Enhancement of pairing in a boson-fermion model for coupled ladders

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Motivated by the presence of various charge inhomogeneities in strongly correlated systems of coupled ladders, a model of spatially separated bosonic and fermionic degrees of freedom is numerically studied. In this model, bosonic chains are connected to fermionic chains by two types of generalized Andreev couplings. It is shown that for both types of couplings the long-distance pairing correlations are enhanced. Near quarter filling, this effect is much larger for the splitting of a pair in electrons which go to the two neighboring fermionic chains than for a pair hopping process. It is argued that the pairing enhancement is a result of the nearest neighbor Coulomb repulsion which tunes the competition between pairing and charge ordering.

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I. INTRODUCTION

Charge inhomogeneities are an ubiquitous feature in strongly correlated electron systems. One of these inhomogeneities is the stripe phase present in some underdoped cuprates. In this phase, it has been recently suggested by theoretical and experimental studies that both stripes and intervening spin regions may be modeled as two-leg ladders. Charge inhomogeneity can also be originated by the structure of the materials. In the layered compound \( \beta\text{-Na}_{0.33}\text{V}_{2}\text{O}_{5} \), the V-O planes consist of two-leg ladders separated by zig-zag chains. This compound undergoes a transition from a charge-ordered state to a superconducting state under pressure. Within a purely electronic mechanism for superconductivity in this material it is tempting to associate the formation of pairs to the ladder units. Similarly, in the compound \( \text{Sr}_{14-x}\text{Ca}_{x}\text{Cu}_{24}\text{O}_{41} \), the Cu-O planes consist of coupled ladders forming a trellis lattice. This material becomes also superconductor under pressure and it also presents a competing charge ordered phase.

Then, it seems natural to study these inhomogeneous systems with Hubbard or \( t-J \) Hamiltonians defined on coupled ladders or quasi-one dimensional structures, with in general different fillings. After all, single ladders contains pairing, pseudogap, charge ordering (CDW) and boson correlations, and the effect of applied pressure which leads to the modification of couplings, site energies.

In general, these effective models will contain fermion and boson hopping terms together with some additional terms mixing bosons and fermions. One of the most important and interesting mixing term is a generalized Andreev coupling which describes the breaking of a pair in two electrons or the reverse process. In Section II the model studied in this paper, formulated on a system of alternating bosonic and fermionic chains, is derived from microscopic models using a projection technique. Results obtained by exact diagonalization are shown in Section III. Finally, the relevance of these results to various physical systems is discussed in Section IV.

II. EFFECTIVE MODEL

The specific model studied in this paper is formulated on a system of alternating bosonic and fermionic chains...
In order to understand the physical origin of these two types of Andreev coupling let us consider an extended t-J or Hubbard model on the 12-site system of Fig. (c) top with 2 electrons. By performing a site to dimer change of basis, and projecting out the one-electron (fermionic) dimer states on the two inner dimers and the double occupied (bosonic) states on the four outer dimers, one gets the effective 6-site boson-fermion model of Fig. (c) bottom. The effective Hamiltonian is given by the standard formula:

$$
\mathcal{H}_{\text{eff}} = \mathcal{P} \mathcal{H}_0 \mathcal{P} - \mathcal{P} \mathcal{H}_0 \mathcal{Q} \frac{1}{Q \mathcal{H}_0 \mathcal{Q} - E_0} Q \mathcal{H}_0 \mathcal{P}
$$

where $\mathcal{P}$ is the projection operator on the subspace of retained states, $Q$ is the projection operator on the subspace of the eliminated states, $\mathcal{H}_0$ is the original Hamiltonian, $\mathcal{H}_0 \mathcal{P} \mathcal{Q} = E_0 \mathcal{P} \mathcal{Q}$. Variants of this procedure were repeatedly performed (14,15) to obtain effective models from the Hubbard or t-J models, specially retaining triplet states and projecting out fermionic states. Similar studies but retaining fermionic states, although using a different projection procedure, have concluded that the most important interactions not involving triplets are the ones contained in Hamiltonian (11). Although Eq. (2) is usually analytically calculated using second order perturbation theory, for the 12-site cluster of Fig. (c) it could easily be numerically solved using standard matrix inversion subroutines. In the mapping shown in Fig. (c), the projection step also leads to second neighbor fermion-fermion and three-site interactions in the horizontal direction which are also negligible in first approximation.

