Electron-Phonon Interactions in the $W = 0$ Pairing Scenario

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We investigate the interplay of phonons and correlations in superconducting pairing by introducing a model Hamiltonian with on-site repulsion and couplings to several vibration branches having the Cu-O plane of the cuprates as a paradigm. We express the electron-phonon coupling (EP) through two force constants for O-Cu and O-O bond stretchings. Without phonons, this reduces to the Hubbard Model, and allows purely electronic $W = 0$ pairing. A $W = 0$ pair is a two-body singlet eigenstate of the Hubbard Hamiltonian, with no double occupancy, which gets bound from interactions with background particles. Indeed, this mechanism produces a Kohn-Luttinger-like pairing from the Hubbard repulsion, provided that its symmetry is not severely distorted. From the many-body theory, a canonical transformation extracts the effective two-body problem, which lends itself to numerical analysis in case studies. As a test, we use as a prototype system the CuO$_4$ cluster. We show analytically that at weak EP coupling the additive contributions of the half-breathing modes reinforce the electronic pairing. At intermediate and strong EP coupling and $U \sim t$, the model behaves in a complex and intriguing way.

73.22.-f Electronic structure of nanoscale materials: clusters, nanoparticles, nanotubes, and nanocrystals
74.20.Mn Nonconventional mechanisms
71.27.+a Strongly correlated electron systems; heavy fermions

I. INTRODUCTION

While the Fröhlich mechanism of conventional superconductivity is driven by phonon exchange, the pairing mechanism in highly correlated, narrow-band systems could have a predominantly electronic origin [1] and the Cu-O plane of cuprates is the most discussed example. Although this remains a very controversial issue, most authors probably accept at least the conceptual importance of a lattice counterpart of the Kohn-Luttinger idea [2] that attractive interactions result from mere repulsion. The Renormalization Group approach [3] to the Hubbard Model shows that such a superconducting instability in the $d_{x^2-y^2}$ channel is dominant near half filling, confirming the results obtained with the FLEX approximation [4]. One definition of pairing is $\Delta < 0$, where

$$\tilde{\Delta}(N + 2) = E(N + 2) + E(N) - 2E(N + 1),$$

and $E(N)$ is the ground state energy of the system with $N$ fermions; this criterion is suitable for finite cluster calculations by exact diagonalization methods. $\Delta < 0$ was indeed observed in particular Hubbard clusters [5] [6], but in many other examples with on-site repulsion on every site a large $\Delta > 0$ was found [7] [8]. The $W = 0$ theory [9] [10] [11] gives a systematic method for producing and analyzing examples of singlet pairing by repulsive interactions; it also allows validating $|\Delta|$ as the pairing binding energy. In this framework the non abelian symmetry group of the underlying graph and the resulting degeneracy is crucial for the pairing mechanism. The fillings and the symmetry channels where $W = 0$ pairing can occur are determined in full generality by the $W = 0$ theorem [12]; these symmetries achieve the same result as high angular momentum and parallel spins in the Kohn-Luttinger [2] continuum approach.

Anyhow, a purely electronic theory misses practically and conceptually important features of this complicated problem. First, many high-$T_c$ compounds exhibit a quite noticeable doping-dependent isotope effect [13], suggesting that electron-phonon (EP) interactions are important and should be included in the theory. In addition, there is experimental evidence [14] that the half breathing Cu-O bond stretching mode at $k = (\pi, 0), (0, \pi)$ is significantly coupled with the doped holes in the superconducting regime and its contribution may be relevant for the $d_{x^2-y^2}$ pairing [15] [16] [17]. A radical, yet serious criticism of all electronic mechanisms was put forth by Mazumdar and coworkers [18]. They suggested that any pairing in Hubbard clusters is of doubtful physical interpretation due to the neglect of the lattice degrees of freedom and the Jahn-Teller (JT) effect. They argued that JT distortions might well cause a larger energy gain of the system with $N + 1$ particles, and that could reverse the sign of $\Delta$ obtained at fixed nuclei; in this case the pairing would be just an artifact of the Hubbard model. This even led the authors to the conjecture that any $\Delta < 0$ due to an electronic mechanism is just a finite size effect, which vanishes for large systems like the JT effect does. Below, we shall show that the Mazumdar et al. argument [18], based on a static Jahn-Teller approximation, can break down in a peculiar and nontrivial way when more flexible wave functions are allowed; thus, phonon pairing and $W = 0$ pairing can be compatible, depending on the symmetries of both pair and vibration and on frequencies.

The Hubbard-Holstein model, where electrons are coupled to a local Einstein phonon, is a simple way to include both strong electronic correlations and EP interactions. Much is known about the possibility of a superconducting phase in this model. Pao and Schuttler [19] applied the numerical renormalization group techniques within the FLEX approximation and found that in the square geometry $s$-wave pairing...
is enhanced by phonons, while $d_{x^2-y^2}$ pairing is suppressed. In the strong EP regime a Lang-Firsov [20] transformation maps the Hubbard-Holstein model in an effective Hamiltonian for hopping polarons with a screened on-site interaction $\hat{U} = U - \frac{\Delta}{2}$, where $U$ is the Hubbard repulsion, $\omega$ is the phonon frequency and $g$ is the EP coupling constant. If over-screening is attained, $\hat{U} < 0$ becomes an effective attraction and one gets bipolaronic bound states [21] [22]; however it is still unclear whether they can exist as itinerant band states [23] [24]. Petrov and Egami [25] found $\Delta < 0$ in a doped 8-site Hubbard-Holstein ring at strong enough EP coupling, while otherwise the normal repulsion prevails. This situation is unavoidable in 1 dimensional repulsive Hubbard model, where no superconducting pairing exist.

In this paper we take the view that one of the sound experimental facts about the CuO plane in all cuprates is that no superconducting pairing exist. Avoidable in 1 dimensional repulsive Hubbard model, where generally, some vibrations could be pairing and others pair-breaking. When lattice effects are introduced in the $W = 0$ scenario, the situation is very different from the Petrov and Egami [25] model, when, as in the conventional (Fröhlich) mechanism, phonons overscreen the electron repulsion; what happens if electronic screening already leads to pairing?

To address these problems we use an extension of the Hubbard model in which bond stretchings dictate the couplings to the normal modes of the $C_{4v}$-symmetric configuration. This is physically more detailed than the Hubbard-Holstein model, and does not restrict to on-site EP couplings that would be impaired by a strong Hubbard repulsion.

The plan of the paper is the following. After introducing the model Hamiltonian in the next Section, we devote Sect.III to a detailed derivation of the effective interactions between holes in the $W = 0$ pair, which is obtained by extending a previous Hubbard Model treatment. Our canonical transformation approach is quite general for weak EP coupling and corresponds to the inclusion of all diagrams involving one-phonon and electron-hole pair exchange due to correlations. We specialize in Sect.IV to the prototype CuO cluster, describing electronic states and vibration modes. The effective interaction is calculated explicitly in Sect.V. Next, we develop a theory based on the Jahn-Teller operator in Sect.VI; in this way we want to test the reliability of that approximation in modeling the behaviour of $W = 0$ pairs in the presence of Jahn-Teller active modes. The numerical results of the full theory are then exposed and discussed in Sect.VII; the exact data for realistic vibration frequencies disagree from those of Sect.VI but are in accord with the canonical transformation approach of Sect. V. The agreement is excellent at weak coupling, but the analytical approach is qualitatively validated also at intermediate coupling. Finally Sect.VIII is devoted to the conclusions.

II. MODEL

We start from the Hubbard model with on-site interaction $U$ and expand the hopping integrals $t_{i,j}(r_i, r_j)$ in powers of the displacements $\rho_i$ around a $C_{4v}$-symmetric equilibrium configuration

$$t_{i,j}(r_i, r_j) \simeq t_{i,j}^0(r_i, r_j) + \sum_\alpha \left[ \frac{\partial t_{i,j}(r_i, r_j)}{\partial \rho_\alpha} \right]_{0, 0} + \sum_\alpha \left[ \frac{\partial t_{i,j}(r_i, r_j)}{\partial \rho_\alpha} \right]_{0, 0} \rho_\alpha,$$

(2)

where $\alpha = x, y$. Below, we write down the $\rho_i^0$ in terms of the normal modes $\bar{q}_\eta$: $\rho_i^0 = \sum_\nu S_{\eta,\nu}(i) q_{\eta,\nu}$, where $\eta$ is the label of an irreducible representation (irrep) of the symmetry group of the undistorted system and $\nu$ is a phonon branch.

