Electron-electron interaction for the dynamical Jahn-Teller effect

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We compute the Fröhlich interaction for the most general two-band Hamiltonian describing the interaction between phonons and electrons. As a special case we obtain the four-electron interaction for the dynamical Jahn-Teller effect corresponding to the model proposed by Yu and Anderson. Our results may have some relevance for the special phonon contribution to the pairing interaction in high- T_c superconductors.

I. INTRODUCTION

The Jahn-Teller effect is a symmetry-breaking phenomenon that manifests itself as a splitting of degenerate energy levels induced by a background field. This can occur statically by a crystal field that breaks the symmetry of the orbitals considered or dynamically by a moving electronic background which has a tendency to restore the degeneracy of the levels, whereby we can associate a characteristic time to the restoration process. More exactly, in the dynamical Jahn-Teller effect the electronic background effectively generates a double-well potential for the oscillating ion that itself influences the electrons and so tunnels between the two minima. Thus the dynamical Jahn-Teller effect has much in common to instanton tunneling in relativistic quantum field theory.

It was the Jahn-Teller polaron model which gave Bednorz and Müller a motivation for the finally successful search of high- T_c superconductors. An electron imbedded in a surrounding distortion field can move through the lattice as a quasiparticle with a high effective mass thus giving strong coupling to the phonons. However, most current approaches to the new superconductors follow a different line, and at present it is not clear which picture contains the essential structures.

Recently the dynamic Jahn-Teller effect has been discussed by several authors as a possible pairing mechanism for high- T_c superconductivity.^{1,2} The discussion proceeds in terms of the BCS theory assuming Fröhlich's form of the pairing interaction that is caused by motion of either copper or oxygen ions in a double potential well. In the zeroth approximation one may assume that we have a situation which may be described equally well by an electron-phonon interaction in a two-band system, where the signs of the couplings are fixed through the double-well picture. One may ask what will we get if we integrate out the phonon degrees of freedom obtaining an effective four-electron Hamiltonian. Are there repulsive terms? These would lead to novel features such as an oscillating gap.

In this paper we show that, because of the description dependence in the two-band system, one has to be careful in the bookkeeping of couplings. Based on a general symmetry argument for the linear electron-phonon interaction-matrix of a two-band model we present the exact form of the Fröhlich pairing interactions and their signs.

II. THE GENERAL THEORY

The most general two-band Hamiltonian describing the interaction between phonons and electrons is given by

$$H = H_{\rm ph} + H_e + H_{e-\rm ph} , \qquad (1)$$

where

$$H_{\rm ph} = \frac{P^2}{2M} + \frac{1}{2}M\Omega^2 Q^2 , \qquad (2)$$

$$H_e = \sum_{k} E_{k1} c_{k1}^{\dagger} c_{k1} + \sum_{k} E_{k2} c_{k2}^{\dagger} c_{k2} , \qquad (3)$$

$$H_{e-\rm ph} = -\sum_{kk'} (c_{k'1}^{\dagger}, c_{k'2}^{\dagger}) \begin{pmatrix} g_{11}Q & g_{12}Q \\ g_{21}Q & g_{22}Q \end{pmatrix} \begin{pmatrix} c_{k1} \\ c_{k2} \end{pmatrix}, \qquad (4)$$

where the matrix containing the phonon Q must be Hermitian, such that the Hamiltonian itself is Hermitian. We use the notation of Ref. 3. If we only allow real-valued coupling constants the matrix must be symmetric, i.e.,

$$g_{12} = g_{21}$$
 (5)