Let us consider first that $\mathcal{H}_0$ is an extended t-J model. Let us assume that we have the usual t, J couplings and a NN Coulomb repulsion $V_0$ on the ladders, and $t_{\text{inter}}, J_{\text{inter}}, V_{\text{inter}}$ between ladders, with $J_{\text{inter}}/J = (t_{\text{inter}}/t)^2$ and $V_{\text{inter}}/V_0 = t_{\text{inter}}/t$. It is reasonable to assume that the main effect of applying pressure is to modify the interladder interactions, which are here related to $t_{\text{inter}}$. The values of the effective couplings $t_b$, $t_f$, $\lambda_{A,s}$ and $\lambda_{A,h}$ are shown in Fig. (d) for $J/t = 0.4$, $V_0/J = 0$, as a function of $t_{\text{inter}}/t$. The most important feature is that $\lambda_{A,s}$ is clearly larger than $\lambda_{A,h}$. It should be noticed that the sign of $\lambda_{A,s}$ corresponding to the process in Fig. (b) is opposite to the process in which the up spin electron goes to the left chain and the down spin electron goes to the right chain. This is related to the fact that the electron pair on a ladder rung form a singlet. One should also notice that $t_b$ and $t_f$ take values close to each other.

On the other hand, let us assume that we have an extended Hubbard model with $U_0 < 0$, $V_0 > 0$, on the 12-site cluster of Fig. (c). This attractive $U_0$ could describe a phonon mediated pairing. In this case, one obtains the effective parameters shown in Fig. (c). It is now apparent that the pair hopping type of Andreev coupling dominates over the pair splitting type. It should also be noticed that in this case $t_b$ is much smaller than $t_f$ and hence it could be neglected which is precisely what has

![Diagram](image-url)
been done in the earlier literature\textsuperscript{14,15} although it was included in the studies related to the pseudogap phase in cuprates\textsuperscript{16} It is possible to think then that the case considered in Fig(4d), with a dominance of \( \lambda_{A,s} \) corresponding to a strongly correlated electron physics with a likely d-wave pairing, while the situation of Fig(4e), would correspond to a more conventional, s-wave, type of superconductivity.

In order to support this interpretation, the probability of double occupancy and the probability of having a singlet on a rung, properly normalized (i.e., the sum of all the possible configurations on a rung equal to 1) was computed. In the case of the extended \( t-J \) model, the probability of electrons forming a rung singlet is much larger than the probability of electrons going to double-occupied sites. The reverse situation occurs for the attractive Hubbard model. It is instructive to consider also a model which interpolates between the Hubbard and the \( t-J \) model, the so-called \( t-J-U \) model, obtained from the \( t-J \) model by relaxing the no double-occupancy constraint but including an onsite Hubbard repulsion. For an intermediate situation, for example, \( J = 1, t = 1, U = 0.5, V = 0 \), there is a crossover from the splitting to the pair-hopping types of Andreev coupling as \( t_{\text{inter}} \) is increased consistent with a crossing from singlet to double-occupancy order. That is, applied pressure can change a s-wave pairing into a d-wave pairing.

The proposed model (1) is far more general than the simple “derivation” schematically shown in Fig.1(c). In the first place, a boson does not necessarily represent a pair on a ladder rung. In fact, it has been shown that on ladders, pairs are located along plaquette diagonals or on more distant sites depending on coupling values\textsuperscript{24.}

In general, this boson-fermion model is applicable to any compound containing quasi-1D units bearing some kind of pairing. The site energy \( \epsilon_i \) would be in general determined by the binding energy of electrons on these quasi-1D units as well as by a potential coming from the whole structure of the material, which can be modified by external applied pressure or by internal chemical substitution, as in \( \text{Sr}_{14-x}\text{Ca}_x\text{Cu}_2\text{O}_{11} \), where Ca doping leads to transfer of holes from the chain to the ladder planes. The boson-fermion model could provide insights to predict the effects produced by these kinds of perturbations on a given compound.

