$H_{ep}^{(1)} = \frac{1}{\sqrt{N}} \sum_{kq\sigma} \left[\gamma_{k,k-q}^{cc} c_{k\sigma}^\dagger c_{k-q\sigma} + \gamma_{k,k-q}^{dd} d_{k\sigma}^\dagger d_{k-q\sigma} + \gamma_{k,k-q}^{cd} \left(c_{k\sigma}^\dagger d_{k-q\sigma} + d_{k\sigma}^\dagger c_{k-q\sigma} \right) \right] \times \left(b_{-q}^\dagger + b_q \right). \quad (18)$$

When transformed to the hybridized fermion representation $H_{ep}^{(1)}$ reads:

$$\widetilde{H}_{ep}^{(1)} = \frac{1}{\sqrt{N}} \sum_{kq\sigma} \left[\Gamma_{k,k-q}^{\alpha\alpha} \alpha_{k\sigma}^\dagger \alpha_{k-q,\sigma} + \Gamma_{k,k-q}^{\beta\beta} \beta_{k\sigma}^\dagger \beta_{k-q,\sigma} + \Gamma_{k,k-q}^{\alpha\beta} \alpha_{k\sigma}^\dagger \beta_{k-q,\sigma} + \Gamma_{k,k-q}^{\beta\alpha} \beta_{k\sigma}^\dagger \alpha_{k-q,\sigma} \right] \left(b_{-q}^\dagger + b_q \right) \quad (19)$$

where the effective couplings are defined as:

$$\Gamma_{k,k-q}^{\alpha\alpha} = \gamma_{k,k-q}^{cc} \cos\varphi_k \cos\varphi_{k-q} + \gamma_{k,k-q}^{dd} \sin\varphi_k \sin\varphi_{k-q} - \gamma_{k,k-q}^{cd} \sin\left(\varphi_k + \varphi_{k-q}\right) \quad (20)$$

$$\Gamma_{k,k-q}^{\beta\beta} = \gamma_{k,k-q}^{cc} \sin\varphi_k \sin\varphi_{k-q} + \gamma_{k,k-q}^{dd} \cos\varphi_k \cos\varphi_{k-q} + \gamma_{k,k-q}^{cd} \sin\left(\varphi_k + \varphi_{k-q}\right) \quad (21)$$

$$\Gamma_{k,k-q}^{\alpha\beta} = \gamma_{k,k-q}^{cc} \cos\varphi_k \sin\varphi_{k-q} - \gamma_{k,k-q}^{dd} \sin\varphi_k \cos\varphi_{k-q} + \gamma_{k,k-q}^{cd} \cos\left(\varphi_k + \varphi_{k-q}\right) \quad (22)$$

$$\Gamma_{k,k-q}^{\beta\alpha} = \gamma_{k,k-q}^{cc} \sin\varphi_k \cos\varphi_{k-q} - \gamma_{k,k-q}^{dd} \cos\varphi_k \sin\varphi_{k-q} + \gamma_{k,k-q}^{cd} \cos\left(\varphi_k + \varphi_{k-q}\right). \quad (23)$$

5 The quadratic electron-phonon interaction

According to references [14,16,18], the electron-phonon Hamiltonian has to include also a quadratic term, which

we write in real space in symmetrized form, as:

$$H_{ep}^{(2)} = \frac{1}{2}\sum_{l\langle j\rangle\sigma}\Bigg[f_{lj}^{cc}\left(c_{l\sigma}^{\dagger}c_{j\sigma}+c_{j\sigma}^{\dagger}c_{l\sigma}\right) + f_{lj}^{dd}\left(d_{l\sigma}^{\dagger}d_{j\sigma}+d_{j\sigma}^{\dagger}d_{l\sigma}\right)\Bigg]\left(u_l-u_j\right)^2 + \frac{1}{2}\sum_{l\langle j\rangle\sigma}f_{lj}^{cd}\left(d_{l\sigma}^{\dagger}c_{j\sigma}+c_{j\sigma}^{\dagger}d_{l\sigma}+d_{j\sigma}^{\dagger}c_{l\sigma}+c_{l\sigma}^{\dagger}d_{j\sigma}\right)\times\left(u_l-u_j\right)^2 \quad (24)$$

