

Gain of the kinetic energy of bipolarons in the t - J -Holstein model based on electron-phonon coupling

L. Vidmar¹ and J. Bonča^{2,1}¹*J. Stefan Institute, 1000 Ljubljana, Slovenia*²*Faculty of Mathematics and Physics, University of Ljubljana, 1000 Ljubljana, Slovenia*

(Received 30 June 2010; published 22 September 2010)

With increasing electron-phonon coupling as described within the t - J -Holstein model, bipolaron kinetic energy is lowered in comparison with that of the polaron. This effect is accompanied with “undressing” of bipolaron from lattice degrees of freedom. Consequently, the effective bipolaron mass becomes smaller than the polaron mass. Magnetic as well as lattice degrees of freedom cooperatively contribute to formation of spin-lattice bipolarons.

DOI: [10.1103/PhysRevB.82.125121](https://doi.org/10.1103/PhysRevB.82.125121)

PACS number(s): 74.20.Mn, 71.38.-k, 74.20.Rp

I. INTRODUCTION

In strongly correlated systems superconductivity (SC) may occur as a consequence of the kinetic-energy lowering as opposed to a standard BCS-type superconductor where there is a slight kinetic-energy raise accompanied by the lowering of the potential energy that stabilizes the SC state.^{1–6} Experimentally, kinetic-energy lowering would reflect in the violation of the low-frequency optical sum rule and lead to a change in high-frequency optical absorption upon entering SC state.^{7,9} The violation of the optical sum rule due to coupling to a single Einstein boson mode has recently been theoretically investigated.⁸

The idea of in-plane kinetic energy driven pairing, originally proposed by Hirsch, is based on the Hubbard-type model where hopping depends upon the occupation number.² The possibility of kinetic-energy gain has been investigated as well in more general models with correlated electrons, such as the standard Hubbard model. Using variational Monte Carlo method authors of Ref. 10 find kinetic-energy gain in SC state with a d -wave symmetry above a critical value of U_c . More recent calculations based on the dynamical cluster approximation show that pairing is driven by the kinetic-energy gain.¹¹

The main motive for the kinetic energy driven pairing in models possessing at least short-range antiferromagnetic correlations relies on the argument that the motion of the single hole is obstructed due to formation of strings of misaligned spins left in the wake of the propagating hole. A pair of holes that propagates coherently should lower its kinetic energy as one hole moves in the wake created by the other hole. This naive argument was challenged by Trugman¹² who suggested, that a pair of holes is less mobile than originally anticipated when assuming the simple string argument. Lower pair mobility occurs due to a frustration effect, which arises from the fermion exchange processes. Cluster dynamical mean-field studies¹³ on the t - J model nevertheless show a small kinetic-energy gain in the underdoped regime as the system enters SC state while there is a slight kinetic-energy raise in the overdoped regime. Authors of Ref. 14 have demonstrated the existence of the kinetic energy driven superconductivity in the t - J model using the spin polaron technique.

A scenario of the kinetic-energy gain upon pair formation is inherently connected with increased pair mobility and con-

sequently with lowering of the effective mass. In Holstein-type models, however, the effective bipolaron mass is in the strong electron-phonon (EP) coupling regime typically much larger than the polaron one. A heavy bipolaron effective mass represents one of the main obstacles for bipolaronic theory of superconductivity.¹⁵ Addition of Coulomb interaction¹⁶ and generalization to physically more relevant Fröhlich-type EP interaction^{17–19} contribute to a substantial decrease in the bipolaron mass. Nevertheless, the bipolaron remains heavier in comparison with the polaron.

While it is widely accepted that strong correlations govern the physics of high- T_c superconductors,²⁰ the notion of the importance of lattice effects with the emphasis on their role in formation of the SC state is as well gaining momentum.²¹ In this paper we compare physical properties of systems with one and two holes coupled to quantum phonons doped in the Heisenberg antiferromagnet.

We first show that there is no kinetic-energy gain upon bipolaron formation in the pure t - J model. Throughout this paper we use the term kinetic energy for the expectation value of the hopping term in the t - J model. We should point out that this term represents only the kinetic energy of the lower Hubbard band, as already noted by Wróbel *et al.* in Ref. 14. Switching on EP coupling we discover that the interplay between the kinetic, magnetic, and elastic energy leads to a formation of a spin-lattice bipolaron that in the crossover regime between the weak and strong EP coupling gains the kinetic energy relative to its polaron constituents. In this regime the effective mass of the spin-lattice bipolaron is decreased relative to the effective mass of the polaron.