Thus, treating the Cu atoms as fixed, for simplicity, one can justify an electron-lattice Hamiltonian:

$$H_{el-latt} = H_0 + V_{el}.$$

(3)

Here $H_0 = H_0^0 + H_0^\eta$ is given by

$$H_0 = \sum_\eta \bar{q}_\eta b_{\eta,\nu}^\dagger b_{\eta,\nu}^\dagger \sum_\nu P_{\eta,\nu}^\dagger P_{\eta,\nu}^\dagger (c_{\alpha,\eta}^\dagger c_{\alpha,\eta}^\dagger + h.c),$$

(4)

where $\omega_{\eta,\nu}$ are the frequencies of the normal modes with creation operator $b_{\eta,\nu}^\dagger$, while $c_{\alpha,\eta}^\dagger$ creates a fermion of spin $\sigma$ in site $i$. Moreover, let $M$ denote the O mass, $\xi_{\eta,\nu} = \lambda_{\eta,\nu} \sqrt{\frac{\hbar}{2 M \omega_{\eta,\nu}}}$ with $\lambda_{\eta,\nu}$ numbers of order unity that modulate the EP coupling strength. Then, $V_{el} = V + W$ reads

$$V_{el} = \sum_{\eta,\nu} \xi_{\eta,\nu} (b_{\eta,\nu}^\dagger + b_{\eta,\nu}) H_{\eta,\nu} + \sum_i n_i t_{i,\sigma} n_{i,\bar{\sigma}},$$

(5)

the $H_{\eta,\nu}$ operators are given by

$$H_{\eta,\nu} = \sum_\nu \sum_{i,j} \sum_\alpha \left[ S_{\eta,\nu}(i) \left[ \frac{\partial t_{i,j}(r_i, r_j)}{\partial \rho_\alpha} \right]_{0, 0} + S_{\eta,\nu}(j) \left[ \frac{\partial t_{i,j}(r_i, r_j)}{\partial \rho_\alpha} \right]_{0, 0} \rho_\alpha \right].$$

(6)

In previous work we have shown that the pure Hubbard model $H_W = H_0^0 + W$ defined on the Cu-O plane and on the simple square as well admits two-body singlet eigenstates with no double occupancy on lattice sites. We referred to them as $W = 0$ pairs. $W = 0$ pairs are therefore eigenstates of the kinetic energy operator $H_0^0$ and of the Hubbard repulsion $W$ with vanishing eigenvalue of the latter. The particles forming a $W = 0$ pair have no direct interaction and are the main candidates to achieve bound states in purely repulsive Hubbard models [26] [27] [28]. In order to study if the $W = 0$ can actually form bound states in the many-body interacting problem, we developed a canonical transformation of the Hubbard Hamiltonian [26], which enables us to extract the effective interaction between the particles forming the pairs. Pairing was found in small symmetric clusters and large systems as well.

In the next Section we wish to derive an effective interaction between the particles in the pair suitable for $H_{el-latt}$, by generalizing the canonical transformation approach of Ref. [26].
III. CANONICAL TRANSFORMATION

In this Section we assume that the system has periodic boundary conditions with particle number \( N \); we denote the phonon vacuum by \( |0\rangle \) and the non-interacting Fermi sphere by \( |\Phi_0(N)\rangle \). The creation operator of a \( W = 0 \) pair is obtained \cite{12} by applying an appropriate projection operator to \( c_\eta^\dagger c_\nu^\dagger \), where the labels denote Bloch states. If we add a \( W = 0 \) pair to \( |\Phi_0(N)\rangle \otimes |0\rangle \), the two extra particles, by definition, cannot interact directly (in first-order). Hence their effective interaction comes out from virtual electron-hole (e-h) excitation and/or phonon exchange and in principle can be attractive. To expand the interacting \((N + 2)\)-fermions ground state \( |\Psi_0(N + 2)\rangle \), we build a complete set of configurations in the subspace with vanishing \( z \)-spin component, considering the vacuum state \( |\Phi_0(N)\rangle \otimes |0\rangle \) and the set of excitations over it.

We start by creating \( W = 0 \) pairs of fermions over \( |\Phi_0(N)\rangle \otimes |0\rangle \); we denote with \(|m\rangle \otimes |0\rangle \) these states. At weak coupling, we may truncate the Hilbert space to the simplest excitations, i.e., to states involving 1 e-h pair or 1 phonon created over the \(|m\rangle \otimes |0\rangle \) states. We define the \(|m \otimes q\rangle \) states, obtained by creating a phonon denoted by \( q = (\eta, \nu) \) over the \(|m \rangle \otimes |0\rangle \) states. Finally we introduce the \(|\alpha \rangle \otimes |0\rangle \) states, obtained from the \(|m \rangle \otimes |0\rangle \) states by creating 1 electron-hole (e-h) pair.

The approximation can be systematically improved by including two or more electron-hole and excitations in the truncated Hilbert space, at the cost of heavier computation. We now expand the interacting ground state in the truncated Hilbert space

\[
|\Psi_0(N + 2)\rangle = \sum_m a_m |m\rangle \otimes |0\rangle + \sum_{m,q} a_{m,q} |m\rangle \otimes |q\rangle + \sum_{\alpha} a_{\alpha} |\alpha\rangle \otimes |0\rangle
\]

and set up the Schrödinger equation

\[
H_{el-trgtt}|\Psi_0(N + 2)\rangle = E |\Psi_0(N + 2)\rangle. \quad (8)
\]

We now consider the effects of the operators \( H_0 \) and \( V_{tot} \) on the terms of \( |\Psi_0(N + 2)\rangle \). Choosing the \(|m\rangle \otimes |0, q\rangle \), \(|\alpha \rangle \otimes |0\rangle \) states to be eigenstates of the noninteracting term \( H_0 \) we have

\[
H_0|m\rangle \otimes |0\rangle = E_m |m\rangle \otimes |0\rangle, \quad (9)
\]

\[
H_0|m\rangle \otimes |q\rangle = (E_m + \omega_q)|m\rangle \otimes |q\rangle, \quad (10)
\]

\[
H_0|\alpha\rangle \otimes |0\rangle = E_\alpha |\alpha\rangle \otimes |0\rangle. \quad (11)
\]

Let us consider the action of \( V \) and \( W \) on the same states, taking in account that \( V \) creates or annihilates up to 1 phonon and 1 e-h pair, and \( W \) is diagonal in the phonon states and can create or destroy up to 2 e-h pairs.

\[
(V + W)|m\rangle \otimes |0\rangle = \sum_{m'} V_{m,m'}^q |m'\rangle \otimes |q\rangle + \sum_{m'} W_{m,m'} |m'\rangle \otimes |0\rangle + \sum_{\alpha} W_{m,\alpha} |\alpha\rangle \otimes |0\rangle \quad (12)
\]

\[
(V + W)|\alpha\rangle \otimes |0\rangle = \sum_{m'} V_{\alpha,m'}^q |m'\rangle \otimes |q\rangle + \sum_{m'} W_{\alpha,m'} |m'\rangle \otimes |0\rangle + \sum_{\alpha'} W_{\alpha,\alpha'} |\alpha'\rangle \otimes |0\rangle \quad (13)
\]

\[
(E_m - E)a_m + \sum_{m'} a_{m,m'} W_{m,m'} + \sum_{m,q} a_{m,q} V_{m,m'}^q + \sum_{\alpha} a_{\alpha} W_{m,\alpha} = 0; \quad (15)
\]

\[
(E_m + \omega_q - E)a_{m,q} + \sum_{m'} a_{m,m'} W_{m,m'} + \sum_{m,q} a_{m,q} V_{m,m'}^q + \sum_{\alpha} a_{\alpha} V_{m,\alpha} = 0; \quad (16)
\]

\[
(E_\alpha - E)a_\alpha + \sum_{\alpha'} a_{\alpha,\alpha'} W_{\alpha,\alpha'} + \sum_{m} a_{m} W_{\alpha,m} + \sum_{m,q} a_{m,q} V_{\alpha,m} = 0. \quad (17)
\]

We define renormalized eigenenergies \( E'_\alpha \) by taking a linear combination of the \( \alpha \) states in such a way that

\[
(H_0 + W)|\alpha,\alpha'\rangle = \delta_{\alpha,\alpha'} E'_\alpha; \quad (18)
\]

Eq.(17) can be solved for the \( a_\alpha \) coefficients:

\[
a_{\alpha} = \frac{1}{E'_\alpha - E_m} \left( \sum_{m} a_{m} W_{\alpha,m} + \sum_{m,q} a_{m,q} V_{\alpha,m}^q \right). \quad (19)
\]

