Effective inter-band coupling in $MgB_2$ due to anharmonic phonons.

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Abstract

We investigate the origin of the inter-band coupling in $MgB_2$ by focusing on its unusual phononic features, namely, the strong anharmonicity of the phonons and the presence of both linear and quadratic electron-phonon interactions of the Su-Schrieffer-Heeger (SSH) type. The bare electronic Hamiltonian has two bands with intra- and inter-band hopping, which lead to two decoupled hybridized bands. The phonon Hamiltonian including the anharmonic terms is diagonalized approximately by a squeezing transformation, which causes the softening of the phonon frequency. The linear SSH coupling amplitude is reduced, consistently with the estimates from first-principle calculations. Additionally, the quadratic coupling generates an effective phonon-induced interaction between the hybridized bands, which is non-vanishing even in the limit of vanishing inter-bare-band hopping amplitude.

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I. INTRODUCTION.

The electronic structure of the 40 K superconductor $MgB_2$ is characterized by the presence at the Fermi level of two hybrid bands ($\sigma$ and $\pi$) of very different character [1]. This feature reflects itself in the experimental evidence of two gaps, which, in the absence of magnetic fields, have a common critical temperature [2]. This implies an interaction between the $\sigma$ and $\pi$ bands contributing to the Fermi surface [3]. The microscopic origin of this interaction is, to the best of our knowledge, not yet clarified. The present work suggests that it might be traced to the unusual phononic structure of $MgB_2$. The dominant electron-phonon interaction is of the Su-Schrieffer-Heeger (SSH) type, namely a modulation of the hopping due to the vibration of the Boron ions along the inter-site bond [4], [5]. The unusual
features 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 \[5\] \[6\] \[7\]. Our aim is to give a qualitative picture of the issue by discussing a physically transparent model, but with no ambition of giving detailed quantitative results. However, we also show that our model is quantitatively consistent with the numerical results of Refs. \[5\] \[6\] \[7\].

II. THE ELECTRONIC HAMILTONIAN.

Our model of the electronic structure of MgB\(_2\) by a Hamiltonian has two bands, labelled \(c\) and \(d\), which hybridize through an inter-site hopping term. Then, in the real space representation, the bare electronic Hamiltonian reads:

\[
H_{el} = \varepsilon^c \sum_{l\sigma} n_{l\sigma}^c + \varepsilon^d \sum_{l\sigma} n_{l\sigma}^d + \sum_{l(j)\sigma} \left[ t_{lj}^{cc} c_{l\sigma}^\dagger c_{j\sigma} + t_{lj}^{dd} d_{l\sigma}^\dagger d_{j\sigma} \right] + \sum_{l(j)\sigma} t_{lj}^{cd} \left( c_{l\sigma}^\dagger d_{j\sigma} + d_{j\sigma}^\dagger c_{l\sigma} \right)
\] (1)

where \(\sum_{l(j)}\) means summing on the \(z\) nearest neighbors \(j\) of a given site \(l\), and then on \(l\). In MgB\(_2\) one expects that \(t_{lj}^{cc}, t_{lj}^{dd} \gg t_{lj}^{cd}\) \[1\], \[4\]. The electron-phonon coupling parameters in the SSH scenario are derivatives of the hopping amplitudes with respect to the inter-site distance. By using \(c_{l\sigma}^\dagger = N^{-1/2} \sum_k c_{k\sigma}^\dagger \exp \left( ikR_l \right)\) we pass to the reciprocal space representation, yielding:

\[
H_{el} = \sum_{k\sigma} \left( \varepsilon^c + z t_{k}^{cc} \right) n_{k\sigma}^c + \sum_{k\sigma} \left( \varepsilon^d + z t_{k}^{dd} \right) n_{k\sigma}^d + \sum_{k\sigma} z t_{k}^{cd} \left( c_{k\sigma}^\dagger d_{k\sigma} + d_{k\sigma}^\dagger c_{k\sigma} \right)
\] (2)