II. MODEL AND METHOD

We employ a recently developed method to solve system of one and two holes in the t - J model defined on an infinite two-dimensional lattice, coupled to lattice degrees of freedom.^{22–24} We investigate the influence of EP coupling via the simplest extension of the t - J model where holes couple to dispersionless phonons. The model describes the influence of apex oxygen vibration on doped holes, propagating in lightly doped CuO planes in cuprates:

$$\begin{aligned}
H = & -t \sum_{\langle i,j \rangle, s} (\tilde{c}_{i,s}^\dagger \tilde{c}_{j,s} + \text{H.c.}) + J \sum_{\langle i,j \rangle} \left(\mathbf{S}_i \mathbf{S}_j - \frac{1}{4} n_i n_j \right) \\
& + g \sum_i n_i^h (a_i^\dagger + a_i) + \omega_0 \sum_i a_i^\dagger a_i,
\end{aligned} \quad (1)$$

where $\tilde{c}_{i,s} = c_{i,s}(1 - n_{i,-s})$ is a projected fermion operator, t represents nearest-neighbor overlap integral, the sum $\langle i,j \rangle$ runs over pairs of nearest neighbors, a_i are phonon annihilation operators and $n_i = \sum_s n_{i,s}$. g and ω_0 represent EP-coupling constant and the Einstein phonon frequency, respectively.

While the numerical method has been in detail described in previous works,^{22–24} we only briefly highlight a few most relevant elements of the method. The construction of the functional space for one and two holes starts from a Néel state with one or two holes located on neighboring Cu sites and with zero phonon quanta. In the case of a high-symmetry point at $\mathbf{k}=(0,0)$, the parent state of two holes can be chosen to exhibit a point symmetry, belonging to a particular irreducible representation of the point group C_{4v} . Such a state is expressed as $|\phi^{(0,0)}\rangle_a = \sum_{\gamma} (-1)^{M_a(\gamma)} c_{0C_\gamma} |\text{Neel}; 0\rangle$, where sum runs over four nearest neighbors in the case of d - and s -wave symmetry and over two in the case of $p_{x(y)}$ -wave while $M_a(\gamma)$, $a \in \{d, s, p\}$ sets the appropriate sign.

We generate new parent states by applying the generator of states $\{|\phi_i^{(N_h, M)}\rangle_a\} = (H_{\text{kin}} + H_g^M)^{N_h} |\phi^{(0,0)}\rangle_a$ where H_{kin} represent the first term in Eq. (1), H_g represents third term in Eq. (1). When parameter $M > 1$ is chosen, the functional generator creates states with additional phonon quanta. This approach ensures good convergence in the strong EP coupling regime where the ground state contains multiple phonon excitations.²² In most cases we have used $N_h=6$ and $M=8$ that lead to $N_{\text{st}}=24 \times 10^6$ states. Full Hamiltonian in Eq. (1) is diagonalized within this limited functional space taking explicitly into account translational symmetry. As of now we refer to one and two hole states as polaron and bipolaron, where polaron (bipolaron) signifies a hole (two holes), dressed with spin as well as lattice excitations.

III. RESULTS

A. t - J model

We first investigate the possibility whether within the framework of the pure t - J model a bipolaron gains the kinetic energy in comparison with a polaron. To this effect we show in Fig. 1(a) the expectation value of the kinetic energy per hole, i.e., $\langle H_{\text{kin}} \rangle / N_{\text{hol}}$, vs J/t of the one and two-hole Hilbert space. Except in the unphysically small $J/t \lesssim 0.15$ we find no kinetic-energy gain of the bipolaron state. This result is in agreement with Trugman's suggestion.¹² The frustration that arises from the fermion exchange processes impedes bipolaron motion. There is no such effect in the polaron case.