where $f_{lj}^{\mu\nu}=\partial^2 t_{lj}^{\mu\nu}/\partial\left(u_l-u_j\right)^2|_0=f_{jl}^{\mu\nu}$, with $\mu,\nu=c,d$. We also develop $\left(u_l-u_j\right)^2=u_l^2+u_j^2-u_lu_j-u_ju_l$. By defining $f_k^{\mu\nu}\equiv z^{-1}\sum_{\langle j\rangle}f_{lj}^{\mu\nu}e^{ik\Delta_{lj}}$ and introducing the coefficients $F_{kpq}^{\mu\nu}\equiv(z/2)\left(f_p^{\mu\nu}+f_k^{\mu\nu}-f_{k-q}^{\mu\nu}-f_{p+q}^{\mu\nu}\right)$, the Fourier transform reads:

$$H_{ep}^{(2)} = \frac{1}{N}\sum_{kpq\sigma}\Bigg[F_{kpq}^{cc}\left(c_{k\sigma}^{\dagger}c_{p\sigma}+c_{-p\sigma}^{\dagger}c_{-k\sigma}\right) + F_{kpq}^{dd}\left(d_{k\sigma}^{\dagger}d_{p\sigma}+d_{-p\sigma}^{\dagger}d_{-k\sigma}\right)\Bigg]u_qu_{k-p-q} + \frac{1}{N}\sum_{kpq\sigma}F_{kpq}^{cd}\left(d_{k\sigma}^{\dagger}c_{p\sigma}+c_{k\sigma}^{\dagger}d_{p\sigma}+d_{-p\sigma}^{\dagger}c_{-k\sigma}+c_{-p\sigma}^{\dagger}d_{-k\sigma}\right)\times u_qu_{k-p-q}. \quad (25)$$

When quantizing the deformations according to equation (8), we shall take into account only the diagonal terms and those which can be diagonalized by squeezing, by enforcing $k=p$. Then u_qu_{k-p-q} reduces to:

$$u_qu_{k-p-q}\Longrightarrow u_qu_{-q}\delta_{pk}= \delta_{pk}L_q^2\left(b_{-q}^{\dagger}b_q^{\dagger}+b_qb_{-q}+\nu_q+\nu_{-q}+1\right). \quad (26)$$

Let us stress that our aim is to show that there are some contributions to $H_{ep}^{(2)}$ which provide an effective inter-band coupling. We do not claim to be able to treat all the terms in $H_{ep}^{(2)}$: we just want to select the subset of "hot" terms. Under this approximation, by using $F_{k,q}^{\mu\nu}=F_{-k,-q}^{\mu\nu}$, equation (25) reduces to:

$$H_{ep}^{(2)}\approx 2\frac{1}{N}\sum_{kq\sigma}L_q^2\Bigg[F_{kq}^{cc}c_{k\sigma}^{\dagger}c_{k\sigma}+F_{kq}^{dd}d_{k\sigma}^{\dagger}d_{k\sigma} + F_{kq}^{cd}\left(d_{k\sigma}^{\dagger}c_{p\sigma}+c_{k\sigma}^{\dagger}d_{p\sigma}\right)\Bigg]\times\left(b_{-q}^{\dagger}b_q^{\dagger}+b_qb_{-q}+\nu_q+\nu_{-q}+1\right). \quad (27)$$