where \(t_{k}^{xy} = z^{-1} \sum_{l(j)} t_{lj}^{xy} \exp \left[ ik \left( R_l - R_j \right) \right]\) with \(x, y = c, d\). To diagonalize \(H_{el}\) we express the bare operators \(c_{k\sigma}^\dagger, d_{k\sigma}^\dagger\) through the hybridized operators \(\alpha_{k\sigma}^\dagger, \beta_{k\sigma}^\dagger\) according to:

\[
\begin{align*}
c_{k\sigma}^\dagger &= \alpha_{k\sigma}^\dagger \cos \varphi_k + \beta_{k\sigma}^\dagger \sin \varphi_k \\
d_{k\sigma}^\dagger &= -\alpha_{k\sigma} \sin \varphi_k + \beta_{k\sigma} \cos \varphi_k
\end{align*}
\] (3)

By choosing

\[
\tan(2\varphi_k) = -\frac{2 z t_{k}^{cd}}{\varepsilon^c_k - \varepsilon^d_k + z \left( t_{k}^{cc} - t_{k}^{dd} \right)}
\] (4)
$H_{el}$ is brought to diagonal form $H_{el} = \sum_{k\sigma} \left( E_k^{\alpha} n_{k\sigma}^\alpha + E_k^{\beta} n_{k\sigma}^\beta \right)$, with the particle energies in the hybridized bands given by:

$$E_k^{\alpha} = \frac{1}{2} \left[ \epsilon^c + \epsilon^d + z \left( t_{cc}^k + t_{dd}^k \right) \right] + \frac{1}{2} \sqrt{\left[ \epsilon^c - \epsilon^d + z \left( t_{cc}^k - t_{dd}^k \right) \right]^2 + (2zt_{cd}^k)^2}$$ (5)

$$E_k^{\beta} = \frac{1}{2} \left[ \epsilon^c + \epsilon^d + z \left( t_{cc}^k + t_{dd}^k \right) \right] - \frac{1}{2} \sqrt{\left[ \epsilon^c - \epsilon^d + z \left( t_{cc}^k - t_{dd}^k \right) \right]^2 + (2zt_{cd}^k)^2}$$ (6)

III. THE PHONONIC HAMILTONIAN WITH ANHARMONIC TERMS.

Following [6], [7] 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. It takes the form:

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

where $M$ is the Boron mass and $\Omega_q$ 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 Ref. [6], one can estimate $x_{qp} \approx 7.8$ eV$^{-1}$.

By quantizing the phonon field according to the usual relations:

$$u_q = \sqrt{\frac{\hbar}{2M\Omega_q}} \left( b_q + b_q^\dagger \right) \quad P_q = i\sqrt{\frac{\hbar\Omega_q}{2M}} \left( b_q^\dagger - b_q \right) \quad L_q = \sqrt{\frac{\hbar}{2M\Omega_q}}$$ (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:

$$\sum_{qp} x_{qp} \left( \frac{\hbar\Omega_q}{4} \right) \left( \frac{\hbar\Omega_p}{4} \right) \left( b_{-q}^\dagger + b_q \right) \left( b_{-p}^\dagger + b_p \right) \left( b_p + b_{-p} \right) \approx$$

$$\approx 4 \sum_q \left( \frac{\hbar\Omega_q}{4} \right) \left( \frac{1}{2} + \nu_q \right) \sum_p x_{qp} \left( \frac{\hbar\Omega_p}{4} \right) \left( 1 + \delta_{qp} \right)$$
\[ +4 \sum_{qp} x_{qp} \left( \frac{\hbar \Omega_q}{4} \right) \left( \frac{\hbar \Omega_p}{4} \right) \nu_q \nu_p \left( 1 + \delta_{q,-p} \right) + 2 \sum_q \left( \frac{\hbar \Omega_q}{4} \right) \left( b_{-q}^\dagger b_q^\dagger + b_{-q} b_q \right) \sum_p x_{qp} \left( \frac{\hbar \Omega_p}{4} \right) \]

\[ -2 \sum_{qp} x_{qp} \left( \frac{\hbar \Omega_q}{4} \right) \left( \frac{\hbar \Omega_p}{4} \right) + \sum_{qp} x_{qp} \left( \frac{\hbar \Omega_q}{4} \right) \left( \frac{\hbar \Omega_p}{4} \right) \]