A higher mobility of the bipolaron should be more pronounced in the case of the t - J_z model due to a lack of spin-flip processes that erase pairs of overturned spins and contribute to the gain of the kinetic energy of polarons in the isotropic case. For this reason we have investigated the difference between kinetic energies per hole between bipolaron and polaron $\Delta_{\text{kin}} = \langle H_{\text{kin}} \rangle^{(2)} / 2 - \langle H_{\text{kin}} \rangle^{(1)}$ in a wider, even

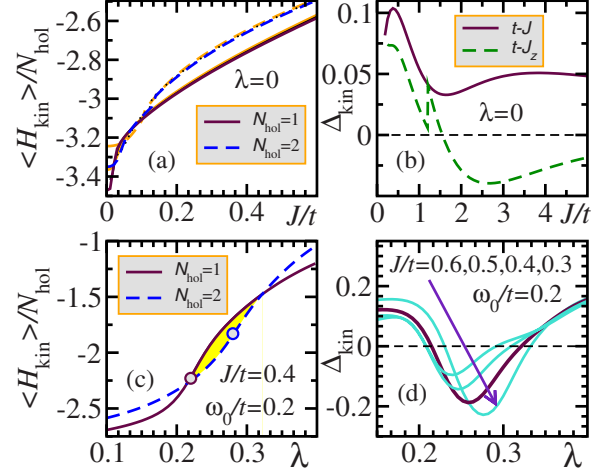


FIG. 1. (Color online) (a) $\langle H_{\text{kin}} \rangle / N_{\text{hol}}$ for the $N_{\text{hol}}=1$ (polaron) and 2 hole (bipolaron) in the t - J model with $\lambda=0$. There are three nearly overlapping curves for each system obtained using the following parameters $N_h=10, 12$, and 14 with $M=0$ in all cases that lead to the following numbers of basis states: $N_{\text{st}}=3.1 \times 10^5$, 2.6×10^6 , and 21×10^6 for the $N_{\text{hol}}=2$ case. Numbers of polaron states ($N_{\text{hol}}=1$) are typically a factor of 4 smaller; (b) Δ_{kin} vs J/t for the t - J model (full curve) and for the anisotropic t - J_z model (dashed line). A discontinuity in the latter case marks the crossover from the p -wave bipolaron ground state at small $J_z/t \lesssim 1.2$ to d wave at large J_z/t ; (c) comparison of $\langle H_{\text{kin}} \rangle / N_{\text{hol}}$ between $N_{\text{hol}}=1$ and 2 systems vs λ . In this and all subsequent plots we used generator of states with $N_h=6$ and $M=8$ that led to a Hilbert space with $N_{\text{st}}=24 \times 10^6$ states and a maximal number of phonons $N_{\text{ph}}=48$, (d) Δ_{kin} representing the difference of kinetic energies between bipolaron and polaron as defined in the text vs λ for different values of the exchange interaction J/t . The thicker curve is for $J/t=0.4$.

though unphysical range of J/t , see Fig. 1(b). We find $\Delta_{\text{kin}} < 0$ for $J_z/t \gtrsim 1.5$. The discontinuity is a consequence of a crossing between p -wave symmetry of the pair at small J_z/t to d -wave symmetry for $J_z/t \gtrsim 1.2$. In contrast, in the isotropic t - J model $\Delta_{\text{kin}} > 0$ in the whole expanded J/t regime, presented in Fig. 1(b).

On the more technical side we report on a test of the convergence of our method. In Fig. 1(a) we present nearly overlapping curves obtained using three different Hilbert spaces, generated by $N_h=10, 12, 14$ and $M=0$. Note, that in our calculation the maximal allowed hole distance is: $l_{\text{max}}=N_h+1=15$ in the case of the largest Hilbert space with no phonons. This should be compared with exact diagonalization calculations on finite square lattices with N sites, where $l_{\text{max}}=\sqrt{N}/2=4$ in the case of $N=32$ sites.²⁵

B. t - J -Holstein model

We now switch on the EP coupling. In Fig. 1(c) we plot the kinetic energy per hole vs dimensionless EP coupling constant $\lambda=g^2/8\omega_0 t$. At small λ kinetic energies of polaron ($N_{\text{hole}}=1$) and bipolaron ($N_{\text{hole}}=2$) increase linearly with λ . Such behavior is characteristic for the weak EP-coupling regime. In the regime $0.22 \lesssim \lambda \lesssim 0.32$ the kinetic energy (per hole) of bipolaron crosses below the kinetic energy of po-