Let' s now pass to the hybridized band picture, through the transformation of equation (3). If we define for short the energies:

$$F_{kq}^{\alpha\alpha}=2L_q^2\left[F_{kq}^{cc}\cos^2\varphi_k+F_{kq}^{dd}\sin^2\varphi_k-F_{kq}^{cd}\sin\left(2\varphi_k\right)\right] \quad (28)$$

$$F_{kq}^{\beta\beta}=2L_q^2\left[F_{kq}^{cc}\sin^2\varphi_k+F_{kq}^{dd}\cos^2\varphi_k+F_{kq}^{cd}\sin\left(2\varphi_k\right)\right] \quad (29)$$

$$F_{kq}^{\alpha\beta}=L_q^2\left[\left(F_{kq}^{cc}-F_{kq}^{dd}\right)\sin\left(2\varphi_k\right)+2F_{kq}^{cd}\cos\left(2\varphi_k\right)\right] \quad (30)$$

where

$$F_{kq}^{\mu\nu}=\sum_{\langle j\rangle}f_{lj}^{\mu\nu}\left\{\cos\left(k\Delta_{lj}\right)\left[1-\cos\left(q\Delta_{lj}\right)\right]\right\} \quad (\mu,\nu=c,d) \quad (31)$$

then equation (27) can be rewritten compactly as:

$$\widetilde{H}_{ep}^{(2)}=\frac{1}{N}\sum_{kq\sigma}\Bigg[n_{k\sigma}^{\alpha}F_{kq}^{\alpha\alpha}+n_{k\sigma}^{\beta}F_{kq}^{\beta\beta}+\left(\alpha_{k\sigma}^{\dagger}\beta_{k\sigma}+\beta_{k\sigma}^{\dagger}\alpha_{p\sigma}\right)\times F_{kq}^{\alpha\beta}\Bigg]\left(b_{-q}^{\dagger}b_q^{\dagger}+b_qb_{-q}+\nu_q+\nu_{-q}+1\right). \quad (32)$$

6 The electron-phonon Hamiltonian in the squeezed phonon representation

Let us now introduce the squeezed phonon representation also for $\widetilde{H}_{ep}^{(1)}+\widetilde{H}_{ep}^{(2)}$. By using the relation $e^S\left(b_{-q}^{\dagger}+b_q\right)e^{-S}=e^{\eta_q}\left(b_{-q}^{\dagger}+b_q\right)$ the linear coupling term becomes:

$$e^S\widetilde{H}_{ep}^{(1)}e^{-S}=\frac{1}{\sqrt{N}}\sum_{kq\sigma}e^{\eta_q}\Bigg[\Gamma_{k,k-q}^{\alpha\alpha}\alpha_{k\sigma}^{\dagger}\alpha_{k-q,\sigma} + \Gamma_{k,k-q}^{\beta\beta}\beta_{k\sigma}^{\dagger}\beta_{k-q,\sigma}+\Gamma_{k,k-q}^{\alpha\beta}\alpha_{k\sigma}^{\dagger}\beta_{k-q,\sigma}+\Gamma_{k,k-q}^{\beta\alpha}\beta_{k\sigma}^{\dagger}\alpha_{k-q,\sigma}\Bigg]\times\left(b_{-q}^{\dagger}+b_q\right). \quad (33)$$

Then the linear coupling has a reduce amplitude, as $\eta_q<0$ (see Eq. (13)), consistently with the numerical analysis of reference [18].

For the quadratic part $\widetilde{H}_{ep}^{(2)}$ we get:

$$e^S\widetilde{H}_{ep}^{(2)}e^{-S}=\frac{1}{N}\sum_{kq}\Bigg[F_{kq}^{\alpha\alpha}n_{k\sigma}^{\alpha}+F_{kq}^{\beta\beta}n_{k\sigma}^{\beta} + F_{kq}^{\alpha\beta}\left(\alpha_{k\sigma}^{\dagger}\beta_{k\sigma}+\beta_{k\sigma}^{\dagger}\alpha_{k\sigma}\right)\Bigg]\times e^{2\eta_q}\left(b_{-q}^{\dagger}b_q^{\dagger}+b_qb_{-q}+\nu_q+\nu_{-q}+1\right). \quad (34)$$