(9)

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

\[ \sum_q \hbar \Omega_q \left( \frac{1}{2} + \nu_q \right) \sum_p x_{qp} \left( \frac{\hbar \Omega_p}{2} \right) \left( \frac{1}{2} + \langle \nu_p \rangle \right) \left( 1 + \delta_{q,-p} \right) \]

\[ + \sum_q \hbar \Omega_q \left( b_{-q}^\dagger b_q^\dagger + b_{-q} b_q \right) \sum_p x_{qp} \left( \frac{\hbar \Omega_p}{8} \right) + \text{const.} \]

(10)

Adding the harmonic contribution and defining

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

(11)

we obtain the purely phononic Hamiltonian as:

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

(12)

This form can be diagonalized by a ”squeezing” transformation \([9]\) \( e^S \equiv \exp \left[-\sum_q \eta_q \left( b_{-q}^\dagger b_q^\dagger - b_{-q} b_q \right) \right] \) under the condition that

\[ \tanh \left( 2 \eta_q \right) = -\frac{1}{X_q} \sum_p x_{qp} \left( \frac{\hbar \Omega_p}{4} \right) \]

(13)

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

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

(14)

By substituting \( \eta_q \) from Eq.13 into Eq.14, the renormalized frequency \( \omega_q \) of the harmonic Hamiltonian for the squeezed phonons is written explicitly as:

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

(15)

where \( \Omega_q X_q \) is the phonon frequency entering the quadratic part of the unsqueezed phononic Hamiltonian (see. Eq.12). Thus \( \omega_q \) is reduced (softened) with respect to the bare frequency \( X_q \Omega_q \), in accordance with the findings of Refs. [5] [6] [7].
IV. THE LINEAR ELECTRON-PHONON INTERACTION.

The linear part of the SSH electron-phonon interaction is written, in real space, as

$$H^{(1)}_{ep} = \frac{1}{\sqrt{N}} \sum_{k\sigma} \left[ g_{ij}^{cc} \alpha_i^{\dagger} \alpha_j \sigma + g_{ij}^{dd} d_i^{\dagger} d_j \sigma \right] (u_i - u_j) + \sum_{l(\sigma)\sigma} g_{ij}^{cd} \left( d_i^{\dagger} c_j \sigma + c_j^{\dagger} d_i \sigma \right) (u_l - u_j)$$  \hspace{1cm} (16)

where \( g_{ij}^{cc} = \partial H_{ij}^{cc} / \partial (u_i - u_j) |_{0} = -g_{ji}^{cc} \) etc., are the coupling constants.

To obtain the Fourier-transformed form of Eq.16 we define \( g_k^{cc} = \langle 1 \rangle \sum_{ij} g_{ij}^{cc} \exp(ik\Delta_{ij}) \) so that

$$\frac{z}{2} \left( g_{k-q}^{cc} + g_{k}^{cc} - g_{-(k-q)}^{cc} - g_{-k}^{cc} \right) = i \sum_{ij} g_{ij}^{cc} \left\{ \sin \left[ (k - q) \cdot \Delta_{ij} \right] - \sin \left[ k \cdot \Delta_{ij} \right] \right\} \equiv \gamma_{k,q}^{cc}$$  \hspace{1cm} (17)

with analogous relations defining \( \gamma_{k,q}^{dd} \) and \( \gamma_{k,q}^{cd} \). Quantization of the phonons according to Eq.8 leads to:

$$H^{(1)}_{ep} = \frac{1}{\sqrt{N}} \sum_{k\sigma} \left[ \gamma_{k,q}^{cc} \alpha_k^{\dagger} \alpha_{k-q} \sigma + \gamma_{k,q}^{dd} d_k^{\dagger} d_{k-q} \sigma + \gamma_{k,q}^{cd} \left( c_k^{\dagger} d_{k-q} \sigma + d_k^{\dagger} c_{k-q} \sigma \right) \right] (b_k^{\dagger} + b_q)$$  \hspace{1cm} (18)