III. NUMERICAL RESULTS

A. 3 \( \times L \) cluster, quarter filling

Model Eq. (1) was studied by exact diagonalization (Lanczos algorithm) on 3 \( \times L \) (\( L = 6, 8 \)) clusters with periodic (open) boundary conditions (BC) along (across) the \( L \)-site chains. The central \( L \)-site chain has bosonic operators while the two external chains contain the fermionic ones. \( t_f \) is adopted as the unit of energy. In the above mentioned basis change, the effective parameters \( U \) and \( V \) result roughly half the NN Coulomb repulsion of the original model \((V_0)\), both for the limits of infinite and zero values of the Hubbard on-site repulsion of the original model \((U_0)\). Hence \( U = V \) in the following. Various properties, specially those related to superconductivity, were computed as a function of \( t_b, \epsilon \) and \( \lambda_A \).

Figure 2 shows results for the \( 3 \times 8 \) cluster, \( \epsilon = 0, U = V = 2 \), at quarter filling \((n = 0.5)\). The first feature to notice is the relative occupation of the fermionic and bosonic chains depends on the parameters of the model. In Figs. (a) and (b), the boson density in the central chain, \( \delta_b = \langle n_b \rangle / L \) \((L = 8 \) in this case) is shown for \( \lambda_{A,s} \) and \( \lambda_{A,h} \) respectively. In both cases, \( \delta_b \) increases as \( t_b \) is increased. This is expected since electrons would move to the central chain to gain kinetic energy. For \( t_b = 1 \) there is a level crossing with a sudden increase of \( \delta_b \). On the other hand, \( \delta_b \) slowly decreases with \( \lambda_{A,h} \) in the interval shown, while its behavior with \( \lambda_{A,s} \) is non monotonic.

The central quantity of the present study is the boson correlation at the maximum distance, \( P_{r_{\text{max}}} = \langle b_r^\dagger b_0 \rangle \) along the central chain. This correlation, which in the current model has the meaning of pairing correlation, is a measure of quasi-long range superconducting order on the bosonic chain. The results for \( P_{r_{\text{max}}} \) are shown in Fig. 2(c),(d) for \( \lambda_{A,s} \) and \( \lambda_{A,h} \) respectively. In both cases, for a fixed value of \( t_b \), \( P_{r_{\text{max}}} \) shows an enhancement as the Andreev coupling increases. The curves of \( P_{r_{\text{max}}} \) vs. \( \lambda_A \) are shifted upward as \( t_b \) increases, as expected. The most important feature of these results is that the enhancement with \( \lambda_A \) is much stronger for the case of pair splitting than for the case of pair hopping. Notice also that for pair splitting, for \( t_b \) fixed, the behavior of \( P_{r_{\text{max}}} \) and the one of \( \delta_b \) are unrelated. It should be emphasized that in the region where \( P_{r_{\text{max}}} \) is enhanced, the pairing correlations as a function of distance, \( \langle b_r^\dagger b_0 \rangle \), have a monotonically decreasing behavior corresponding...
to true long-distance pairing. A non-monotonic behavior would be indicative of phase separation or CDW.

For $U = V = 0$, energy, boson occupancy and pairing correlations are identical for $\lambda_{A,s}$ and $\lambda_{A,h}$. This comes from the fact that the respective Hamiltonians are related by the transformation $H_0^{(h)} = T^{-1}H_0^{(s)}T$, where $T$ relates the two processes depicted in Fig. 1(b) as $H_b = T^{-1}H_s T$, and $T^{-1} = T^T$. Quantities defined solely in terms of bosonic operators are preserved by this transformation. The important result is that in this case, $P_{r\text{max}}$ is not enhanced by $\lambda_A$, although it is considerably larger than for $U = V = 2$.