By choosing the appropriate coherent superpositions of the two bands we are able to diagonalize the Hamiltonian giving

$$H_{e-\mathrm{ph}} = -\sum_{kk'} (c_{k'\mathrm{I}}^{\dagger}, c_{k'\mathrm{II}}^{\dagger}) \begin{pmatrix} g_\mathrm{I} \mathcal{Q} & 0\\ 0 & g_\mathrm{II} \mathcal{Q} \end{pmatrix} \begin{pmatrix} c_{k\mathrm{I}}\\ c_{k\mathrm{II}} \end{pmatrix}, \qquad (6)$$

where

$$g_{I} = \frac{g_{11} + g_{22}}{2} + \left[\frac{g_{11}^{2}}{4} - \frac{g_{11}g_{22}}{2} + \frac{g_{22}^{2}}{4} + g_{12}^{2}\right]^{1/2}$$
(7)

and

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$$g_{\rm II} = \frac{g_{11} + g_{22}}{2} - \left[\frac{g_{11}^2}{4} - \frac{g_{11}g_{22}}{2} + \frac{g_{22}^2}{4} + g_{12}^2\right]^{1/2}$$
(8)

are nothing but the eigenvalues of the Hermitian matrix

appearing in Eq. (4).

Using phonon field operators and integrating over all momenta we are able to write down the phonon second quantized form of the diagonalized Hamiltonian:

$$H_{\rm ph} = \sum_{q} \hbar \omega_{q} a_{q}^{\dagger} a_{q} , \qquad (9)$$

$$H_e = \sum_{\mathbf{k}\sigma} E_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} , \qquad (10)$$

$$H_{e-\mathrm{ph}} = \sum_{\mathbf{k},\mathbf{k}+\mathbf{q}} \left(c_{\mathbf{k}+\mathbf{q}\mathbf{I}}^{\dagger}, c_{\mathbf{k}+\mathbf{q}\mathbf{I}}^{\dagger} \right) \begin{pmatrix} g_{\mathbf{I}}(a_{-\mathbf{q}}^{\dagger}+a_{\mathbf{q}}) & 0\\ 0 & g_{\mathbf{II}}(a_{-\mathbf{q}}^{\dagger}+a_{\mathbf{q}}) \end{pmatrix} \begin{vmatrix} c_{\mathbf{k}\mathbf{I}}\\ c_{\mathbf{k}\mathbf{I}} \end{vmatrix},$$
(11)

where, of course, g_1 and g_{11} have been conveniently rescaled to account for the displacement amplitudes. Let us now perform a canonical transformation according to

$$H_{S} = e^{-S} H e^{S} = H_{0} + (H_{e-\text{ph}} + [H_{0}, S]) + \frac{1}{2} (H_{e-\text{ph}} + [H_{0}, S]) S + \frac{1}{2} [H_{e-\text{ph}}, S] + \dots,$$
(12)

where $H_0 := H_{ph} + H_e$. One always chooses $H_{e-ph} + [H_0, S] = 0$, i.e.,

$$H_{S} = H_{0} + \frac{1}{2} [H_{e-ph}, S] + \dots$$
(13)

As usual the generator S of the canonical transformation has a form similar to H_{e-nh} :

$$S = -\sum_{\mathbf{k},\mathbf{k}+\mathbf{q}} \left(c_{\mathbf{k}\ \mathbf{q}\mathbf{I}}^{\dagger}, c_{\mathbf{k}+\mathbf{q}\mathbf{I}\mathbf{I}}^{\dagger} \right) \begin{bmatrix} g_{\mathbf{I}}(\alpha a_{-\mathbf{q}}^{\dagger} + \beta a_{\mathbf{q}}) & 0\\ 0 & g_{\mathbf{II}}(\alpha a_{-\mathbf{q}}^{\dagger} + \beta a_{\mathbf{q}}) \end{bmatrix} \begin{bmatrix} c_{\mathbf{k}\mathbf{I}}\\ c_{\mathbf{k}\mathbf{I}} \end{bmatrix}.$$
(14)

From the consistency condition we immediately get

$$\alpha^{-1} = E(\mathbf{k}) - E(\mathbf{k} + \mathbf{q}) - \hbar \omega_{\mathbf{q}} , \qquad (15)$$

$$\beta^{-1} = E(\mathbf{k}) - E(\mathbf{k} + \mathbf{q}) + \hbar \omega_{\mathbf{q}} .$$
⁽¹⁶⁾

Notice that the calculation runs in complete analogy to the classical case. A possibly occurring "wrong" sign in H_{e-ph} is compensated for by the corresponding sign in S and there are no terms appearing in the evaluation of the consistency condition mixing I and II.