Substituting \( a_\alpha \) in Eq.(16) one gets:

\[
(E_m + \omega_q - E)a_{m,q} + \sum_{m'} a_{m,m'} W_{m,m'} + \sum_{m,q} a_{m,q} V_{m,m'}^q + \sum_{m'} a_{m',q} \left( \sum_{\alpha} \frac{V_{\alpha,m}^q}{E'_\alpha - E_m} \right) + \sum_{\alpha} a_{\alpha} V_{\alpha,m} = 0. \quad (20)
\]

Here, two important simplifications allow to proceed. First, as in Ref. \cite{10}, Eq.(49), one can show that

\[
W_{m,m'} = W_{m,m'}^{(d)} + \delta_{m,m'} W_F; \quad (21)
\]

\( W_{m,m'}^{(d)} \) is the direct interaction among the particles forming the pair and \( W_F \) comes from the average over the occupied states on the Fermi sphere and is a \( m \)-independent constant; since \( W_{m,m'}^{(d)} \) vanishes for the \( W = 0 \) property, it holds
\[ \sum_{m'} a_{m',q} W_{m,m'} = a_{m,q} W_F. \]  

(22)

Moreover,
\[ \sum_{m',q} a_{m',q} (\sum_{a} V_{q,a} V_{q,a}') = \]
\[ = a_{m,q} \sum_{a} |V_{q,a}|^2 (E_{m} - E). \]  

(23)

Indeed, \( V \) is a one-body operator for the fermions; so the electron-hole pair in the \( \alpha \) state must be created by one \( V \) factor and annihilated by the other; in this way, the \( W = 0 \) pair is not touched. With these simplifications, the contributions in Eqs.(22) and (23) can be taken over to the l.h.s. of Eq.(20), where they just renormalize the eigen-energies of the \( |m\rangle \otimes |q\rangle \) states. Thus, \( E_m + \omega_q \rightarrow E'_m + \omega_q \), and the Eq.(20) can easily solved for the \( a_{m,q}'s \), as we did for the \( a_{\alpha}'s \) in Eq.(19):
\[ a_{m,q} = \frac{1}{E_m + \omega_q - E} \sum_{m'} a_{m'} (V_{q,m,m'}^q + \sum_{a} \frac{V_{q,a} W_{a,m,m'}}{E_{\alpha} - E}). \]  

(24)

Finally, substituting Eqs.(19, 24) into Eq.(15), we can write the Schrödinger equation in terms of only the \( |m\rangle \) states, with the excitations-mediated interactions and with renormalized quantities:
\[ 0 = (E_m - E)a_m + a_m W_F + \]
\[ + \sum_{m',m'',q} a_{m'} (V_{q,m,m''}^q + \sum_{\alpha} \frac{V_{q,a} W_{a,m,m''}}{E_{\alpha} - E}) + \]
\[ + \sum_{m',q} a_{m'} (E_{m'}^q + \omega_q - E)(E_{\alpha} - E)) \]
\[ + 2 \sum_{m',m'',q,a} a_{m'} (V_{q,m,m''}^q V_{q,a,m''}^q W_{a,m'',m'}) \]  

(25)

Here, the last two terms are of higher order and must be dropped; \( E \) is the ground state of the system with \( N + 2 \) Fermions; yet, Eq.(25) is of the form of a Schrödinger equation with eigenvalue \( E \) for the added pair. We interpret \( a_m \), as the expansion coefficients over the \( W = 0 \) pairs of the wave function of the dressed pair, \( |\varphi\rangle \equiv \sum_m a_m |m\rangle \otimes |0\rangle \). This obeys the Cooper-like equation
\[ H_{\text{pair}} |\varphi\rangle = E |\varphi\rangle \]  

(26)

with the same \( E \) as in Eq.(8), but with an effective two-body Hamiltonian:
\[ H_{\text{pair}} \equiv H_0 + W_F + S[E]. \]  

(27)

Here \( S \) is the \( E \)-dependent effective scattering operator
\[ S[E]_{m,m'} = \sum_{a} W_{a,m} W_{a,m'} + \sum_{m'',q} V_{q,m,m''}^q \frac{V_{q,a,m''}}{E_{\alpha}^q + \omega_q - E}. \]  

(28)

and therefore Eq.(26) must be solved self-consistently. Let us examine in detail the structure of the \( S[E] \) contribution. The matrix elements \( S_{m,m'} \) may be written as
\[ S_{m,m'} = \langle W_{\text{eff}} \rangle_{m,m'} + F_{m\delta m,m'}. \]  

(29)

where \( W_{\text{eff}} \) is the true effective interaction between the electrons in the \( m \) states, while the other term represents the forward scattering amplitude \( F \).

The first-order self-energy \( W_F \delta m,m' \) and the forward scattering term \( F_{m\delta m,m'} \) are diagonal in the indices \( m \) and \( m' \), and therefore they renormalize the non-interacting energy \( E_m \) of the \( m \) states:
\[ E_m \rightarrow E_{m}^{(R)} = E_m + W_F + F_m. \]  

(30)

If the effective interaction \( W_{\text{eff}} \) is attractive and produces bound, localized states the spectrum of the Schrödinger equation with the Hamiltonian in Eq.(27) contains discrete states below the unpaired states. In an extended system, we have bound states below the threshold of the continuum. The threshold may be defined (in clusters and in extended systems) by
\[ E_T^{(R)} \equiv \min_{|m\rangle} [E_{m}^{(R)}(E)], \]  

(31)

which, according to Eq.(30), takes into account all the pair-wise interactions except those between the particles in the pair. Note that this is an extensive quantity, i.e. an \( N + 2 \)-particle energy. The ground state energy \( E \) may be conveniently written as
\[ E = E_T^{(R)} + \Delta; \]  

(32)

\( \Delta < 0 \) indicates a Cooper-like instability of the normal Fermi liquid and its magnitude represents the binding energy of the pair.

Below, we solve Eq.(26) explicitly for the CuO\(_4\) cluster with open boundary conditions, where the above theory is readily applied.

**IV. PROTOTYPE CLUSTER**

As an illustrative application of the above pairing scheme, in this preliminary work we focus on CuO\(_4\), the smallest cluster yielding \( W = 0 \) pairing in the Hubbard model. This requires 4 holes, (total number, not referred to half filling); such a doping is somewhat unrealistic, but larger \( 4t \)-symmetric clusters and the full CuO\(_2\) plane also show \( W = 0 \) pairing in the doping regime relevant for cuprates [9] [26]. Remarkably, in the pure Hubbard model, one can verify that \( \Delta = \tilde{\Delta}(4) \) at least at weak coupling [9], which demonstrates that \( \Delta \) has the physical meaning of an effective interaction. CuO\(_4\) represents a good test of the interplay between electronic and phononic pairing mechanisms since we can compare exact diagonalization results with the analytic approximations of the canonical transformation. A further merit of this model is that it demonstrates dramatically the decisive role of symmetry in the electronic pairing mechanism: any serious distortion of the square symmetry restores the normal \( \Delta > 0 \) situation [9].

Since vibrations cause distortions it is not evident a priori.
that they tend to help pairing; in particular we may expect that Jahn-Teller distortions are going to prevent \( W = 0 \) pairing altogether. On the other hand, the Fröhlich mechanism of conventional superconductivity is based on phonon exchange. This suggests that the role of EP coupling is complex.

\( \text{CuO}_4 \) allows only the coupling to phonons at the centre or at the edge of the Brillouin Zone; however, phonons near the edge are precisely those most involved [14] [15]. Even in this small system the virtually exact diagonalizations are already hard and the next \( C_{4v} \)-symmetric example, the \( \text{Cu}_2\text{O}_4 \) cluster [27], is much more demanding for the number of vibrations and the size of the electronic Hilbert space.

![Diagram of CuO4 cluster and its modes](image)

FIG. 1. Pictorial representation of the ionic displacements in the eight normal modes of the CuO4 cluster, labelled according to the irreps of the \( D_4^h \) Group.

Starting with the \( C_{4v} \)-symmetric arrangement, any displacement of the Oxygen in the plane can be analysed in \( \text{irreps} \), \( \text{A}_1, \text{A}_2, \text{B}_1, \text{B}_2, \text{E}_1, \text{E}_2 \), see Fig.1.