When transformed to the hybridized fermion representation \( H^{(1)}_{ep} \) reads:

$$H^{(1)}_{ep} =$$  \hspace{1cm} (19)

where the effective couplings are defined as:

$$\Gamma_{k,k-q}^{\alpha} = \gamma_{k,k-q}^{cc} \cos \varphi_k \cos \varphi_{k-q} + \gamma_{k,k-q}^{dd} \sin \varphi_k \sin \varphi_{k-q} - 2\gamma_{k,k-q}^{cd} \cos \varphi_k \sin \varphi_{k-q}$$  \hspace{1cm} (20)

$$\Gamma_{k,k-q}^{\beta} = \gamma_{k,k-q}^{cc} \sin \varphi_k \sin \varphi_{k-q} + \gamma_{k,k-q}^{dd} \cos \varphi_k \cos \varphi_{k-q} + 2\gamma_{k,k-q}^{cd} \sin \varphi_k \cos \varphi_{k-q}$$  \hspace{1cm} (21)

$$\Gamma_{k,k-q}^{\alpha\beta} = \gamma_{k,k-q}^{cc} \cos \varphi_k \sin \varphi_{k-q} - \gamma_{k,k-q}^{dd} \sin \varphi_k \cos \varphi_{k-q} + \gamma_{k,k-q}^{cd} \left( \cos \varphi_k \cos \varphi_{k-q} + \sin \varphi_k \sin \varphi_{k-q} \right)$$  \hspace{1cm} (22)

$$\Gamma_{k,k-q}^{\alpha\beta} = \gamma_{k,k-q}^{cc} \sin \varphi_k \cos \varphi_{k-q} - \gamma_{k,k-q}^{dd} \cos \varphi_k \sin \varphi_{k-q} - \gamma_{k,k-q}^{cd} \left( \cos \varphi_k \cos \varphi_{k-q} + \sin \varphi_k \sin \varphi_{k-q} \right)$$  \hspace{1cm} (23)
V. THE QUADRATIC ELECTRON-PHONON INTERACTION.

According to Refs. [5] [6] [7], the electron-phonon Hamiltonian has to include also a quadratic term, which we write in real space as:

\[
H^{(2)}_{ep} = \sum_{l,j(\sigma)} \left[ f^{cc}_{lj} c_{l\sigma} c_{j\sigma} + f^{dd}_{lj} d_{l\sigma}^\dagger d_{j\sigma} \right] (u_l - u_j) + \sum_{l,j(\sigma)} f^{cd}_{lj} \left( d_{l\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger d_{l\sigma} \right) (u_l - u_j)^2
\]

(24)

where \( f^{cc}_{lj} = \partial^2 f^{cc}_{lj} / \partial \left( u_l - u_j \right)^2 \big|_0 = f^{cc}_{jl} \), etc. By defining \( f^{cc}_{kl} = z^{-1} \sum_{l,j} f^{cc}_{lj} e^{i k \Delta_{lj}} \) and the coefficients \( F^{xy}_{kpq} = z \left( f^{xy}_{kp} + f^{xy}_{kp} - 2 f^{xy}_{k-p} \right) \) with \( x, y = c, d \), the Fourier transform reads:

\[
\frac{1}{N} \sum_{kpq(\sigma)} c_{k\sigma}^\dagger c_{p\sigma} u_q u_{k-p-q} F^{cc}_{kpq} + \frac{1}{N} \sum_{kpq(\sigma)} d_{k\sigma}^\dagger d_{p\sigma} u_q u_{k-p-q} F^{dd}_{kpq}
\]

\[+ \frac{1}{N} \sum_{kpq(\sigma)} \left( d_{k\sigma}^\dagger c_{p\sigma} u_q u_{k-p-q} + c_{p\sigma}^\dagger d_{k\sigma} u_q u_{p-k-q} \right) F^{cd}_{kpq}
\]