However, such terms will be present, if we compute the commutator $[H_{e-ph}, S]$. In addition to the conventional four-I-electron and conventional four-II-electron self-couplings, which are always attractive, we have "interband" terms, which will be repulsive if $g_1g_{11} < 0$ and will be attractive if $g_1g_{11} > 0$. Thus the result of the Fröhlich transformation is

$$H = \sum_{q} \hbar \omega_{q} a_{q}^{\dagger} a_{q} + \sum_{k\sigma} E_{k\sigma} c_{k\sigma}^{\dagger} c_{k\sigma} + g_{I}^{2} \sum_{kk'q} \frac{\hbar \omega_{q}}{[E(\mathbf{k}+\mathbf{q})-E(\mathbf{k})]^{2} - (\hbar \omega_{q})^{2}} c_{\mathbf{k}+\mathbf{q}I}^{\dagger} c_{\mathbf{k}'-\mathbf{q}I} c_{\mathbf{k}'I} c_{\mathbf{k}I} + g_{I}^{2} \sum_{kk'q} \frac{\hbar \omega_{q}}{[E(\mathbf{k}+\mathbf{q})-E(\mathbf{k})]^{2} - (\hbar \omega_{q})^{2}} c_{\mathbf{k}+\mathbf{q}II}^{\dagger} c_{\mathbf{k}'II} c_{\mathbf{k}II} + g_{I} g_{II} \sum_{kk'q} \frac{\hbar \omega_{q}}{[E(\mathbf{k}+\mathbf{q})-E(\mathbf{k})]^{2} - (\hbar \omega_{q})^{2}} c_{\mathbf{k}+\mathbf{q}II}^{\dagger} c_{\mathbf{k}'I}^{\dagger} c_{\mathbf{k}II} c_{\mathbf{k}II} + g_{I} g_{II} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \frac{\hbar \omega_{q}}{[E(\mathbf{k}+\mathbf{q})-E(\mathbf{k})]^{2} - (\hbar \omega_{q})^{2}} c_{\mathbf{k}+\mathbf{q}II}^{\dagger} c_{\mathbf{k}'I}^{\dagger} c_{\mathbf{k}II} c_{\mathbf{k}II} + g_{I} g_{II} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \frac{\hbar \omega_{q}}{[E(\mathbf{k}+\mathbf{q})-E(\mathbf{k})]^{2} - (\hbar \omega_{q})^{2}} c_{\mathbf{k}+\mathbf{q}II}^{\dagger} c_{\mathbf{k}'I}^{\dagger} c_{\mathbf{k}II} c_{\mathbf{k}II}$$

$$(17)$$

The physical interpretation is quite clear: Naively we expect that, in the I-II band picture, BCS-like "intraband" pairing *always* occurs. We may assume that there are (I)(I)- and (II)(II)-Cooper pairs leading to superconductivity, whereas an attractive BCS-like "interband" pairing, with the two mates in I and II, will be realized only if $g_1g_{II} > 0$. Otherwise we have a "four-fermion" realization of the Jahn-Teller effect.

Alternatively we also could compute the fourelectron-interaction directly from Eq. (4). Formally we could get 16 four-electron terms, which also may be reproduced by expressing the I- and II-band electron operators in terms of the 1- and 2-band ones, respectively. In addition to the two "intraband" terms and the two "interband" terms we get interactions, which may be conventionally called "switch", respectively, "crossband" interactions, i.e., four terms like

$$c_{k+q2}^{\dagger}c_{k'-q2}^{\dagger}c_{k'1}c_{k1}, \qquad (18)$$

$$c_{k+ql}^{\dagger}c_{k'-ql}^{\dagger}c_{k'2}c_{k2}, \qquad (19)$$

$$c_{k+q2}^{\dagger}c_{k'-q1}^{\dagger}c_{k'1}c_{k2}, \qquad (20)$$

$$c_{\mathbf{k}+\mathbf{q}1}^{\dagger}c_{\mathbf{k}'-\mathbf{q}2}^{\dagger}c_{\mathbf{k}'2}c_{\mathbf{k}1}$$
, (21)

and eight terms, in which the phonon couples to the one vertex in a band-changing way and to the other in a brand-preserving way.