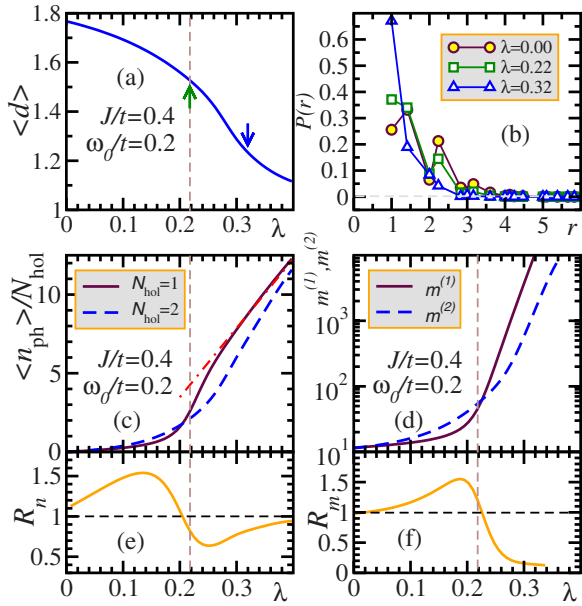


FIG. 2. (Color online) (a) Average hole distance vs $\langle d \rangle$. Vertical dashed line indicates the onset of the regime of the kinetic-energy gain, $\Delta_{\text{kin}} < 0$ as seen in Fig. 1(a). (b) Probability $P(r)$ of finding holes at a distance of r computed at three different values of $\lambda = 0, 0.22$, and 0.32 , the latter two coinciding with positions of two arrows in (a), (c) $\langle n_{\text{ph}} \rangle / N_{\text{hol}}$ vs λ of polaron (full line) and bipolaron system (dashed line). The dotted-dashed line represents the fit of the polaron result to a straight line in the regime $\lambda > 0.375$ that is given by $y = C + 8.8\lambda t / \omega_0$ (d) effective masses per hole $m^{(1)}$ and $m^{(2)}$ of polaron (full line) and bipolaron (dashed line) system, (e) and (f) R_n and R_m ratios between phonon numbers and effective masses as presented in (c) and (d), respectively (see also definitions in the text).

laron. The onset of this regime coincides with the crossover to strong-coupling regime of the spin-lattice polaron.^{22,26} If we roughly define the crossover to the strong EP-coupling regime as a point of the steepest increase in $\langle H_{\text{kin}} \rangle$ vs λ , we discover, that the polaron state enters strong EP-coupling regime at smaller $\lambda_c^{(1)} \sim 0.22$ than the bipolaron state, where $\lambda_c^{(2)} \sim 0.28$. The two inflection points are as well indicated with open circles in Fig. 1(c).

The dependence of the kinetic-energy gain on the magnetic exchange interaction J/t is investigated in Fig. 1(d) where we follow Δ_{kin} vs λ using different values of the exchange interaction. As J/t increases the kinetic-energy gain is reduced. This behavior is in contrast with the anisotropic case where at $\lambda = 0$, Δ_{kin} becomes negative only at large J_z/t , see Fig. 1(b). The kinetic-energy gain, observed in the isotropic case, is driven by the EP coupling. It is positioned in the crossover from weak to strong EP-coupling regime. In terms of the magnetic exchange interaction it is located well within the physically relevant regime of $J/t \in [0.3, 0.4]$.

In Fig. 2(a) we present the average hole distance $\langle d \rangle = \sum_r r P(r)$, of a bipolaron state, where $P(r)$ represents the probability of finding a hole pair at a distance of r : $P(r) = \langle \sum_{(i \neq j)} n_i^h n_j^h \delta[|i-j|-r] \rangle / \langle \sum_{(i \neq j)} n_i^h n_j^h \rangle$. At $J/t = 0.4$ and $\lambda = 0$ two holes form a bound bipolaron with the largest probability at a distance of $r = \sqrt{2}$, as consistent with previous calculations.^{25,27,28} With increasing EP coupling λ , $\langle d \rangle$ expe-

riences the steepest decrease in the middle of the regime where $\Delta_{\text{kin}} < 0$, i.e., for $0.22 \lesssim \lambda \lesssim 0.32$. This is reflected in the change in the shape of bipolaron where the hole distance with the largest probability $P(r)$ crosses over from $r = \sqrt{2}$ at $\lambda = 0$ to $r = 1$ at $\lambda = 0.32$, see Fig. 2(b). It is somewhat counter intuitive that such shrinking of the bipolaron size simultaneously gives rise to $\Delta_{\text{kin}} < 0$. Close proximity of holes, namely, restricts the range of hopping that consequently leads to a raise of the kinetic energy, as well seen in Fig. 1(c).