In order to characterize the physics of this model more completely, the static charge structure factor $C(q)$ and the current-current correlations at the maximum distance along one of the fermionic chains were computed. The first quantity is indicative of CDW while the second one is related to the conduction of the fermionic chains. For the same parameters as before ($U = V = 2$, $\epsilon = 0$, $n = 0.5$), $C(q)$ presents a maximum at $q_{\text{max}} = (3\pi/4, 2\pi/3)$ in the whole range of $t_b$ and $\lambda_A$ examined. Figures 3(a),(b) show $C_{\text{max}} = C(q_{\text{max}})$ for $\lambda_{A,s}$ and $\lambda_{A,h}$ respectively. It can be seen that this quantity is suppressed, particularly by $\lambda_{A,s}$. The charge structure factor for the whole cluster behaves in a similar way than the one computed from the charge-charge correlations along a single fermionic chain. Now, for $U = V = 0$, $C(q)$, as it was found for $P_{r\text{max}}$, is roughly independent of $\lambda_A$. The same behavior is also found for other clusters and densities considered below. It is possible then to sum up these features by suggesting that $\lambda_{A,s}$ works against the tendency to CDW, favored by $V$, thus leading to an enhancement of long distance pairing.

The current operator between sites $i$ and $i+\vec{y}$ is defined as usual as $j_{\vec{y},i} = i\epsilon_t \sum_\sigma (c_{i+\vec{y}\sigma}^\dagger c_{i\sigma} - h.c.)$, and current-current correlations at the maximum distance as $\sigma_{r\text{max}} = \langle j_{\vec{y},r\text{max}} j_{\vec{y},0} \rangle$. Results for $\sigma_{r\text{max}}$ along a fermionic chain are shown in Fig. 3(c),(d) for $\lambda_{A,s}$ and $\lambda_{A,h}$ respectively. It can be seen that $\sigma_{r\text{max}}$ is suppressed in both cases although this effect is much larger for $\lambda_{A,s}$ than for $\lambda_{A,h}$. This behavior indicates that the effect of $\lambda_A$ is to favour the conduction mainly through the bosonic chain.

B. Other clusters and fillings

It is also important to determine if the behavior shown in Figs. 2 and 3 is also present at larger electron fillings, specially because some possible applications of the present model, for example Sr$_{14−x}$Ca$_x$Cu$_2$O$_{24}$, correspond to systems close to half-filling. As electron filling increases from $n = 0.5$, the dimension of the Hilbert space increases rapidly and it soon makes this problem very hard for exact diagonalization. Hence we have to limit the study to the smaller $3 \times 6$ cluster.

Results for the $3 \times 6$ cluster with 12 electrons ($n = 0.67$) and 16 electrons ($n = 0.89$) are shown in Fig. 4. For $U = V = 1$, $\epsilon = -0.5$, $t_b = 0.8$, the boson density varies slowly with $\lambda_A$ (Fig. 4(a)). At $n = 0.67$, $\delta_b \sim 0.35$, which implies an identical charge density on fermionic and bosonic chains. At $n = 0.89$, $\delta_b \sim 0.5$ implying a larger charge density on the bosonic than on the fermionic chains. The overall behavior of the pairing correlation at the maximum distance along the central chain, shown in Fig. 4(b), is the same as in Fig. 2, i.e., there is an enhancement of $P_{r\text{max}}$ with $\lambda_A$ which is more pronounced for pair splitting process. For these values of the parameters, $C_{\text{max}}$, peaked at $q_{\text{max}} = (\pi, \pi)$ is monotonically suppressed by $\lambda_A$.

To obtain larger charge density on the bosonic chain,
the couplings $U = V = 0.5$ and $\epsilon = -2$ were studied; $t_b = 0.8$ as before. It can be seen in Fig. 4(c), that at $n = 0.67$, $\delta_b$ becomes slightly larger than 0.5 and at $n = 0.89$, $\delta_b \sim 0.6$. For both global fillings, the charge density on the bosonic chain is approximately twice the one on the fermionic chains. Notice that now $P_{\text{max}}$ (Fig. 4(d)) is larger than the one shown in Fig. 4(b). This larger value, for $n = 0.89$, could be related to the behavior of simple hard-core boson (or spinless fermion) chain with NN repulsion, where superconductivity is suppressed at half-filling ($\delta_b = 0.5$), which is the case for $U = V = 1$ and $\epsilon = -0.5$ (Fig. 4(a)). On the other hand, the opposite happens for the case of $n = 0.67$, indicating that the Andreev coupling changes the physics of an isolated bosonic chain. However, at $\lambda_A \leq 0.2$, the pairing correlations as a function of distance has a non monotonic behavior, signaling CDW. It should also be noticed that for all cases in Fig. 4(d), there is a saturation and further decreasing of $P_{\text{max}}$ for larger $\lambda_A$. This may indicate that the behavior shown in Figs. 4(c) and 4(b) is mostly a property of low bosonic density ($\delta_b < 0.5$). It should be stressed that by going from $\epsilon = -0.5$ to $-2$, with $U = V = 1$ fixed, the changes are smoother than by going from $U = V = 1$ to $U = V = 0.5$, keeping $\epsilon = -2$ fixed. In this parameter space, results interpolate smoothly between those of Fig. 4(a),(b) and those of Fig. 4(c),(d).