But the "diagonalized" version, Eq. (17), makes more transparent what is happening and thus is more comfortable for the computation of higher-order graphs.

Finally, in order to get an overview let us introduce a "bookkeeping matrix" (which is nothing but the tensor square of the symmetric phonon coupling matrix) displaying all possible four-fermion couplings:

$$\begin{bmatrix} g_{11} & g_{12} & g_{21} & g_{22} \\ g_{11} & g_{11}g_{11} & g_{12}g_{11} & g_{21}g_{11} & g_{22}g_{11} \\ g_{12} & g_{11}g_{12} & g_{12}g_{12} & g_{21}g_{12} & g_{22}g_{12} \\ g_{21} & g_{11}g_{21} & g_{12}g_{21} & g_{21}g_{21} & g_{22}g_{21} \\ g_{22} & g_{11}g_{22} & g_{12}g_{22} & g_{21}g_{22} & g_{22}g_{22} \end{bmatrix},$$
(22)

which through diagonalization reduces to

III. THE YU-ANDERSON MODEL

Equations (7) and (8) will be considerably simplified if we assume that $g_{11} = g_{22}$. Then we get

$$g_{\rm I} = g_{11} + g_{12} , \qquad (24)$$

$$g_{\rm II} = g_{11} - g_{12} \ . \tag{25}$$

To study the effect of the dynamical Jahn-Teller effect on superconductivity it would suffice to neglect the g_{11} term. Thus we get a model reminiscent of the one proposed by Yu and Anderson.³

They take as the 1- and 2-bands the bands associated with the oxygen s and p orbitals and set $g_{12} = \lambda$. Notice that the s orbitals have even and the p orbitals odd parity, respectively, and diagonalizing the phonon matrix means to introduce their *chiral*, i.e., left-handed and righthanded linear combinations:

$$c_{kL} = \frac{1}{\sqrt{2}} (c_{ks} - c_{kp}) , \qquad (26)$$

$$c_{\mathbf{k}R} = \frac{1}{\sqrt{2}} (c_{\mathbf{k}s} + c_{\mathbf{k}p}) , \qquad (27)$$

which correspond to our I- and II-band operators. Essentially Yu and Anderson now proceed by "integrating out" the electron degrees of freedom and calculate the dynamical modification of the harmonic oscillator potential giving a "dynamical double well."

We will proceed into a different direction. Performing the standard Fröhlich transformation, i.e., inserting this special choice of coupling constants into our result Hamiltonian we immediately get the diagonalized "bookkeeping" matrix

and the associated Hamiltonian

$$H_{\text{eff}} = \sum_{\mathbf{q}} \hbar \omega_{\mathbf{q}} a_{\mathbf{q}}^{\dagger} a_{\mathbf{q}} + \sum_{\mathbf{k}\sigma} E_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \lambda^{2} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \frac{\hbar \omega_{q}}{[E(\mathbf{k}+\mathbf{q})=E(\mathbf{k})]^{2} - (\hbar \omega_{q})^{2}} c_{\mathbf{k}+\mathbf{q}R}^{\dagger} c_{\mathbf{k}'-\mathbf{q}R}^{\dagger} c_{\mathbf{k}'R} c_{\mathbf{k}R}^{\dagger} c_{\mathbf{k}'R}^{\dagger} c_{\mathbf{k}R}^{\dagger} c_{\mathbf{k}'R}^{\dagger} c_{\mathbf{k}'R}^{\dagger}$$