We gain additional insight into the mechanism leading to $\Delta_{\text{kin}} < 0$ by presenting comparison of the average number of phonons per hole between polaron and bipolaron. In Fig. 2(c) we plot $\langle n_{\text{ph}} \rangle / N_{\text{hol}}$ vs λ . At small λ the average $\langle n_{\text{ph}} \rangle / N_{\text{hol}}$ is for bipolaron slightly larger from that of the polaron while at $\lambda \sim 0.22$ it crosses below the polaron result. In the large λ limit both expectation values should approach the strong-coupling regime. Indeed, $\langle n_{\text{ph}} \rangle / N_{\text{hol}}$ for polaron for $\lambda \geq 0.27$ approaches a straight-line characteristic for the strong-coupling result: $\langle n_{\text{ph}} \rangle = g^2 / \omega_0^2 = 8\lambda t / \omega_0$, see the fit in Fig. 2(c). The same is not true for the bipolaron, where $\langle n_{\text{ph}} \rangle / N_{\text{hol}}$ is below polaron result for $\lambda \geq 0.22$ and finally approaches the strong-coupling result above $\lambda \geq 0.35$. We should also note that in the $\Delta_{\text{kin}} < 0$ regime, say around $\lambda = 0.26$, $\langle n_{\text{ph}} \rangle / N_{\text{hol}}$ for the polaron system exceeds result for bipolaron by nearly 50%. Results are consistent with the observation that the bipolaron crosses over to the strong-coupling regime within a wider crossover regime and at larger λ than the polaron.

In connection with Fig. 2(c) we note that in the vicinity of the physically relevant values of $\lambda \in [0.22, 0.32]$ the average number of phonons in the bipolaron state is $\langle n_{\text{ph}} \rangle < 20$. This is to be compared with the maximum number of phonon quanta contained in the Hilbert space $N_{\text{ph}} = N_h \times M = 48$. We can conclude that Hilbert space used in our method contains sufficient amount of phonon degrees that empowers our calculation reaching full convergence. To further investigate the difference in the phonon number between bipolaron and polaron state we plot in Fig. 2(e) the corresponding ratio $R_n = \langle n_{\text{ph}} \rangle^{(2)} / 2 \langle n_{\text{ph}} \rangle^{(1)}$ that approaches $R_n \sim 0.7$ in the regime $\Delta_{\text{kin}} < 0$. Note that in the strong-coupling regime $R_n \rightarrow 1$.

We proceed by presenting comparison of effective polaron and bipolaron masses. The polaron dispersion of the t - J model has a minimum at $\mathbf{k} = (\pi/2, \pi/2)$ and is highly anisotropic. We compute the effective-mass tensor in its eigendirections $m_{\alpha\alpha} = 2t(\partial^2 E(\mathbf{k}) / \partial \mathbf{k} \partial \mathbf{k})_{\alpha\alpha}^{-1}$. Taking into account anisotropic dispersion we define the polaron mass as $m^{(1)} = \sqrt{m_{\parallel} m_{\perp}}$, where m_{\parallel} and m_{\perp} are effective polaron masses along nodal and antinodal directions, respectively. In contrast, bipolaron has the energy minimum at $k=0$ with locally isotropic dispersion. We compute effective bipolaron mass per hole from $m^{(2)} = m_{xx}/2$. In Fig. 2(d) we present $m^{(1)}$ and $m^{(2)}$ vs λ . In the weak-coupling regime we find the expected result where $m^{(2)} > m^{(1)}$. For $\lambda \geq 0.23$ the opposite becomes true. Results in Fig. 2(d) represent, at least to our knowledge, the first example where $m^{(2)} < m^{(1)}$. The ratio $R_m = m^{(2)} / m^{(1)}$ in Fig. 2(f) drops down to $R_m \sim 0.2$ around $\lambda \sim 0.3$. This result is highly unusual. For comparison we draw attention to a well-known result for the Holstein model where the effective mass of two particles forming a lattice bipolaron singlet, scales in the strong-coupling regime as $m^{(2)} \propto \exp[4(g/\omega_0)^2]$