(25)

To pass over to the hybridized-fermion representation, let us define for short:

\[
F^{\alpha\alpha}_{kpq} = F^{cc}_{kpq} \cos \varphi_k \cos \varphi_p + F^{dd}_{kpq} \sin \varphi_k \sin \varphi_p - F^{cd}_{kpq} \sin \varphi_k \cos \varphi_p
\]

(26)

\[
F^{\beta\beta}_{kpq} = F^{cc}_{kpq} \sin \varphi_k \sin \varphi_p + F^{dd}_{kpq} \cos \varphi_k \cos \varphi_p + F^{cd}_{kpq} \cos \varphi_k \sin \varphi_p
\]

(27)

\[
F^{\alpha\beta}_{kpq} = F^{cc}_{kpq} \cos \varphi_k \sin \varphi_p - F^{dd}_{kpq} \sin \varphi_k \cos \varphi_p - F^{cd}_{kpq} \sin \varphi_k \sin \varphi_p
\]

(28)

\[
F^{\beta\alpha}_{kpq} = F^{cc}_{kpq} \sin \varphi_k \cos \varphi_p - F^{dd}_{kpq} \cos \varphi_k \sin \varphi_p + F^{cd}_{kpq} \cos \varphi_k \cos \varphi_p
\]

(29)

Then, the quadratic coupling can be cast in the form:

\[
H^{(2)}_{ep} = \frac{1}{N} \sum_{kpq} \left( \alpha_{k\sigma}^\dagger \alpha_{p\sigma} F^{\alpha\alpha}_{kpq} + \beta_{k\sigma}^\dagger \beta_{p\sigma} F^{\beta\beta}_{kpq} + \alpha_{k\sigma}^\dagger \beta_{p\sigma} F^{\alpha\beta}_{kpq} + \beta_{k\sigma}^\dagger \alpha_{p\sigma} F^{\beta\alpha}_{kpq} \right) u_q u_{k-p-q}
\]

\[+ \frac{1}{N} \sum_{kpq} \left( \alpha_{p\sigma}^\dagger \alpha_{k\sigma} F^{\alpha\alpha}_{kpq} + \beta_{p\sigma}^\dagger \beta_{k\sigma} F^{\beta\beta}_{kpq} + \alpha_{p\sigma}^\dagger \beta_{k\sigma} F^{\alpha\beta}_{kpq} + \beta_{p\sigma}^\dagger \alpha_{k\sigma} F^{\beta\alpha}_{kpq} \right) u_{-q} u_{-(k-p-q)}
\]

(30)

Next, we quantize the phonons according to Eq.8. By enforcing \( k = p \) we take into account only the terms which do not change the number of phonons in a given mode:
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. Selecting the \( p=q \) terms, then, Eq.30 can be written compactly as

\[
H_{ep}^{(2)} \approx \frac{1}{N} \sum_{kq} \left( 2F_{kkq}^{\alpha\alpha} n_{k\sigma}^{\alpha} + 2F_{kkq}^{\beta\beta} n_{k\sigma}^{\beta} \right) L_q^2 \left( b_{-q}^\dagger b_q^\dagger + b_q b_{-q} + \nu_q + \nu_{-q} + 1 \right) \\
+ \frac{1}{N} \sum_{kq} \left( F_{kkq}^{\beta\alpha} + F_{kkq}^{\alpha\beta} \right) \left( \alpha_{k\sigma}^\dagger \beta_{k\sigma} + \beta_{k\sigma}^\dagger \alpha_{k\sigma} \right) L_q^2 \left( b_{-q}^\dagger b_q^\dagger + b_q b_{-q} + \nu_q + \nu_{-q} + 1 \right)
\]

(31)