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We have exactly four terms whose coupling strengths equal, whereby the interband RL and LR terms are repulsive. In the off-diagonalized representation we only get the "switch" and "cross-band" terms corresponding to the "bookkeeping" matrix

[0	λ	λ	0
0	0	0	0	0
lλ	0	λ^2	λ^2	0
λ	0	λ^2	λ^2	0
0	0	0	0	0

and explicitly giving the Hamiltonian

$$H_{\text{eff}} = \sum_{\mathbf{q}} \hbar \omega_{\mathbf{q}} a_{\mathbf{q}}^{\dagger} a_{\mathbf{q}} + \sum_{\mathbf{k}\sigma} E_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \lambda^{2} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \frac{\hbar \omega_{q}}{[E(\mathbf{k}+\mathbf{q})-E(\mathbf{k})]^{2} - (\hbar \omega_{q})^{2}} c_{\mathbf{k}+\mathbf{q}s}^{\dagger} c_{\mathbf{k}'-\mathbf{q}s}^{\dagger} c_{\mathbf{k}'\sigma} c_{\mathbf{k}p} c_{\mathbf{k}'p} c_{\mathbf{k}'p$$

(

IV. OTHER MODELS

A very similar but by no means identical model was considered by Englman, Halperin, and Weger.² Their interaction Hamiltonian is fixed by

$$g_{11} = g_{\theta} , \qquad (32)$$

 $g_{22} = g_{\epsilon} , \qquad (33)$

and

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$$g_{12} = g_{21} = g_{\theta \epsilon}$$
, (34)

corresponding to a phonon coupling to the d_{ϵ} and the d_{θ} copper bands. This case is nothing but an example for the most general case introduced in the beginning. Notice that both orbitals have the same parity and therefore we have no physically distinguished basis. After performing the diagonalization we get a Hamiltonian with two attractive and two repulsive terms, since

$$g_{\theta}g_{\epsilon} < 0 , \qquad (35)$$

the reason being that g_{θ} and g_{ϵ} have opposite signs is pointed out in Ref. 2. The corresponding off-diagonal and diagonal "bookkeeping" matrices are given by Eqs. (22) and (23), respectively, from which we can read off the associated Hamiltonians.

The above authors also get terms that, in our notation, correspond to a "bookkeeping" matrix

$$\begin{vmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & 0 & 0 & 0 & g_{\theta}g_{\epsilon} \\ \cdot & 0 & -g_{\theta\epsilon}^{2} & -g_{\theta\epsilon}^{2} & 0 \\ \cdot & 0 & -g_{\theta\epsilon}^{2} & -g_{\theta\epsilon}^{2} & 0 \\ \cdot & g_{\theta}g_{\epsilon} & 0 & 0 & 0 \end{vmatrix}, \quad (36)$$

where the minus sign is attributed to the "exchange of the θ and the ϵ states."

We argue that the action of an exchange-scattering term, as compared with the BCS direct-scattering term, manifests itself not as a sign of certain coupling constants in the Hamiltonian but enters the calculation during the evaluation of pairing of operators. Especially this term will give a nontrivial contribution if one considers the pairing of electrons which are *not* in "pure" spin-up and spin-down states, cf. Ref. 4. Here, however, our "bookkeeping" matrix shows that the diagonalization implicitly proposed is not consistent because a first column and a first row cannot be reconstructed from the entries in the middle. This observation may not affect the qualitative conclusions of Ref. 2, since $2|g_{\theta}g_{\epsilon}|$ is probably much larger than $g_{\theta\epsilon}^2$.

Suhl, Matthias, and Walker⁵ consider a two-band (sand d-band) BCS theory corresponding to a "bookkeeping" matrix such as

$$\begin{vmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & V_{ss} & 0 & 0 & 0 \\ \cdot & 0 & V_{sd} & V_{sd} & 0 \\ \cdot & 0 & V_{sd} & V_{sd} & 0 \\ \cdot & 0 & 0 & 0 & V_{dd} \end{vmatrix} ,$$
 (37)

If one assumes that the terms describing the interaction of band-changing with band-preserving "currents" are different from zero then one can diagonalize the problem and obtain an electron-phonon Hamiltonian with two attractive "intraband" and two attractive "interband" terms.