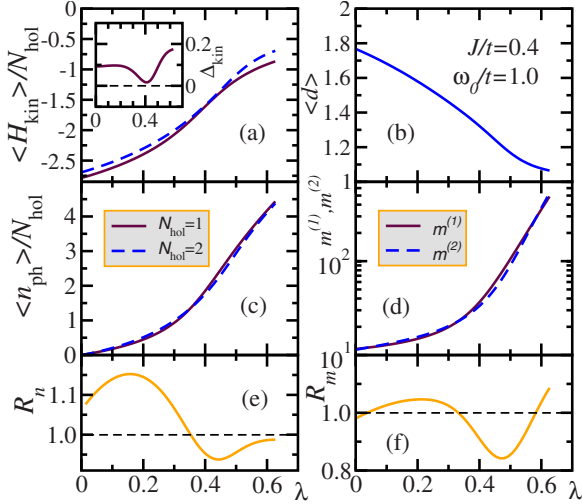


FIG. 3. (Color online) (a) $\langle H_{\text{kin}} \rangle / N_{\text{hol}}$ for $N_{\text{hol}}=1$ and 2 systems vs λ , (b) average hole distance $\langle d \rangle$ vs λ , (c) $\langle n_{\text{ph}} \rangle / N_{\text{hol}}$ vs λ of polaron (full line) and bipolaron system (dashed line), (d) effective masses per hole $m^{(1)}$ and $m^{(2)}$ for polaron (full line) and bipolaron (dashed line) system, (e) and (f) R_n and R_m ratios between phonon numbers and effective masses as presented in (c) and (d), respectively. Parameters of the model in all pictures (a,...,f) are: $J/t=0.4$ and $\omega_0/t=1.0$.

in comparison to $m^{(1)} \propto \exp[(g/\omega_0)^2]$ that leads to $m^{(2)} \gg m^{(1)}$. In the Holstein-Hubbard model, however, the on-site Coulomb interaction gives rise to a formation of an intersite bipolaron with an effective mass that is comparable, nevertheless always larger than the polaron mass.¹⁶ Recently Hague *et al.*¹⁸ examined a bipolaron defined on a triangular lattice and found unusually small effective bipolaron mass due to a crablike motion. Nevertheless, bipolaron effective mass remains larger than that of the polaron.

A note of caution: as seen in Fig. 2(d) the absolute value of the effective bipolaron mass is rather large already at the onset of the $\Delta_{\text{kin}} < 0$ regime, $m^{(1)} \sim m^{(2)} \sim 60$ (in units of free-electron mass) at $\lambda=0.23$. This shortcoming can be easily alleviated by taking into account physically more relevant longer-range Fröhlich EP interaction that may reduce $m^{(2)}$ and $m^{(1)}$ up to an order of magnitude.^{17–19} Experimental results on the effective mass seem to be slightly ambiguous. Nevertheless, latest de Haas-van Alphen measurements of the cyclotron effective mass inside of the superconducting dome of YBCO (Yttrium Barium Copper Oxide cuprate) show divergence with decreasing doping. They have measured effective masses as large as 4.5 free-electron masses.²⁹

In our search for deeper understanding of the phonon driven kinetic energy lowering and bipolaron mass renormalization we have investigated as well the regime with larger ω_0 , i.e., $\omega_0/t=1.0$. In this case the effect of EP coupling on the kinetic energy lowering disappears as seen from Fig. 3(a) even though around $\lambda \sim 0.4$ Δ_{kin} approaches zero, see also the insert of Fig. 3(a). On the other hand the effective bipolaron mass still shows a slight decrease with respect to the polaron mass in the regime $0.35 \leq \lambda \leq 0.6$, as shown in Figs. 3(d) and 3(e). This effect is closely connected to the average number of phonons that shows barely detectable decrease in