It is tempting to relate the relatively small effect of pair hopping on pairing correlations to its possible suppression by the onsite Coulomb repulsion on the fermionic chains. This is actually not the case. One should notice first that pair splitting is also affected by such repulsion since an electron could be already present in one or both of the final sites on the fermionic chains. For noninteracting electrons simple combinatorics lead to the result that double-occupancy is more likely on the splitting than on the pair processes for electron densities larger than $\sim 0.6$. A similar effect caused by the NN repulsion $V$ is more difficult to predict. Alternatively, it is possible to compute the contribution of the Andreev term to the total energy, $E_A$, as a measure of how much this term is actually "working". It may be convenient then to plot $P_{\text{max}}$ as a function of $E_A$, rather than as a function of the bare parameter $\lambda_A$. This is done in Fig. 5 for some typical cases of Figs. 2 and 4. It can be seen that the qualitative behavior of these figures is not modified. Only in Fig. 5(d), corresponding to a density $\epsilon = 0.89$, there is a jump in $P_{\text{max}}$ for the pair hopping case but this occurs at a rather large value of the bare coupling, $\lambda_A, h = 1.2$. Figs. 5(a) and (b) allows the comparison between two different values of $\epsilon$. For both types of Andreev couplings, a smaller (negative) value of $\epsilon$ gives a smaller enhancement of $P_{\text{max}}$, an even a suppression in the case of the pair type of Andreev coupling.

Computer limitations make it difficult to go to larger clusters in order to assess finite size effects but it is possible to study clusters with different geometry. The $2 \times 12$ cluster was considered to estimate finite size effects on the pair hopping between the fermionic and bosonic chains. Results for the same parameters as in Fig. 2 show that $P_{\text{max}}$ takes values very close to those found for the $3 \times 8$ cluster with a very similar (small) dependence with $\lambda_A, h$. This asymmetric two-chain system is essentially the same studied by Le Hur, by bosonization techniques, although in this work the boson mediated pairing of unpaired electrons is mainly investigated. Finally, the cluster with 4 coupled chains of length 6, with periodic BC also in the transversal direction, with 12 and 14 electrons, and the same couplings as in Figs. 2 and 4 was considered. The overall behavior is the same as that depicted in those Figures -in particular $P_{\text{max}}$ is much more robust for $\lambda_A, h$ than for $\lambda_A, h$- with the additional feature of an enhancement of pairing correlations also in the direction perpendicular to the chains. For $U = V = 0$, as for the $3 \times L$ clusters studied above, $C(q)$ and longitudinal $P_{\text{max}}$ are almost independent of $\lambda_A$ although transversal pairing correlations are trivially enhanced by $\lambda_A$.