In equation (34) we can decouple the electronic and phononic terms in MFA. Indeed, assuming

$$\langle b_{-q}^{\dagger} b_q^{\dagger} + b_q b_{-q} + \nu_q + \nu_{-q} + 1 \rangle \approx 2\langle \nu_q \rangle + 1 \tag{35}$$

and defining

$$\Phi_q = \frac{1}{N} \sum_{k\sigma} \Big[F_{kq}^{\alpha\alpha} \langle n_{k\sigma}^{\alpha} \rangle + 2F_{kq}^{\beta\beta} \langle n_{k\sigma}^{\beta} \rangle + F_{kq}^{\alpha\beta} \big(\langle \alpha_{k\sigma}^{\dagger} \beta_{k\sigma} \rangle + \langle \beta_{k\sigma}^{\dagger} \alpha_{k\sigma} \rangle \big) \Big] = \Phi_{-q} \tag{36}$$

yields:

$$e^S \widetilde{H}_{ep}^{(2)} e^{-S} \approx \frac{1}{N} \sum_{kq\sigma} \Big[F_{kq}^{\alpha\alpha} n_{k\sigma}^{\alpha} + F_{kq}^{\beta\beta} n_{k\sigma}^{\beta} + F_{kq}^{\alpha\beta} \left(\alpha_{k\sigma}^{\dagger} \beta_{k\sigma} + \beta_{k\sigma}^{\dagger} \alpha_{k\sigma} \right) \Big] \times e^{2\eta_q} \left(2\langle \nu_q \rangle + 1 \right) + \sum_q e^{2\eta_q} \Phi_q \Big(b_{-q}^{\dagger} b_q^{\dagger} + b_q b_{-q} + \nu_q + \nu_{-q} + 1 \Big) + \text{const.} \tag{37}$$

By writing $\sum_q \hbar\omega_q \left(\nu_q + \frac{1}{2} \right) = \frac{1}{2} \sum_q \hbar\omega_q \left(\nu_q + \nu_{-q} + 1 \right)$ and reordering the Hamiltonian in the hybridized basis we get:

$$e^S \widetilde{H} e^{-S} = \sum_{k\sigma} E_k^{\alpha} n_{k\sigma}^{\alpha} + \sum_{k\sigma} E_k^{\beta} n_{k\sigma}^{\beta} + \sum_q \hbar\omega_q \left(\nu_q + \frac{1}{2} \right) + e^S \widetilde{H}_{ep}^{(1)} e^{-S} + e^S \widetilde{H}_{ep}^{(2)} e^{-S}. \tag{38}$$

Inserting $e^S \widetilde{H}_{ep}^{(2)} e^{-S}$ from equation (37) into equation (38) and reordering yields:

$$e^S \widetilde{H} e^{-S} = \mathcal{H}_{el.}^{diag} + \mathcal{H}_{el}^{hyb} + \mathcal{H}_{ph} + e^S H_{ep}^{(1)} e^{-S} + \text{const.} \tag{39}$$

where the diagonal electronic Hamiltonian is:

$$\mathcal{H}_{el.}^{diag} \equiv \sum_{k\sigma} \left[E_k^{\alpha} + \frac{1}{N} \sum_q F_{kq}^{\alpha\alpha} e^{2\eta_q} \left(2\langle \nu_q \rangle + 1 \right) \right] n_{k\sigma}^{\alpha} + \sum_{k\sigma} \left[E_k^{\beta} + \frac{1}{N} \sum_q F_{kq}^{\beta\beta} e^{2\eta_q} \left(2\langle \nu_q \rangle + 1 \right) \right] n_{k\sigma}^{\beta} \tag{40}$$

and describes a phonon-depending renormalization of the band energies. The hybrid electronic Hamiltonian is:

$$\mathcal{H}_{el}^{hyb} \equiv \frac{1}{N} \sum_{kq\sigma} e^{2\eta_q} F_{kq}^{\alpha\beta} \left(2\langle \nu_q \rangle + 1 \right) \left(\alpha_{k\sigma}^{\dagger} \beta_{k\sigma} + \beta_{k\sigma}^{\dagger} \alpha_{k\sigma} \right). \tag{41}$$