VI. THE ELECTRON-PHONON HAMILTONIAN IN THE SQUEEZED PHONON REPRESENTATION.

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

\[
e^S H_{ep}^{(1)} e^{-S} = \\
= \frac{1}{\sqrt{N}} \sum_{kq\alpha\beta} L_q e^{\eta_q} \left[ \Gamma_{k,k,q}^{\alpha\beta} \alpha_{k\sigma}^\dagger \beta_{k\sigma} - \Gamma_{k,k,q}^{\beta\alpha} \alpha_{k\sigma} \beta_{k\sigma}^\dagger + \Gamma_{k,k,q}^{\alpha\beta} \alpha_{k\sigma} \beta_{k\sigma}^\dagger \right] \left( b_{-q}^\dagger + b_q \right)
\]

(32)

Then the linear coupling has a reduce amplitude, as \( \eta_q < 0 \) (see Eq.13), consistently with the numerical analysis of Ref. [7].

For the quadratic part \( H_{ep}^{(2)} \) we get:

\[
e^S H_{ep}^{(2)} e^{-S} = \frac{1}{N} \sum_{kq} \left( 2F_{kkq}^{\alpha\alpha} n_{k\sigma}^{\alpha} + 2F_{kkq}^{\beta\beta} n_{k\sigma}^{\beta} \right) L_q^2 e^{2\eta_q} \left( b_{-q}^\dagger b_q^\dagger + b_q b_{-q} + \nu_q + \nu_{-q} + 1 \right) \\
+ \frac{1}{N} \sum_{kq} \left( F_{kkq}^{\beta\alpha} + F_{kkq}^{\alpha\beta} \right) \left( \alpha_{k\sigma}^\dagger \beta_{k\sigma} + \beta_{k\sigma}^\dagger \alpha_{k\sigma} \right) L_q^2 e^{2\eta_q} \left( b_{-q}^\dagger b_q^\dagger + b_q b_{-q} + \nu_q + \nu_{-q} + 1 \right)
\]

(33)

(34)
The Eqs.33 and 34 show that the phonons induce an effective inter-band coupling through both the linear and the quadratic SSH interaction. However, the quadratic term in the second line of Eq.34 is the only one providing an inter-band coupling term which is non-vanishing even if \( \langle \nu_q \rangle = 0 \). It reads:

\[
L^2 \frac{e^{2\eta_0}}{4} \left( F_{\alpha\beta}^{\alpha\alpha} + F_{\beta\alpha}^{\alpha\alpha} \right) \left( \alpha_{k\sigma}^\dagger \beta_{k\sigma} + \beta_{k\sigma}^\dagger \alpha_{k\sigma} \right) \tag{35}
\]

where \( \tanh \left( 2\eta_0 \right) = \lim_{\langle \nu_q \rangle \to 0} \tanh \left( 2\eta_q \right) \). It is interesting to discuss its behaviour in the limit of small hybridization of the bare bands. From the definition of \( F_{\alpha\beta}^{\alpha\alpha} \), \( F_{\beta\alpha}^{\alpha\alpha} \) (Eq.28 and 29) and of \( \varphi_k \) (Eq.4) one sees that, when the inter-band hybridization \( t_{ij}^{cd} \to 0 \), then either \( \varphi_k \to 0 \), or \( \varphi_k \to \pm \pi/2 \). In the two cases we have, from Eqs.28 and 29:

\[
\lim_{\varphi_k \to 0} F_{\alpha\beta}^{\alpha\alpha} = 0 \quad \lim_{\varphi_k \to -\pi/2} F_{\alpha\beta}^{\alpha\alpha} = F_{\alpha\beta}^{cd} \quad \lim_{\varphi_k \to +\pi/2} F_{\alpha\beta}^{\alpha\alpha} = -F_{\alpha\beta}^{cd} \quad \lim_{\varphi_k \to \pm \pi/2} F_{\alpha\beta}^{\alpha\alpha} = 0 \tag{36}
\]