We suppose that the hopping integrals depend only on the bond lengths*. Hence, the EP coupling is expressed through just two parameters \( g \) and \( g_{ox} \), defined as follows: denoting e.g. by \( t^1 \) the hopping integral between Oxygen 1 and the Cu and by \( t_{ox}^1,2 \) the one between Oxygens 1 and 2 (see Fig.1), \( g \equiv \left[ \begin{array}{c} \frac{\partial \nu^1}{\partial \nu^1} \end{array} \right]_0 \) and \( g_{ox} \equiv \left[ \begin{array}{c} \frac{\partial \nu^2}{\partial \nu^2} \end{array} \right]_0 \). We take \( g < 0 \) since a positive Cu-O hopping integral decreases as the Cu-O distance is increased. On the other hand \( g_{ox} > 0 \), since physically the O-O hopping integral has the opposite sign with respect the Cu-O one. Following Eqs. (3-6), the second-quantized electron-lattice Hamiltonian reads

\[
H_{\text{el-latt}}^{\text{CuO}_4} = \varepsilon_p \sum_{i,\sigma} n_{i,\sigma} + \varepsilon_d \sum n_{d,\sigma} + \\
\sum_{\eta} \hbar \omega_{\eta} b_\eta^+ b_\eta + t \sum_{i,\sigma} (d_{i,\sigma}^+ p_{i+1,\sigma} + h.c.) + \\
t_{ox} \sum_{\eta} (p_{\eta,\sigma}^+ p_{\eta,\sigma+1,\sigma} + h.c.) + U \sum_{i} n_{i,\sigma}^+(n_{i,\sigma}^- + n_{\eta,\sigma}^+(n_{\eta,\sigma}^-)) + \\
+ \sum_{\eta} \xi_{\eta} (b_\eta^+ b_\eta) H_\eta;
\]

where \( p_{\eta,\sigma}^+ \) and \( p_{i,\sigma} \) are the hole creation and annihilation operators onto the oxygen \( i = 1, \ldots, 4 \) with spin \( \sigma = \uparrow, \downarrow \), \( d_{i,\sigma}^+ \) and \( d_{\eta,\sigma} \) are the hole creation and annihilation operators onto the central copper site, while \( n_{i,\sigma}^+ = p_{i,\sigma}^+ p_{i,\sigma} \) and \( n_{\eta,\sigma} = d_{\eta,\sigma}^+ d_{\eta,\sigma} \) are the corresponding number operator. Henceforth we set \( \varepsilon_p = \varepsilon_d = 0 \) for convenience, since this simple choice is adequate for the present qualitative purposes. Also, we are assuming for simplicity that the Oxygen-Oxygen hopping \( t_{ox} \) is zero, and O-O hoppings are important only once the ions are moved. Similar results are obtained using a realistic \( t_{ox} \), except that pair binding energies are somewhat reduced.

The \( H_\eta \) matrices are given by

\[
H_{A_1} = \frac{1}{2} g \sum_{\eta} (d^+_{\eta,\sigma} p_{\eta,\sigma} + \eta.c.) + \\
\frac{1}{\sqrt{2}} g_{ox} \sum_{\eta} (p_{\eta,\sigma}^+ p_{\eta,\sigma+1,\sigma} + h.c.); \\
H_{A_2} = 0; \\
H_{B_1} = \frac{1}{2} g \sum_{\sigma} (d^+_{\eta,\sigma} p_{\eta,\sigma} - d^+_{\eta,\sigma} p_{3\sigma} + d^+_{\eta,\sigma} p_{4\sigma} + h.c.); \\
H_{B_2} = \frac{1}{\sqrt{2}} g_{ox} \sum_{\sigma} (p_{\eta,\sigma}^+ p_{2\sigma} - p_{\eta,\sigma}^+ p_{3\sigma} + p_{\eta,\sigma}^+ p_{4\sigma} + h.c.); \\
H_{E_{1x}} = \frac{1}{\sqrt{2}} g \sum_{\sigma} (-d^+_{\eta,\sigma} p_{3\sigma} + d^+_{\eta,\sigma} p_{4\sigma} + h.c.); \\
H_{E_{1y}} = \frac{1}{\sqrt{2}} g \sum_{\sigma} (d^+_{\eta,\sigma} p_{3\sigma} - d^+_{\eta,\sigma} p_{4\sigma} + h.c.); \\
H_{E_{2x}} = \frac{1}{2} g_{ox} \sum_{\sigma} (p_{\eta,\sigma}^+ p_{2\sigma} + p_{\eta,\sigma}^+ p_{3\sigma} - p_{\eta,\sigma}^+ p_{4\sigma} + h.c.); \\
H_{E_{2x}} = \frac{1}{2} g_{ox} \sum_{\sigma} (p_{\eta,\sigma}^+ p_{2\sigma} - p_{\eta,\sigma}^+ p_{3\sigma} + p_{\eta,\sigma}^+ p_{4\sigma} + h.c.); \\
H_{E_{2y}} = \frac{1}{2} g_{ox} \sum_{\sigma} (-p_{\eta,\sigma}^+ p_{2\sigma} - p_{\eta,\sigma}^+ p_{3\sigma} + p_{\eta,\sigma}^+ p_{4\sigma}; \quad (34)
\]

*Some Authors use an alternating sign convention for the bonds from a given Cu site. However, this is just a gauge; in the present CuO4 case, this corresponds to changing the sign of two opposite Oxygen orbitals. Even in the full plane, starting from positive \( t \) integrals, one can introduce staggered signs by negating a sublattice of O orbitals; then, one can arrange opposite signs for the bonds of each O by simply negating a sublattice of Cu. All this has no physical implications, and in our opinion does not help to visualize the real symmetry of the problem.
In order to make contact with the physics of cuprates, let us discuss the connection between the normal modes of the CuO$_4$ cluster and the phonon modes of the Cu-O planes. There is experimental evidence [15] that the possibly relevant modes for superconductivity lie on the CuO$_2$ planes and have a Cu-O bond stretching origin. In particular the LO half-breathing mode with $k = (\pi, 0)$, $(0, \pi)$ is believed to couple significantly with the doped holes in the superconducting regime. In the CuO$_4$ cluster the half-breathing modes are contained in the breathing mode $A_1$ and in the quadrupolar mode $B_1$ by means of the linear combination $q_{A_1} \pm q_{B_1}$. We argue that qualitatively the effect of the coupling with the $A_1$ and $B_1$ modes should give us clues about the interplay between electronic $W = 0$ pairing and phonon exchange.

V. LOWEST-ORDER EFFECTIVE INTERACTION IN CuO$_4$

The mere Hubbard CuO$_4$ cluster with O-O hopping $t_{ox} = 0$ yields [9] $\Delta(4) < 0$, due to a couple of degenerate $W = 0$ bound pairs, in the $A_1$ and $B_2$ irreps of the $C_{4v}$ group; therefore in Eq.(28) we set the $m = m'$ labels accordingly. At weak coupling, we may simplify Eq.(28), neglecting all renormalizations; the phonon-mediated interaction for the $B_2$ pair reads:

$$\sum_{m'' \neq m'} \frac{V^{q}_{B_2,m''} V^{q}_{m',B_2}}{E_{m''} + \omega_q - E} = -\frac{4g_{ox}^2}{3} \frac{\lambda_{B_2}^2}{2E_{A_1} + \omega_{B_2} - E}. \quad (35)$$

Note that in the denominator in the r.h.s., $2E_{A_1} + \omega_{B_2}$ is the energy of an unrenormalized excited $|q\rangle$ state, which at weak coupling is higher than the ground state energy $E$; hence the r.h.s. must be negative and the $B_2$ phonon is synergic with electronic pairing. On the other hand, the vibronic effective interaction for the $A_1$ pair is:

$$\sum_{m'' \neq m'} \frac{V^{q}_{A_1,m''} V^{q}_{m',A_1}}{E_{m''} + \omega_q - E} = -\frac{4}{3} \frac{g_{ox}^2}{E_{A_1}} \left( \frac{\lambda_{B_2}^2}{2E_{A_1} + \omega_{B_2} - E} \right). \quad (36)$$

This shows that in the $A_1$ sector the total sign depends on the relative weight of attractive and repulsive contributions. Eqs.(35,36) show that at weak coupling $A_1$ and $B_2$ modes are synergetic to the $W = 0$ pairing, while both longitudinal and transverse $E$ modes are pair-breaking. The half-breathing modes that are deemed most important [15] [16] are $A_1 \pm B_1$ combinations, but $B_1$ does not appear in Eqs.(35,36). The numerical calculations reported below confirm these findings in a broad range of parameters.