It represents a phonon-depending band hybridization term. This is, we believe, the term responsible for the coupling between the bands in MgB_2 which results in a single critical temperature for both gaps. We would like to point out that, in the limit of small inter-bare-band hopping, *i.e.* $t_{lj}^{cd}/t_{lj}^{cc} \to 0$, and at zero temperature, where $\langle \nu_q \rangle$ can be neglected, one finds:

$$\lim_{t_{lj}^{cd}/t_{lj}^{cc} \to 0} e^{2\eta_q} F_{kq}^{\alpha\beta} = 2L_q^2 e^{2\eta_q} F_{kq}^{cd} = 2L_q^2 e^{2\eta_q} \sum_{\langle j \rangle} f_{lj}^{cd} \left\{ \cos\left(k\Delta_{lj} \right) \left[1 - \cos\left(q\Delta_{lj} \right) \right] \right\}. \tag{42}$$

Apart from geometric factors, this amplitude depends only on the intensity of the squeezing (through $e^{2\eta_q}$) and on the strength of the quadratic inter-band SSH electron-phonon coupling f_{lj}^{cd}. As f_{lj}^{cd} is a second derivative of t_{lj}^{cd}, it can be non-negligible even if t_{lj}^{cd} itself is very small. Different evaluations of f_{lj}^{cd} [1] all agree that in MgB_2 it has an appreciable value. More specifically, an effective two-band model derived from first-principle calculations [14] yields $\lambda_{\sigma\pi}/\lambda_{\sigma\sigma} = 0.21$ and $\lambda_{\pi\sigma}/\lambda_{\sigma\sigma} = 0.15$ [26].

At nonzero temperatures, the hybridization amplitude gets an additional contribution proportional to $2\langle \nu_q \rangle$, hence it increases with temperature, consistently with the findings of reference [13]

The purely phononic term

$$\mathcal{H}_{ph} \equiv \sum_q \left(\frac{1}{2} \hbar\omega_q + e^{2\eta_q} \Phi_q \right) \left(\nu_q + \nu_{-q} + 1 \right) + \sum_q e^{2\eta_q} \Phi_q \left(b_{-q}^{\dagger} b_q^{\dagger} + b_q b_{-q} \right) \tag{43}$$

is diagonalized by a second squeezing transformation $e^T \equiv \exp\left[-\sum_q \vartheta_q \left(b_{-q}^{\dagger} b_q^{\dagger} - b_{-q} b_q \right) \right]$ with the value of ϑ_q set by:

$$\tanh\left(2\vartheta_q \right) = \frac{\hbar\omega_q}{\hbar\omega_q + 2e^{2\eta_q} \Phi_q} - 1 \tag{44}$$

Notice that the sign of ϑ_q is opposite to the sign of Φ_q. Also, as the relevant phonons are optical ones, $\hbar\omega_q$ never vanishes in the Brillouin zone, then $\tanh\left(2\vartheta_q \right) \neq -1$, and ϑ_q is always well defined. Due to the presence of Φ_q in equation (44), the parameter ϑ_q depends on the band-filling factors $\langle n_{k\sigma}^{\alpha(\beta)} \rangle$ and on the band hybridization $\langle \alpha_{k\sigma}^{\dagger} \beta_{k\sigma} + \beta_{k\sigma}^{\dagger} \alpha_{k\sigma} \rangle$.

The diagonalized free-phonon Hamiltonian reads therefore:

$$e^T \mathcal{H}_{ph} e^{-T} = \sum_q \left[\hbar\omega_q \cosh\left(2\vartheta_q \right) + 2e^{2\eta_q} e^{2\vartheta_q} \Phi_q \right] \nu_q + \text{const.} = \sum_q \hbar\varpi_q \nu_q + \text{const.} \tag{45}$$

We have obtained a band-filling and hybridization-depending renormalization of the phonon frequencies:

$$\hbar\varpi_q = \hbar\omega_q \cosh\left(2\vartheta_q \right) + 2e^{2\eta_q} e^{2\vartheta_q} \Phi_q \tag{46}$$