The reason for the minus sign in \( \lim_{\varphi_k \to \pm \pi/2} F_{\alpha\beta}^{\alpha\alpha} = -F_{\alpha\beta}^{cd} \) can be understood by recalling that, from Eq.3, \( \lim_{\varphi_k \to \pm \pi/2} c_k^\dagger (\varphi_k) = \pm \alpha_k^\dagger \). It follows:

\[
\lim_{\varphi_k \to \pm \pi/2} \left( F_{\alpha\beta}^{\alpha\alpha} + F_{\beta\alpha}^{\alpha\alpha} \right) \left( \alpha_{k\sigma}^\dagger \beta_{k\sigma} + \beta_{k\sigma}^\dagger \alpha_{k\sigma} \right) = -F_{\alpha\beta}^{cd} \left( -d_k^\dagger c_{k\sigma} - c_k^\dagger d_{k\sigma} \right) = F_{\alpha\beta}^{cd} \left( d_k^\dagger c_{k\sigma} + c_k^\dagger d_{k\sigma} \right) \tag{37}
\]

Hence in both cases \( \varphi_k \to 0, \pm \pi/2 \) we get the same expression for the effective inter-band coupling term, namely:

\[
\lim_{t_{ij}^{cd} \to 0} \left( F_{\alpha\beta}^{\alpha\alpha} + F_{\beta\alpha}^{\alpha\alpha} \right) \left( \alpha_{k\sigma}^\dagger \beta_{k\sigma} + \beta_{k\sigma}^\dagger \alpha_{k\sigma} \right) L^2 \frac{e^{2\eta_0}}{4} = F_{\alpha\beta}^{cd} \frac{L^2 e^{2\eta_0}}{4} \left( d_k^\dagger c_{k\sigma} + c_k^\dagger d_{k\sigma} \right) =
\]

\[
= L^2 \frac{e^{2\eta_0}}{4} \sum_{l(i,j)} f_{ij}^{cd} \left\{ \cos \left( k \cdot \Delta_{ij} \right) - \cos \left[ \left( k - q \right) \cdot \Delta_{ij} \right] \right\} \left( d_k^\dagger c_{k\sigma} + c_k^\dagger d_{k\sigma} \right) \tag{38}
\]

Apart from geometric factors, this term depends only on the intensity of the squeezing (through \( e^{2\eta_0} \)) and on the amplitude of the quadratic inter-band SSH electron-phonon coupling \( f_{ij}^{cd} \). As \( f_{ij}^{cd} \) is a second derivative of \( t_{ij}^{cd} \), it can be appreciable even if \( t_{ij}^{cd} \) itself is very small. Different evaluations of \( f_{ij}^{cd} \) [1] all agree that it has an appreciable value.
The weakening of the linear and quadratic electron-phonon interactions is expressed by the coefficients $e^{n_q}$ and $e^{2n_q}$. Their value is, in turn, set by the diagonalization condition of the anharmonic phonon Hamiltonian, Eq.13 according to:

$$e^{2n_q} = \frac{1 + \tanh(2\eta_q)}{\sqrt{1 - \tanh(2\eta_q)}}$$  \(39\)

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 softening of the harmonic frequency and the reduction of the electron-phonon coupling strength is consistent with the estimates of those quantities as given, e.g., in Refs. [5], [6] and [7]. The softening of the frequency is evaluated as 15% [5], 25% [6] and 20% [7]. For our check we assume the intermediate estimate by Ref. [7]. If $\omega_q/X_q\Omega_q = 0.80$ then, from Eq.15, it follows $\theta(2\eta_q) = -0.60$ and therefore $e^{n_q} = 0.70$, which agrees with the estimate [7] of a weakening of the linear electron-phonon coupling by 30%.

VII. CONCLUSIONS.

We have presented an analytic treatment of a two-band Hamiltonian with anharmonic phonons and both linear and quadratic electron-phonon interactions of the Su-Schrieffer-Heeger type, which should represent the essential physics of MgB$_2$. We have shown that the numerical results of Ref. [7] about the phononic features of the material, namely the softening of the effective harmonic frequency $\omega_q$ and the reduction of the linear electron-phonon coupling amplitude, can be interpreted as due to the phonons accommodating themselves in a "squeezed" state. Additionally, we have found that the quadratic electron-phonon interaction generates an effective coupling between the hybridized bands due to virtual phonons.

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