For the sake of argument, in the explicit calculations we took all the normal modes with the same energy $\omega_0 = \hbar \omega_0 = 10^{-1}$ eV and $\lambda_0 = 1$. This sets the length scale of lattice effects $\xi_0 = \sqrt{\frac{\hbar}{2M\omega_0}} \approx 10^{-1}$ Å where we used $M = 2.7 \times 10^{-28}$ Kg for Oxygen.

With this choice, the Cooper-like equation (25) reads

$$\sum_{A_1 \neq E} \frac{U^2}{16} \left( \frac{1}{\varepsilon_{B_1} + \varepsilon_{A_1} - E} - \frac{1}{2\varepsilon_{A_1} + \varepsilon_{A_1} - E} \right) - \frac{4}{3} g_{ox}^2 \frac{1}{2E_{A_1} + \omega_0 - E} = 0 \quad (37)$$

in the $A_1$ channel and

$$\sum_{A_1 \neq E} \frac{U^2}{16} \left( \frac{1}{\varepsilon_{B_1} + \varepsilon_{A_1} - E} - \frac{1}{2\varepsilon_{A_1} + \varepsilon_{A_1} - E} \right) - \frac{4g_{ox}^2}{2E_{A_1} + \omega_0 - E} = 0. \quad (38)$$

for $B_2$ pairs. The eigenvalue $E$, like in Eq.(8), is the total energy of the cluster; it must be compared with the threshold $E_{T}^{(R)}$ of Eq.(31), whose noninteracting limit is $E_{T}^{(R)} = 2\varepsilon_{A_1}$ since the degenerate level energy (see Table II, Appendix A) is $\varepsilon_{p} = 0$. It turns out that using Eq.(32) in the weak coupling approximation, that ignores renormalizations, the effective interaction is $\Delta = E - 2\varepsilon_{A_1}$; in Appendix B we verify by perturbation theory that like in the Hubbard model, $\Delta = \Delta(4)$; this supports our interpretation of $\Delta$ as minus the pairing energy.

The trend of $\Delta$ in both channels is shown in Fig.2. The vibrations split the degeneracy of the $W = 0$ pairs, effectively lowering the symmetry like a nonvanishing $t_{ox}$. Pairing is enhanced in the $A_1$ sector as well, albeit less than in $B_2$; without phonons, $\Delta \approx -20$ meV for both the $W = 0$ pairs.

FIG. 2. Analytical results of the canonical transformation: pair binding energy in the $A_1$ and $B_2$ sectors as a function of $g_{ox}$. Here we used $\lambda_0 = 1$ for every mode, $t = 1$ eV, $t_{ox} = 0$, $U = 1$ eV; $g_{ox}$ is in units of $\varepsilon_0/\xi_0 = 1$ eV $\times$ Å$^{-1}$, $\Delta$ is in eV.

VI. JAHN-TELLER MIXING OF ELECTRONIC GROUND STATES AND PAIRING

If really the inclusion of the lattice degrees of freedom systematically leads to $\Delta > 0$, purely electronic cluster models become totally irrelevant to superconductivity, as it was argued [18]. However small, the CuO$_4$ cluster yields electronic pairing and allows to test this important point.

In this Section we set up a conventional calculation of the JT effect involving degenerate electronic ground states and their mixing with the vibrations. We first take the nuclei as
frozen in a $C_{4v}$-symmetric configuration and diagonalize the purely electronic part of the Hamiltonian:

$$
H_{el}^{CuO_4} = t \sum_{i \sigma} \langle d_i^\sigma p_{i\sigma} + h.c \rangle + U \sum_i n_i^{(p)} n_i^{(p)} + n_i^{(d)} n_i^{(d)}.
$$

(39)

As before, we are using $\varepsilon_p = \varepsilon_d = \varepsilon_d = 0$.

The JT effect arises if the ground state of $H_{el}^{CuO_4}$ is degenerate, with a ground state multiplet $\{|\Psi_1\rangle, \ldots, |\Psi_n\rangle\}$ such that $H_{el}^{CuO_4}|\Psi_k\rangle = E_0|\Psi_k\rangle$. If we take matrix elements of $H_{el-latt}$ in this truncated (n-dimensional) electronic basis integrating over electrons and keeping boson operators we get the dynamical JT Hamiltonian, [29], [30] with matrix elements:

$$
H_{a\beta}^{JT} = (E_0 + \sum_{\eta} \hbar \omega_\eta b_\eta^\dagger b_\eta) \delta_{\alpha\beta} + \langle \Psi_\alpha | V | \Psi_\beta \rangle.
$$

(40)

It is worth noting that neglecting the nuclear kinetic energy (i.e. $-\hbar^2 \sum_i \frac{\partial^2}{\partial r_i^2} \rightarrow 0$) and treating the nuclear positions as variational parameters corresponds to the static JT Hamiltonian, but we follow the dynamic treatment which is superior.

In the following we assume that the initial configuration is stable with respect to the mode $A_1$ which only changes the scale of the CuO$_4$ molecule. Since this mode does not produce any JT distortion, it is not involved in the arguments of Ref. [18]. In this Section, we study $\Delta(4)$ in this approximation, according to Eq.(1). The ground state with 2 holes is a nondegenerate total-symmetric singlet unaffected by the JT effect; in the other cases, the use of the Hamiltonian (40) is justified provided that the excited states are several phonon energies above the ground state.

A. Three-hole ground state mixing

With three holes the ground state belongs to the 3-dimensional irrep of $S_4$ which in $C_{4v}$ breaks into $B_2 \oplus E$. To illustrate the electronic structure and its dependence on distortions, in Fig.3 we show the adiabatic potential energy surface projected along the $B_2$ distortion. Projecting on the other directions, we obtain similar trends. It is clear that the ground state multiplet is well separated from the excited states and hence this treatment of the JT effect is well justified.

![FIG. 3. Adiabatic potential energy surfaces along $B_2$ for the ground and first excited 3-hole states of CuO$_4$. Here, $q_{B_2}$ denotes the classical normal coordinate; $U = 5eV$, $t = 1eV$, $g = -2.4$, $g_{0x} = 0.6$ in units eV/Å and $\hbar \omega_\eta = 0.1eV \forall \eta$; the displacement $q_{B_2}$ is in Å, energies are in eV. The ground state multiplet is below the first excited state by $\sim 1eV$.](image)

Since $E \otimes E$ contains all the irreps of $C_{4v}$, all the normal modes are JT active in this case. Following Eqs.(40), we computed the following $V$ matrix elements in the 3-hole ground state multiplet with the Hubbard interaction, using Eq.(34). The 4 independent elements at the optimal value $U/t \sim 5$, where the $W = 0$ pair binding energy is maximum, are:

$$
\gamma_1 = \langle \Psi_{B_1} | H_{el}^{B_1} | \Psi_{E_1} \rangle = 0.17 g_{0x} \tag{41}
$$

$$
\gamma_2 = \langle \Psi_{B_1} | H_{el}^{B_2} | \Psi_{E_1} \rangle = 0.24 g + 0.17 g_{0x} \tag{42}
$$

$$
\gamma_3 = \langle \Psi_{E_1} | H_{el}^{B_1} | \Psi_{E_1} \rangle = 0.24 g \tag{43}
$$

$$
\gamma_4 = \langle \Psi_{E_1} | H_{el}^{B_2} | \Psi_{E_1} \rangle = -1.05 g_{0x} \tag{44}
$$

The JT Hamiltonian reads

$$
H_{JT}(3) = \left[ E_0(3) + \sum_{\eta} \hbar \omega_\eta b_\eta^\dagger b_\eta \right] \otimes 1_{3x3} + \sum_{\eta} \xi_\eta (b_\eta^\dagger + b_\eta) M_\eta \tag{45}
$$

where $E_0(3)$ is the ground state energy of $H_{el}^{CuO_4}$ with 3 holes and

$$
M_{B_1} = \gamma_3 \begin{pmatrix} 0 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & -1 \end{pmatrix}, \tag{46}
$$

$$
M_{B_2} = \gamma_4 \begin{pmatrix} 0 & 0 & 0 \\
0 & 0 & 1 \\
0 & 1 & 0 \end{pmatrix}, \tag{47}
$$

$$
M_{E_1 x} = \begin{pmatrix} 0 & \gamma_2 & -\gamma_1 \\
\gamma_2 & 0 & 0 \\
-\gamma_1 & 0 & 0 \end{pmatrix}, \tag{48}
$$

$$
M_{E_1 y} = \begin{pmatrix} 0 & -\gamma_1 & -\gamma_2 \\
-\gamma_1 & 0 & 0 \\
-\gamma_2 & 0 & 0 \end{pmatrix}. \tag{49}
$$
\[ M_{E_{2x}} = \gamma_1 \begin{pmatrix} 0 & -1 & 1 \\ -1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \]  
(50)

and

\[ M_{E_{2y}} = \gamma_1 \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}. \]  
(51)

We numerically diagonalized \( H_{JT}(3) \) in the Hilbert space spanned by \( |\Psi_\eta\rangle \otimes |\Phi_{N_{ph}}\rangle \), where \( \eta = B_1, E_x, E_y \) is the electronic state and \( |\Phi_{N_{ph}}\rangle \) is a vibration state in the truncated Hilbert space with all modes having vibrational quantum numbers \( \leq N_{ph} \). Excluding the breathing mode the size of the problem is \( 3(N_{ph} + 1)^6 \). We consider \( N_{ph} = 3 \), since already in the weak coupling regime \( \Delta \) changes sign. We studied \( \omega_0 = \omega = 0.1eV, \lambda_0 = 1 \forall \eta \) in the range of \( |g| \) and \( |g_{ox}| \) between 0 and 2.4eV/\( \nu \). We observe that \( |g_{B_1}| \) is in units of \( 1eV, g \) and \( |g_{ox}| \) are in units of \( \nu_0/\xi_0 = 1eV \times \Lambda \).