The final Hamiltonian therefore reads:

$$e^T\mathcal{H}e^{-T} = \sum_{k\sigma}\left(\mathcal{E}_k^\alpha n_{k\sigma}^\alpha + \mathcal{E}_k^\beta n_{k\sigma}^\beta\right) + \frac{1}{N}\sum_{kq\sigma}\left[e^{2\eta_q}F_{kq}^{\alpha\beta}\left(2\langle\nu_q\rangle+1\right)\right]\left(\alpha_{k\sigma}^\dagger\beta_{k\sigma}+\beta_{k\sigma}^\dagger\alpha_{k\sigma}\right) + \sum_q \hbar\varpi_q\nu_q + e^Te^S\widetilde{H}_{ep}^{(1)}e^{-S}e^{-T} + \text{const.} \quad (47)$$

where

$$\mathcal{E}_k^\zeta = E_k^\zeta + \frac{1}{N}\sum_q F_{kq}^{\zeta\zeta}e^{2\eta_q}\left(2\langle\nu_q\rangle+1\right) \qquad (\zeta=\alpha,\beta)\,. \quad (48)$$

This has the shape of a standard (*i.e.* harmonic and linear) SSH Hamiltonian for two hybridizing bands. However, also the linear SSH term has acquired a band-filling and hybridization dependence, because it now reads:

$$e^Te^S\widetilde{H}_{ep}^{(1)}e^{-S}e^{-T} = \frac{1}{\sqrt{N}}\sum_{kq\sigma}e^{\eta_q+\vartheta_q}\Big[\Gamma_{k,k-q}^{\alpha\alpha}\alpha_{k\sigma}^\dagger\alpha_{k-q,\sigma}+\Gamma_{k,k-q}^{\beta\beta}\beta_{k\sigma}^\dagger\beta_{k-q,\sigma} + \Gamma_{k,k-q}^{\alpha\beta}\alpha_{k\sigma}^\dagger\beta_{k-q,\sigma}+\Gamma_{k,k-q}^{\beta\alpha}\beta_{k\sigma}^\dagger\alpha_{k-q,\sigma}\Big] \times\left(b_{-q}^\dagger+b_q\right). \quad (49)$$

Therefore also the phonon linewidths, due to the SSH interaction, will depend, through $\exp(\vartheta_q)$, on $\langle n_{k\sigma}^{\alpha(\beta)}\rangle$ and $\langle\alpha_{k\sigma}^\dagger\beta_{k\sigma}+\beta_{k\sigma}^\dagger\alpha_{k\sigma}\rangle$.

The weakening of the linear electron-phonon interaction is expressed by the coefficient $\exp(\vartheta_q)\exp(\eta_q)$. The value of $\exp(\eta_q)$ is set by the diagonalization condition of the anharmonic phonon Hamiltonian, equation (13) according to the identity:

$$e^{2\eta_q} = \sqrt{\frac{1+\tanh\left(2\eta_q\right)}{1-\tanh\left(2\eta_q\right)}}. \quad (50)$$

Therefore the squeezing effect related to the anharmonicity of the phonons also reduces the electron-phonon interactions.

To conclude, let us check if the link that our model establishes between the renormalization of the harmonic frequency from Ω_q to ω_q and the reduction of the electron-phonon coupling strength is consistent with the estimates of those quantities as given, *e.g.*, in references [14,16,18]. The ratio $\Omega_q\ /\omega_q$ is evaluated as 85%. [14], 75% [16] and 80% [18]. We assume that the value of $\exp(\vartheta_q)$ (Eq. (44)), which we can not estimate at this stage, is not far from unity. By taking from reference [16] $x_{qq}\sim 7.8\ \text{eV}^{-1}$, $\hbar\Omega_q = 60$ meV, and assuming a dispersionless mode in equation (11) we obtain, at zero temperature, where we can neglect $\langle\nu_q\rangle$, that $X_q\sim 1.12$. Then $\tanh\left(2\eta_q\right)\sim -0.105$ yielding, from equation (15), $\Omega_q/\omega_q\sim 0.85$ and, from equation (50), $\exp\left(2\eta_q\right)=0.90$. In Eliashberg's theory [22] $\lambda\sim\langle|g^2|\rangle/\langle\omega^2\rangle$, where $\langle ...\rangle$ are suitable averages. In our model then $\lambda_{anhar}/\lambda_{har}\sim e^{2\eta_q}/X_q^2\left[1-\tanh^2\left(2\eta_q\right)\right]=0.65$. which agrees with the estimate [18] of a 30% weakening of λ_{anhar}. From the fact that $\tanh\left(2\eta_q\right)\sim -0.105$ we also conclude that the large phonon softening found on passing from AlB_2 to MgB_2 [16,20,21] is probably not due only to the harmonic-to-anharmonic phonon change, because the squeezing-induced softening effect in equation (15) is not strong enough. The filling-dependent effect of $\exp(\vartheta_q)$ should also be taken into account quantitatively before drawing more reliable conclusions on this point.