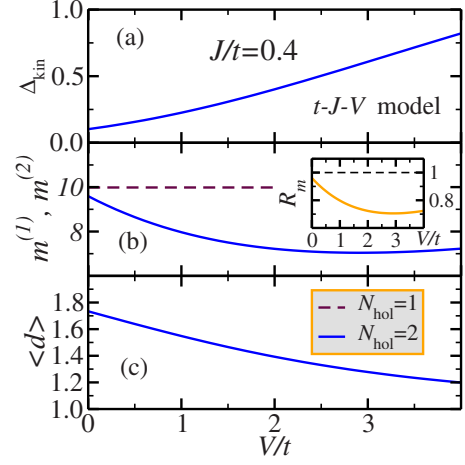


FIG. 4. (Color online) (a) Δ_{kin} vs V/t for the t - J - V model, (b) effective masses per hole $m^{(1)}$ and $m^{(2)}$ for polaron (dashed line) and bipolaron (full line) system vs V/t , and (c) average hole distance $\langle d \rangle$ vs V/t . We have used basis, generated by $N_h=12$ and $M=0$.

the same parameter regime, see Figs. 3(d) and 3(e).

C. Attractive t - J - V model

We have tried to reproduce the kinetic energy lowering and the effective bipolaron mass renormalization using a t - J - V model where the effect of phonons is replaced by an effective nearest-neighbors attractive interaction V . To this effect we have added an attractive term of the form $H_V = -V \sum_{\langle i,j \rangle} n_i^h n_j^h$ where n_i^h represents the hole-density operator, to a standard t - J model. From Fig. 4(a) we conclude that with increasing V/t Δ_{kin} remains positive and monotonically increases. We find no kinetic-energy gain in this simplified model. Nevertheless, we find a decrease in the effective mass of the bipolaron system as presented in Fig. 4(b). Effective-mass ratio reaches its minimum value $R_m \sim 0.75$ around $V/t=3.0$. This should be compared to $R_m \sim 0.13$ in the case of $\omega_0=0.2$ and $\lambda=0.3$, Fig. 2(f). Even though the effect of nearest-neighbor attraction V on the average distance $\langle d \rangle$ is similar to the effect of increasing λ [compare Figs. 2(a), 3(b), and 4(c)], the influence of the EP coupling on hole motion in the t - J model cannot be entirely explained using an effective attraction between holes. Using the simplified model we nevertheless discover an important mechanism whereby the effective bipolaron mass decreases at fixed value of J/t as the average distance between holes decreases by increasing V . In contrast to spin-lattice bipolaron where its cumulative effective mass at $\omega_0=0.2$ and $\lambda \sim 0.3$ becomes lower than that of a polaron, $R_m \sim 0.13 < 0.5$, spin bipolaron with attractive hole-hole interaction remains heavier than the polaron since $R_m \sim 0.75 > 0.5$.

IV. DISCUSSION

The main mechanism behind the gain of the kinetic energy as well as lowering of the effective mass of bipolaron emerges from the competition between kinetic, magnetic and lattice degrees of freedom. As two holes form a bipolaron in

the regime where $\Delta_{\text{kin}} < 0$, the system minimizes the kinetic energy at the expense of increased elastic energy. The gain of the kinetic energy contributes to energy splitting between states of different point-group symmetries. This is in agreement with recent results of Ref. 24 where it has been shown, that EP coupling to transverse modes in-plane oxygen vibrations stabilizes d -wave symmetry. The increase in the elastic energy emerges as undressing of bipolaron from lattice degrees of freedom as seen as the decrease in $\langle n_{\text{ph}} \rangle / N_{\text{hol}}$ below the respective polaron values. The gain in the kinetic energy does not represent the “glue” for the formation of the bipolaron since for $J/t \geq 0.2$ bipolaron is already formed in the pure t - J model where no gain in the kinetic energy is found. Instead, it emerges as a side product of the competition between the kinetic, magnetic, and elastic energies.

Our results lead to a distinct paradigm where in a correlated system, coupled to quantum lattice degrees of freedom,

upon pair formation the bipolaron mobility increases due to a lower effective mass as well as due to a detectable gain in bipolaron kinetic energy. The attractive potential for binding of bipolaron appears as a cooperative interplay between magnetic and lattice degrees of freedom. While the original idea of the kinetic-energy gain as a mechanism for hole-pairing has been proposed for a system of correlated electrons, our finding opens the possibility where lowering of the kinetic energy in a correlated model is driven by the EP interaction.

ACKNOWLEDGMENTS

J.B. acknowledges stimulating discussions with I. Sega, C.D. Batista, S.A. Trugman, and T. Tohyama and the financial support of the SRA under Grant No. P1-0044.

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