The lower surface represents the ground state energy shift \( \Delta E \) for electronic states belonging to the degenerate irrep \( E \), while the higher one is \( \Delta E \) refers to the \( B_1 \) state. The JT effect partially removes the three-fold degeneracy and the ground state is a \( E \) doublet. Note that according to the textbook, static JT effect, one should observe a total removal of the degeneracy. This is however not borne out by the dynamical calculation and, for \( g_{ox} = 0 \), all the three states remain degenerate (see Fig.4b).

The way the system dynamically distorts is also of interest. The only vibration having the coordinate on the diagonal of \( H_{JT}(3) \) is \( B_1 \); thus, the \( E \) doublet can only distort along the \( B_1 \) normal mode. In other terms, with \( \hat{q}_{B_1} = \xi_{B_1}(\hat{b}_{B_1}^\dagger + \hat{b}_{B_1}) \), \( \langle \hat{q}_{B_1} \rangle \equiv \langle \Psi_{E_x}\rangle |\hat{q}_{B_1}| \langle \Psi_{E_x}\rangle = -\langle \Psi_{E_y}\rangle |\hat{q}_{B_1}| \langle \Psi_{E_y}\rangle \neq 0 \). The trend of \( \langle \hat{q}_{B_1} \rangle \) as a function of \( g \) and \( g_{ox} \) is shown in Fig.5. We observe that \( \langle \hat{q}_{B_1} \rangle \rightarrow 0 \) as \( g \rightarrow 0 \); we also remark that the deformation depends essentially by \( g \) and only weakly on \( g_{ox} \). Because according to Eq.(43) the coupling constant \( \gamma_3 \) responsible for the distortion along \( B_1 \) depends on \( g \) and not on \( g_{ox} \). The \( E-B_1 \) splitting, on the contrary, depends on \( g_{ox} \) and only weakly on \( g \). The naive expectation that splittings go along with distortions only holds for static ones.

![Fig. 4.](image)

**B. Four-hole ground state mixing**

With 4 holes, \( H_{CuO_4} \) has a two-fold degenerate ground state; it belongs to the two dimensional irrep of \( S_1 \) that breaks in \( A_1 \oplus B_2 \) in \( C_{4v} \). Thus, the only JT-active mode is \( B_2 \), which makes the problem exactly resoluble in terms of a continued fraction [31].

Following again Eqs.(40) the second-quantized JT Hamiltonian with four particles reads

\[ H_{JT}(4) = [\hbar \omega B_1 \hat{b}_{B_2}^\dagger \hat{b}_{B_2} + E_0(4)] \otimes 1_{2 \times 2} + \xi B_2 \gamma_3 \hat{b}_{B_2}^\dagger \hat{b}_{B_2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \]  
(52)

in the space spanned by the electronic ground states. The coupling constant \( \gamma_3 \) is given by

\[ \gamma_3 = \langle \Psi_{A_1} \| H_{B_2} \| \Psi_{B_2} \rangle = 1.19 \ g_{ox}, \]  
(53)

where as usual, the matrix element in Eq.(53) is evaluated at \( U/t \sim 5 \).

The ground state energy of \( H_{JT}(4) \) in the sector of symmetry \( \eta \) coincides with the lowest pole of the Green function

\[ G_{\eta,\eta}(E) = \langle 0 \| \langle \Psi_\eta \| E - H_{JT}(4) + i0^+ \| \Psi_\eta \rangle \| 0 \rangle = \frac{1}{\chi(0) - \sum_{\eta = (1)}^{(3)} \frac{(\xi B_2 \gamma_3)^2}{\chi_{(\eta)} - \sum_{\eta = (1)}^{(3)} \frac{5(\xi B_2 \gamma_3)^2}{\chi_{(\eta)} - \sum_{\eta = (1)}^{(3)} \frac{7(\xi B_2 \gamma_3)^2}{\chi_{(\eta)} - \sum_{\eta = (1)}^{(3)} \cdots}}}} \]  
(54)

where \( \eta = A_1, B_2 \) and \( \chi(n) = E - E_0(4) - n\hbar \omega B_2 \). \( G_{\eta,\eta}(E) \) does not depend on \( \eta \) and the energy corrections in the \( A_1 \) and \( B_2 \) sectors are the same. The ground state energy shift \( \Delta E \) as a function of \( g_{ox} \) is plotted in Fig.6.

![Fig. 5.](image)
There are no diagonal couplings in Eq.(52), which implies no distortions; the energy correction is much smaller than in the three holes case.

In Fig.7 we show the adiabatic potential curve, with the same parameters as in Fig.7. In contrast with the three-hole case, the ground state multiplet is separated from the excited states by $\sim 100 \div 150\,\text{meV}$ which is comparable the phonon energies. Hence we expect that in this case the approximation restricting the Hilbert space to the lowest multiplet is not justified. However, in the case of weak coupling to soft vibrations, with $\omega$ small compared to the gap in the electronic spectrum, this approximation should work well.

**C. $W=0$ pairing in the presence of Jahn-Teller distortions**

Collecting together the results of the present Section we obtain the behaviour of $\tilde{\Delta}$ in a popular approximation that neglects the excited electronic states. In Fig.8 we show the plot of $\tilde{\Delta}$ as a function of $-g$ and $g_{ox}$, shown with the zero-energy plane. The maximum distortion along $B_1$ compatible with $\tilde{\Delta} < 0$ (see Fig.8.b) is $\langle \beta_{B_1}^{\max} \rangle \sim 3 \times 10^{-2} \, \tilde{\Delta}$, which is attained at $g \simeq 1\,\text{eV} \times \tilde{\Delta}$ and $g_{ox} = 0$.

Both the systems with four and three holes gain energy by the JT effect; $\tilde{\Delta}$ remains negative only in the weak EP coupling regime, since the decrease of $2E(3)$ overcomes the decrease of $E(4)$. This is due to the fact that the system with three holes can gain energy by mixing with $B_1, B_2, E_{1x}, E_{1y}, E_{2x}, E_{2y}$ vibrations, while the system with four holes can do it only with the $B_2$ mode. Moreover the factor 2 in front of $E(3)$ in the expression for $\tilde{\Delta}$ further favours the distortion in the 3-holes case.

These results in line with Ref. [18], would imply that the electronic pairing is limited to relatively weak EP couplings and that at any rate the vibrations are invariably detrimental to $W = 0$ pairing. However we know from Sect.V that this conclusion is remarkably but definitely wrong, because the full theory predicts synergy of vibrations and $W = 0$ pairing at least at weak coupling. This failure of the JT Hamiltonian is due to the neglect of the electronic excited states, causing a severe overestimate of the 4 hole energy. The physical reason is that if we restrict the mixing to the degenerate states the electronic wave function is too rigid. On the other hand, including all the multiplet of states arising from the degenerate one-electron level the pair can achieve the flexibility which allows it to follow adiabatically the vibration-induced deformations, as we shall see in the next Section.

Detecting the failure of a textbook procedure is by itself a potentially very interesting result; it is a merit of a relatively simple model like this that allows to understand in detail how this arises.