7 Conclusions

We have obtained a model Hamiltonian which should contain the essential physics of MgB_2.

Our starting point was a two-band Hamiltonian with anharmonic phonons and both linear and quadratic electron-phonon interactions of the bond-stretching type, as dictated by the results of LDA calculations [14,16–18,20]. The final Hamiltonian followed by applying a sequence of unitary transformations to both the electronic and phononic terms. In particular, we have been able to go beyond the Hartree-Fock approximation in treating the anharmonic effects. We have thus obtained an effective Hamiltonian (Eqs. (47) and (49)) of a very simple structure. The electronic part has two bands with a phonon-depending hybridization, generated by the quadratic electron-phonon interaction, which increases with temperature as observed [13]. The phononic part has an effective harmonic free-phonon term with a frequency which depends from the band filling factors. Finally, the effective electron-phonon interaction is reduced to a linear one, but with an amplitude also depending from the band filling factors, which would result in a similar dependence of the phonon linewidths [19,21]. One could ask if it might have been possible to obtain the same results starting from a simpler Hamiltonian, as, for instance, the one proposed in reference [23]. We do not think so. Indeed, all our results depend basically from taking into account the quartic anharmonicity and the second order EPI, as can be checked by considering the limits for $\eta_q\to 0$ and $\vartheta_q\to 0$ of equations (46, 47) and (49). Namely, if both $\eta_q,\vartheta_q\to 0$, from equation (49) one finds no reduction of the effective EPI. If there is no second-order EPI, then $\Phi_q=0$ follows, implying $\vartheta_q\to 0$, so that there is no filling dependence of ϖ_q (Eq. (46)), no phonon-number effect on the hybridization (Eq. (47)) and no filling dependence of the phonon linewidths (Eq. (49)).

We have also shown that the numerical results of Ref. [18] about the phononic features of the material, namely the renormalization of the effective harmonic frequency ω_q and the reduction of the Eliashberg's λ, can be consistently interpreted as due to the phonons accomodating themselves in a "squeezed" state. On the other side, squeezing effects alone are not strong enough to account for the large E_{2g} phonon softening on passing from AlB_2 to MgB_2 [16,20,21].