C. A “toy” model of stripes

With respect to the application of the present model to the stripe phase in the cuprates, one should take into account that the $t$-$J$ model considered as a microscopic model from which the couplings in Fig. 4(d) were derived, was meant to be the strong-coupling limit of the one-band Hubbard model. In these models pairs involve electrons with opposite spins. In the $t$-$J$ model, as applied to cuprates, pairing involves doped holes which are described by singlets. Although a derivation of an effective model from this version of the $t$-$J$ model is possible, it is instructive to use the already obtained results to
To study a “toy” model of stripes. To do this, a fermion should have the meaning of a doped hole, and the half-filled state of the cuprates should be the “vacuum” of model (1). From Fig. 1(d), the approximate values of the couplings are \( t_b = t_f = 1 \), \( \lambda_{A,s} = 0.33 \), \( \lambda_{A,h} = 0.06 \), \( U = V = 0 \). On the 4 \( \times \) 6 cluster described above, in order that the stripes be at a linear filling of one quarter, there should be 6 doped holes, corresponding to a doping on the original cluster of 0.125. In this study the variable is the site energy at the stripes, \( \epsilon \), which may also depend of various mechanisms such as structural details, phonons. Results are shown in Fig. 6. The main conclusion is that pairing is enhanced in both longitudinal and transversal directions, even though doped holes are increasingly localized at the “stripes”.

IV. CONCLUSIONS

In summary, a model of coupled bosonic and fermionic chains was proposed to describe the physics of compounds in which pairing takes place in quasi-1D structures such as two-leg ladders. Starting from a microscopic model, an exact projection procedure on a small cluster suggests that a pair splitting kind of Andreev process is related to the physics of repulsive \( U \) systems, characterized by d-wave pairing, while a pair hopping Andreev process is more related to a negative \( U \) kind of physics leading to s-wave pairing. This elementary projection also gives indication of how the effective couplings are changed with pressure. The values of these couplings for a specific compound should be obtained from a realistic, in general complex, microscopic model, and in this case an exact diagonalization procedure dealing with much larger clusters than the ones of Fig. 1(c) should be used. Although in principle both types of Andreev couplings are going to be present in the effective model irrespective of the nature of the pairing, the purpose of the present study was to determine the more general and important properties of those processes taken separately. The conclusion was that, close to quarter-filling, a pair splitting process is more efficient to enhance long-distance pairing than pair hopping from the superconducting to the non superconducting chains. So far this result would suggest that if the effect of pressure translates in an increasing of \( \lambda_A \) in, for example, \( \beta \)-\( \text{Na}_0.33 \text{V}_2\text{O}_5 \), then the presence of pairing would be more likely the result of strongly correlated electron physics in these compounds. More detailed predictions would require to determine the effective couplings more precisely as discussed above. In any case, even at this general level, more predictions for example for ARPES experiments could be obtained by studying dynamical properties.

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13 E. Altman and A. Auerbach, Phys. Rev. B 65, 104508 (2002).
14 M. Cuoco, C. Noce, J. Ranninger, and A. Romano, Phys. Rev. B 67, 224504 (2003), and references therein.
15 S. Robaszkiewicz, R. Micnas and J. Ranninger, Phys. Rev. B 36, 180 (1987); J. Ranninger and S. Robaszkiewicz, Physica B 135, 468 (1985).
16 V. B. Geshkenbein, L. B. Ioffe, and A. I. Larkin, Phys. Rev. B 55, 3173 (1997).
17 K. Le Hur, Phys. Rev. B 64, 060502 (2001).
18 V. J. Emery, S. A. Kivelson, and O. Zachar, Phys. Rev. B 56, 6120 (1996).
19 J. A. Riera, Phys. Rev. B 65, 064524 (2002).
20 M. C. Aronson, S. B. Dierker, B. S. Dennis, S. W. Cheong, and Z. Fisk, Phys. Rev. B 44, 4657 (1991); J. S. Zhou and J. B. Goodenough, Phys. Rev. Lett. 89, 087201 (2002).
21 The symbol $\lambda_A$ is used to denote indistinctly $\lambda_{A,s}$ or $\lambda_{A,h}$.
22 The derivation of Eq. (2) involves elementary matrix algebra and can be seen in P. Fulde, *Electron Correlation in molecules and solids*, (Springer, Berlin, 1991), Chap. 12.2.2.
23 The codes implementing Eq. (2) are available upon request at riera@ifir.edu.ar.
24 J. A. Riera and E. Dagotto, Phys. Rev. B 57, 8609 (1998).
25 More appropriate quantities, such as the Drude weight are studied in a following paper, J. A. Riera, in preparation.
26 F. C. Zhang and T. M. Rice, Phys. Rev. B 37, 3759 (1988).