**VII. NUMERICAL RESULTS OF THE FULL THEORY**

Since the conventional JT Hamiltonian is not enough, to see what really happens in this model with increasing EP coupling, where the analytic treatment of Sect.V loses validity, we resort to numerical methods. In this Section we explore the pairing scenario numerically, which offers an independent check of the weak-coupling calculations and permits to go beyond the weak coupling regime. First, we analyze one phonon at a time ($\lambda_n = 1$), turning off the all others ($\lambda_n = 0$); $\omega_n \equiv 0.1$ for all modes. In this way we see which kind of phonon is cooperative with the $W = 0$ pairing and which is not. We have performed these calculations in a virtually exact way, by including a number of phonons $N_{ph}$ up to 20. To this end we take advantage of the recently proposed spin-disentangled diagonalization technique [11]. The results are shown in Figs.9,10 and 11.
Here we used \( t = 1 \text{eV}, t_{ox} = 0, U = 1 \text{eV}, g_{ox} \) and \( g \) are in units of \( \varepsilon_0/\xi_0 = 1 \text{eV} \times A \).

The plots show the trend of \( \Delta(4) \) as a function of \( g_{ox} \) and \( g \). It appears (see Figs. 9 and 10) that if \( g_{ox} \) is increased, the \( A_1 \) and \( B_2 \) phonons enhance the pairing, even beyond the weak coupling regime. The further enhancement of \( |\Delta(4)| \) due to \( A_1 \) as \( |g| \) is increased is not predicted by the weak coupling theory [Eq.(36)]. The \( B_1 \) phonon is slightly suppressive, but it affects the pairing energy on a scale of \( 10^{-3} \text{eV} \) and hence its contribution is negligible. On the other hand the (longitudinal and transverse) \( E \) phonons (see Figs. 10 and 11) have an unambiguous tendency to destroy the pairing. In particular the \( E_1 \) mode does it both by increasing \( g_{ox} \) and by increasing \( |g| \).

The presented results show that the behaviour of the individual phonons is essentially the same as predicted analytically in Sect.V: some of them \((A_1 \text{ and } B_2)\) act in a cooperative way with the electronic pairing mechanism; some other \((E \text{ phonons})\) does not; the \( B_1 \) mode is quite inoperative. However, for a proper understanding of the conflicting vibronic effects we need to include as many phonon modes as possible at the same time. In this case the exact diagonalizations become hard even with a modest \( N_{ph} \) per vibration. We performed exact diagonalizations of \( H^{\text{CuO}_4}_{el-\text{phon}} \) with five active modes; with 4 holes, the size of the problem is \( 100(N_{ph} + 1)^3 \); we could afford \( N_{ph} = 3 \) for each. Some results are shown in Figs. 12.

In Fig. 12.a we included the vibrations with \( \eta = A_1, B_1, B_2, E_{2x}, E_{2y} \); one notes a strong, monotonic increase of the binding energy with both \( g_{ox} \) and \( |g| \). The weak-coupling theory of Sect.V qualitatively explains the \( g_{ox} \) dependence but not the \( |g| \) one: when the EP coupling gets strong, the Cu-O stretching grows important. In Fig. 10 (diamonds) we noted that the \( E_2 \) vibrations alone tend to destroy pairing; here we observe that when they compete with \( A_1 \) and \( B_2 \) their effects are utterly suppressed. It is possible that the couplings to the pair-breaking \( E \) modes are somewhat underestimated by the choiche of \( \lambda \) parameters.

In Fig. 12.b we included the vibrations with \( \eta = A_1, B_1, B_2, E_{1x}, E_{1y} \), and we observe that \( \Delta \) now becomes

\[ \sim \Delta \]
positive at moderate \(g_{\text{ox}}\). Comparing with the above results on individual modes, we observe that in going from Fig.12.a to Fig.12.b we are replacing the pair-breaking transversal \(E_2\) phonons by the pair-breaking, longitudinal \(E_1\) modes. We conclude that the longitudinal ones are more efficient in restoring the repulsion and at intermediate coupling they overwhelm the pair-healing \(A_1\) and \(B_2\).

However for \(g_{\text{ox}} \gtrsim 0.15 \text{ eV} \times \xi^{-1}\), the cooperative modes win and \(\tilde{\Delta}(4)\) gets negative again. This remarkable behavior could not be anticipated by the weak coupling approach of Sect.V, where only the one-phonon exchange diagrams were included as in the BCS theory.

In Fig.12.c the active modes are \(\eta = B_1, E_{1x}, E_{1y}, E_{2x}, E_{2y}\); these are all pair-breaking individually and switching them all together, they readily unbind pairs, leading to strong positive \(\Delta\). However, unexpectedly, we again find attraction at large enough \(g_{\text{ox}}\).

It is likely that the couplings to the pair-breaking \(E\) modes are somewhat overestimated by the choice of \(\lambda\) parameters in Fig.12.b,c. The pairing at strong coupling observed in Figs.12.b,c results from more complicated interactions leading to bipolaron formation. This recalls the charge-ordered super-lattice phase found in Ref [25]; however they used a Hubbard-Holstein model and, since the system is one-dimensional, the electronic pairing does not occur in their case.

FIG. 12. \(\tilde{\Delta}(4)\) in eV as a function of \(g_{\text{ox}}\) for different values of \(g\). \(\lambda_{\eta} = 1\) all the vibrations, except: \(\lambda_{\eta} = 0\) for \(\eta = E_1\) (a); \(\lambda_{\eta} = 0\) for \(\eta = E_2\) (b); \(\lambda_{\eta} = 0\) for \(\eta = A_1, B_2\) (c). \(N_{\text{ph}}=3\) for each active mode; \(g = -0.2\) (diamonds); \(g = -0.5\) (triangles); \(g = -1\) (crosses). Here we used \(t = 1\text{eV};\ t_{\text{ox}} = 0, \t U = 1\text{eV};\ g_{\text{ox}}\) and \(g\) are in units of \(\varepsilon_0/\xi_0 = 1\text{eV}\times\xi^{-1}\).
VIII. CONCLUSIONS

Introducing vibrations and vibronic couplings into a strongly correlated model opens up a rich scenario where, among other possibilities, pairing can be achieved by a synergy of electronic correlation and phonon-exchange. A possible outcome, however, is competition among different symmetry vibration modes and electronic excitations. We illustrate the situation by using a CuO$_4$ model that allows a full treatment of all degrees of freedom and hosts bound $W = 0$ pairs when undistorted, has vibrations of the same symmetries as the CuO plane and is numerically affordable. A popular recipe for computing JT distorted molecules prescribes restricting to the degenerate electronic levels letting them interact with the JT active modes. A static treatment invariably leads to a complete removal of the symmetry and a nodegenerate ground state. We put forth a fuller dynamical theory which partly preserves the degeneracy; however, the vibrations are always opposing $W = 0$ pairing which is thereby reduced to a weak EP coupling effect. This restricted basis, however, may only be valid provided that the excited states of the unperturbed electronic Hamiltonian are far removed from the ground state on the energy scale set by the frequency of the relevant phonon modes. With the cuprates in mind, we consider a situation when the phonon energies and the superconducting gap are comparable, in the 0.1 eV range; we diagonalize the full model keeping up to 5 simultaneous modes and vibrational quantum numbers $N_{ph} \leq 3$. Depending on the parameters, a rich phenomenology emerges from the numerical data. Pairing prevails at weak EP coupling, as expected, but the phonon contributions which dominate in such a case turns out to contribute to the pairing rather than opposing it. The correct trend is predicted by a canonical transformation approach, which also explains the pairing or pair-breaking character of the modes. In particular it is found that the half-breathing modes give a synergic contribution to the purely electronic pairing; since they are believed to be mainly involved in optimally doped cuprates, our findings suggest a joint mechanism, with the Hubbard model that captures a crucial part of the physics.

This agreement validates the canonical transformation approach, which allows to carry out useful calculations even in large systems that o not lend themselves to exact diagonalization.

At intermediate coupling the outcome of the theory depends essentially on the relative weight of the coupling to the longitudinal and transverse vector modes, which destabilize pairing most effectively.

Remarkably, however, the vibrations restore pairing again at strong coupling, when a bipolaronic regime prevails. This scenario was also drawn in the context of an extended t-J model, where the half-breathing mode was found to enhance electronic pairing [17] [32].

Finally, experimental data on nanopowders [33] also indicate that one should not be overly pessimistic about cluster calculations. The pairing that shows up there can be relevant and physically insightful concerning the interplay of various degrees of freedom on pair structure and formation.