V. CONCLUSION

Let us summarize our point. The two-band electronphonon picture for the dynamical Jahn-Teller gives a Fröhlich-type Hamiltonian, which suggests that the pairing mechanism in the class of models considered is not very much different from the ordinary BCS pairing—at least in the lowest order. Nevertheless novel features such as oscillating gaps or a tendency toward a pairing in configuration space rather than in momentum space may occur, if we go beyond this ansatz. A careful strong coupling treatment (such as that of Eliashberg) is necessary to get a good theory for these nonlinear phonon models allowing for a comparison of experimental results and, hopefully, experimental predictions.

Our interaction Hamiltonian (4) is, of course, not the most general one, in that it contains only one phonon. Even more generally we have to set

$$H_{e-\mathrm{ph}} = -\sum_{\mathbf{k}\mathbf{k}'} \left(c_{\mathbf{k}'1}^{\dagger}, c_{\mathbf{k}'2}^{\dagger} \right) \begin{bmatrix} g_{11}Q_{11} & g_{12}Q_{12} \\ g_{21}Q_{21} & g_{22}Q_{22} \end{bmatrix} \begin{bmatrix} c_{\mathbf{k}1} \\ c_{\mathbf{k}2} \end{bmatrix}, \quad (38)$$

with $g_{12} = g_{21}$, $Q_{12} = Q_{21}$, and it is physically reasonable

to set $Q_{11} = Q_{22}$ (cf. Ref. 2).

The signs do not change and this can be seen as follows. We introduce orthogonalized multicomponent phonons

$$\mathbf{Q} = \begin{bmatrix} \mathcal{Q}_{11} & \mathcal{Q}_{12} \\ \mathcal{Q}_{21} & \mathcal{Q}_{22} \end{bmatrix} \tag{39}$$

and projection operator-valued coupling constants g_{ij} , such that

$$g_{ij}\mathbf{Q} = g_{ij}Q_{ij} \ . \tag{40}$$

Thus if $g_{ij} \perp g_{kl}$ we will have $g_{ij}g_{kl} = 0$. Our interaction Hamiltonian is now written as

$$H_{e\text{-ph}} = -\sum_{\mathbf{k}\mathbf{k}'} (c_{\mathbf{k}'1}^{\dagger}, c_{\mathbf{k}'2}^{\dagger}) \begin{bmatrix} g_{11}\mathbf{Q} & g_{12}\mathbf{Q} \\ g_{21}\mathbf{Q} & g_{22}\mathbf{Q} \end{bmatrix} \begin{bmatrix} c_{\mathbf{k}1} \\ c_{\mathbf{k}2} \end{bmatrix}. \quad (41)$$

Thus the "bookkeeping matrix" (22) becomes

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$$\begin{bmatrix} g_{11} & g_{12} & g_{21} & g_{22} \\ g_{11} & g_{11}g_{11} & 0 & 0 & g_{22}g_{11} \\ g_{12} & 0 & g_{12}g_{12} & g_{21}g_{12} & 0 \\ g_{21} & 0 & g_{12}g_{21} & g_{21}g_{21} & 0 \\ g_{22} & g_{11}g_{22} & 0 & 0 & g_{22}g_{22} \end{bmatrix}.$$
 (42)

This is our counterpoint to Eq. (36) and clearly shows that—ordering all operators consistently—a "switch" or "cross-band" interaction has the same sign as the conventional intraband BCS-type interaction. Although a "cross-band" interaction exchanges the labels of the particles it never must be confused with an exchange interaction. In physical terms, a "cross-band" process is a "flavor" changing particle process whereas an exchange term is due to the "braiding" of the particle trajectories.

ACKNOWLEDGMENTS

We thank R. Englman and M. Weger for useful discussions.

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