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References

1. I.I. Mazin, V.P. Antropov, Physica C **385**, 49 (2003)
2. F. Bouquet, R.A. Fisher, N.E. Phillips, D.G. Hinks, D.J. Jorgensen, Phys. Rev. Lett. **87**, 047001 (2001)
3. F. Giubileo, D. Roditchev, W. Sacks, R. Lamy, D.X. Thanh, J. Klein, S. Miraglia, D. Fruchart, J. Marcus, P. Monod, Phys. Rev. Lett. **87**, 177008 (2001)
4. H. Schmidt, J.F. Zasadzinski, K.E. Gray, D.G. Hinks, Phys. Rev. Lett. **88**, 127002 (2002)
5. M. Iavarone, G. Karapetrov, A.E. Koshelev, W.K. Kwok, G.W. Crabtree, D.G. Hinks, Phys. Rev. Lett. **89**, 187002 (2002)
6. S. Tsuda, T. Yokoya, Y. Takano, H. Kito, A. Matsushita, F. Yin, H. Harima, S. Shin, `cond-mat/0303636` (2003)
7. H.J. Choi, D. Roundy, H. Sun, M.L. Cohen, S.G. Louie, Nature, **418**, 758 (2002)
8. S.L. Bud'ko, G. Lapertot, C. Petrovic, C.E. Cunningham, N. Anderson, P.C. Canfield, Phys. Rev. Lett. **86**, 1877 (2001); D.G. Hinks, H. Claus, J.D. Jorgensen, Nature, **411**, 457 (2001)
9. J. Kondo, Prog. Theor. Physics **29**, 1 (1963); M. Imada, J. Phys. Soc. Jpn **70**, 1218 (2001); J. Kondo, J. Phys. Soc. Jpn **71**, 1353 (2002)
10. H. Suhl, B.T. Matthias, L.R. Walker, Phys. Rev. Lett. **3**, 552 (1959)
11. I.I. Mazin, O.K. Andersen, O. Jepsen, O.V. Dolgov, J. Kortus, A.A. Golubov, A.B. Kuz'menko, D. van der Marel, Phys. Rev. Lett. **89**, 107002 (2002)
12. S. Jemima Balaselvi, A. Bharathi, V. Sankara Sastry, G.L.N. Reddy, Y. Hariharan, `cond-mat/0303022` (2003); submitted to Phys. Rev. B
13. T. Dahm, N. Schopohl, Phys. Rev. Lett. **91**, 017001 (2003)
14. A.Y. Liu, I.I. Mazin, J. Kortus, Phys. Rev. Lett. **87**, 087005 (2001)
15. Y. Kong, O.V. Dolgov, O. Jepsen, O.K. Andersen, Phys. Rev. B **64**, 020501(R) (2001)
16. T. Yildirim, O. Gülseren, J.W. Lynn, C.M. Brown, T.J. Udovic, Q. Huang, N. Rogado, K.A. Regan, M.A. Hayward, J.S. Sluski, T. He, M.K. Haas, P. Khalifah, K. Inumaru, R.J. Cava, Phys. Rev. Lett. **87**, 037001 (2001)
17. K. Kunc, I. Loa, K. Syassen, R.K. Kremer, K. Ahn, J. Phys.: Condens. Matter **13**, 9945 (2001)
18. H.J. Choi, D. Roundy, H. Sun, M.L. Cohen, S.G. Louie, Phys. Rev. B **66**, 020513(R) (2002)
19. P. Postorino, A. Congeduti, P. Dore, A. Nucara, A. Bianconi, D. Di Castro, S. De Negri, A. Saccone, Phys. Rev. B **65**, 020507 (2001)
20. K.-P. Bohnen, R. Heid, B. Renker, Phys. Rev. Lett. **86**, 5771 (2001)
21. B. Renker, K.B. Bohnen, R. Heid, D. Ernst, H. Schlober, M. Koza, P. Adelmann, P. Schweiss, T. Wolf, Phys. Rev. Lett. **88**, 067001 (2002)
22. S. Barisic, J. Labbé, J. Friedel, Phys. Rev. Lett. **25**, 919 (1970)
23. L. Boeri, G.B. Bachelet, E. Cappelluti, L. Pietronero, Phys. Rev. B **65**, 214501 (2002)
24. see, for instance, Ch.3 in: W. Jones, N.H. March, *Theoretical Solid State Physics* (Dover Publications, Inc., New York 1973)
25. Wei-Min Zhang, Da Hsuan Feng, R. Gilmore, Rev. Mod. Phys. **62**, 867 (1990); D. Feinberg, S. Ciuchi, F. De Pasquale, Int. J. Mod. Phys. B **4**, 1317 (1990)
26. A.A. Golubov, J. Kortus, O.V. Dolgov, O. Jepsen, Y. Kong, O.K. Andersen, B.J. Gibson, K. Ahn, R.K. Kremer, J. Phys.: Condens. Matter **14**, 1353 (2002)