IX. APPENDIX A: $W = 0$ PAIRS IN THE CuO$_4$ CLUSTER

The CuO$_4$ Hubbard Hamiltonian has $C_{4v}$ symmetry. When the Oxygen-Oxygen hopping is absent, the symmetry group is the permutation group $S_4$ and although for convenience we continue to use the subgroup $C_{4v}$ labels, it is $S_4$ that must be used for the $W = 0$ theorem [12]. The character table reads:

| $C_{4v}$ | $C_2$ | $C_4^{(+)}$, $C_4^{-(-)}$ | $\sigma_x$, $\sigma_y$, $\sigma_z$, $\sigma$ | Symmetry |
|---------|-------|-----------------------------|---------------------------------|----------|
| $A_1$   | 1     | 1                           | 1                               | $x^2 + y^2$ |
| $A_2$   | 1     | 1                           | -1                              | $(x/y) - (y/x)$ |
| $B_1$   | 1     | -1                          | 1                               | $x^2 - y^2$ |
| $B_2$   | 1     | -1                          | -1                              | $xy$ |
| $E$     | 2     | -2                          | 0                               | $(x, y)$ |

Table I: Character table of the $C_{4v}$ symmetry group. Here 1 denotes the identity, $C_2$ the 180 degrees rotation, $C_4^{(+)}$, $C_4^{(-)}$ the counterclockwise and clockwise 90 degrees rotations, $\sigma_x$, $\sigma_y$, $\sigma_z$, $\sigma$ the reflection with respect to the $y = 0$ and $x = 0$ axis and $\sigma_x$ the reflection with respect to the $x = y$ and $z = -y$ diagonals. In the last column we show typical basis functions.

Setting for simplicity $\varepsilon_d = \varepsilon_p = 0$, the one-body spectrum of the CuO$_4$ Hamiltonian has the following eigenvalues:

| $\varepsilon_1$ | $\varepsilon_2$ | $\varepsilon_3$ | $\varepsilon_4$ | $\varepsilon_4'$ |
|-----------------|-----------------|-----------------|-----------------|-----------------|
| $\tau - \sqrt{4 + \tau^2}$ | $-2\tau$ | $0$ | $0$ | $\tau + \sqrt{4 + \tau^2}$ |

Table II: One-body levels of the CuO$_4$ cluster in units of $t$; the last line reports the values for $t_{ox} = 0$ which are used in the text.

Here we label the eigenvalues by the irreps of the corresponding eigenfunctions. The level energies are in units of $t$, $\tau \equiv t_{ox}/t$; for $t_{ox} = 0$, $\varepsilon_{E_x} = \varepsilon_{E_y} = \varepsilon_{B_1} = 0$. The corresponding one body creation operators of a particle in each of these eigenstates are:

$$c_{E_x} = \frac{1}{\sqrt{2}} \left( p_{2\sigma}^\dagger - p_{4\sigma}^\dagger \right)$$

(55)

$$c_{E_y} = \frac{1}{\sqrt{2}} \left( p_{1\sigma}^\dagger - p_{3\sigma}^\dagger \right)$$

(56)

$$c_{B_1} = \frac{1}{2} \left( p_{1\sigma}^\dagger - p_{2\sigma}^\dagger + p_{3\sigma}^\dagger - p_{4\sigma}^\dagger \right)$$

(57)

$$c_{A_1} = \frac{1}{\alpha^2} \left( \alpha d_{1\sigma}^\dagger + p_{1\sigma}^\dagger + p_{2\sigma}^\dagger + p_{3\sigma}^\dagger + p_{4\sigma}^\dagger \right)$$

(58)

$$c_{A_1} = \frac{1}{\beta^2} \left( \beta d_{1\sigma}^\dagger + p_{1\sigma}^\dagger + p_{2\sigma}^\dagger + p_{3\sigma}^\dagger + p_{4\sigma}^\dagger \right)$$

(59)

where $\alpha$ and $\beta$ depend on $\tau$ as follows:

$$\alpha = \frac{4 \left( -1 + \tau^2 + \tau \sqrt{4 + \tau^2} \right)}{-5 \tau - 2 \tau^3 + \sqrt{4 + \tau^2} + 2 \tau^2 \sqrt{4 + \tau^2}}$$

(61)
These are readily verified to create singlet eigenstates with no double occupation. Projecting one which is not represented in the one-body spectrum must yield the same holds for the pair with $\Delta$ obtained by solving Eqs.(37,38). Basically the second-order perturbation theory in both quantities represent the effective interaction of the dressed $B_2W = 0$ pair. Indeed, much information about the ground state energies cancels out if one applies Eq. (1); the canonical transformation is a much more practical way to represent the effective interaction.

**X. APPENDIX B: PAIR BINDING ENERGY**

Here we calculate $\tilde{\Delta}$ of the $B_2$ pair in the CuO$_4$ cluster by second-order perturbation theory in both $W$ and $V$ and compare with $\Delta$ obtained by solving Eqs.(37,38). Basically the same holds for the $A_1$ pair. $\lambda_0 \equiv 1$ throughout this Appendix.

The ground state with two particles belongs to $A_1$ and, using the notations of Table III, its ground state reads

$$E(2) = 2\varepsilon_{A_1} + \frac{5}{16} U + U^2 \left[ \frac{3}{128 \varepsilon_{A_1}} - \frac{61}{512} d_1 \right] -$$

$$g^2 (d_2 + d_3) - g_{ox}^2 (d_2 + d_3) + 2 \sqrt{2} g_{ox} g d_3.$$  (64)

$$\phi_{A_1} = \frac{2}{\sqrt{3}} \phi_{B_1} \phi_{B_1}^\dagger + \frac{1}{\sqrt{3}} \left( \phi_{E_{1u}} \phi_{E_{1u}}^\dagger + \phi_{E_{2g}} \phi_{E_{2g}}^\dagger \right)$$

$$\phi_{B_2} = \frac{1}{\sqrt{2}} \left( \phi_{E_{1u}} \phi_{E_{1u}}^\dagger + \phi_{E_{2g}} \phi_{E_{2g}}^\dagger \right).$$  (63)

These are readily verified to create $W = 0$ pairs.

**Table III: Shorthand notations used in Eqs.(64,65,66).**

With 3 particles the ground state is a $E$ doublet, and

$$E(3) = 2\varepsilon_{A_1} + \frac{7}{16} U + U^2 \left[ \frac{5}{64 \varepsilon_{A_1}} - \frac{53}{512} d_1 \right] -$$

$$g^2 \left[ d_3 + \frac{d_3}{2} + \frac{d_2}{2} \right] -$$

$$g_{ox}^2 \left[ \frac{2}{\omega_{B_2}} + \frac{1}{2 \omega_{E_1}} + \frac{1}{2 \omega_{E_2}} \right]$$

$$\frac{d_3}{4} + \frac{d_4}{4} + \frac{3d_4}{4} + \frac{3d_4}{4} -$$

$$g_{ox} g \left[ \frac{3 \sqrt{2} d_3}{2} + \frac{\sqrt{2} d_2}{2} \right].$$  (65)

The ground state with 4 particles belongs to $B_2$, as predicted by the canonical transformation; one gets:

$$E(4) = 2\varepsilon_{A_1} + \frac{9}{16} U + U^2 \left[ \frac{25}{128 \varepsilon_{A_1}} - \frac{29}{512} d_1 \right] -$$

$$g^2 \left[ d_3 + d_3 + d_3 \right] -$$

$$g_{ox}^2 \left[ \frac{8}{\omega_{B_2}} + \frac{1}{\omega_{E_1}} + \frac{1}{\omega_{E_2}} \right]$$

$$\frac{d_3}{2} + \frac{d_4}{2} + \frac{d_3}{2} + \frac{d_4}{2} + \frac{d_4}{2} + \frac{d_4}{2} +$$

$$g_{ox} g \sqrt{2} \left[ d_3 - d_2 \right].$$  (66)

Finally using Eq.(1) and setting $\omega_0 = \omega_0$, we obtain

$$\tilde{\Delta}(4) = - \frac{U^2}{16} \left[ - \frac{1}{\varepsilon_{A_1}} - \frac{1}{2(-\varepsilon_{A_1} + \varepsilon_{A_1}^\dagger)} \right] - g_{ox}^2 \frac{4}{\omega_0}. \quad (67)$$

This must be compared with Eq.(38), Sect.V, that can be solved iteratively for $\Delta(4) = E - 2\varepsilon_{A_1}$ inserting $\varepsilon_{B_1} = 0$ from Appendix A. The second iteration yields Eq.(67), supporting the identification $\Delta(4) = \Delta(4)$ at this order. Both quantities represent the effective interaction of the dressed $B_2W = 0$ pair. Indeed, much information about the ground state energies cancels out if one applies Eq.(1); the canonical transformation is a much more practical way to represent the effective interaction.

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