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Mobile inter-site bipolarons in presence of long-range interactions

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ABSTRACT

We report an exact diagonalization study of strongly correlated electron–phonon (EP) systems like doped polar insulators within the framework of the polaronic $t - J_p$ model considering realistic long-range Coulomb and EP (Fröhlich) interactions on linear and square clusters. For a small ratio of polaronic hopping amplitude (t) and exchange interaction (J_p), polarons predominantly occupy the nearest-neighbor (NN) position with NN spin–singlet pairing (d-wave type). With the increase in the t/J_p ratio, bipolaron size increases and finally becomes large and constant depending on the lattice size. The crossover from small to large bipolaron is nearly independent of system size but depends on the cluster geometry. Bipolaron effective mass and kinetic energy calculation show that at $t/J_p \sim 0.3$, light and small bipolarons are perfectly mobile. In linear chain, bipolaron composite is formed within a region of $0 < t/J_p < 0.5$. Results suggest the existence of the superconducting phase at the vicinity of $t/J_p \sim 0.3$.

1. Introduction

The study of strong electron–electron ($e - e$) correlation along with electron–phonon (EP) interaction remains an intriguing many-body problem. It is widely believed that the most relevant features of a strongly correlated electron system are due to the interplay between these two competing interactions. For example, the spin fluctuations induced by strong $e-e$ interactions in high-T_c cuprates mediate pairing between electrons to produce anisotropic Cooper pairs for superconducting condensation [1]. On the other hand, isotropic Cooper pairs are formed by phonon-mediated attraction leading to condensation to superconducting states. The presence of 'kinks' in the angle-resolved photoemission spectrum gives strong evidence of EP interaction in high-T_c cuprates [2]. In addition to high-T_c cuprates, sizeable EP interaction is also found to be present in different materials like Colossal magnetoresistance manganites [3], fullerenes [4], magnesium diborides [5], etc.

The basic models to study the properties of strongly correlated systems with these competing interactions are the Hubbard–Holstein and Holstein-tJ model [6]. The phenomena of the high-T_c superconductivity in cuprates were addressed both analytically [7] and numerically [8] in the framework of these two models [9] considering short-range electron–phonon interaction. A more realistic Coulomb–Fröhlich model considering long-range interactions was also proposed [10] and studied in the context of high-temperature superconductivity [11–13]. The relative strength of the long-range EP interaction and Coulomb repulsion determine whether the system is Fermi- or (Luttinger) liquids, bipolaronic superconductors or charge segregated insulators. Results show that relatively weak long-range EP interaction induces d-wave superconducting phase in doped Mott–Hubbard insulators without the necessity of additional mechanisms like spin fluctuation. It has been argued that the low Fermi energy and strong EP coupling with high-frequency phonons are the roots of high critical temperature in cuprate superconductors [12].

A polaron, charge carrier dressed by phonon clouds, and bipolarons (polarons bound by phonon-mediated interaction), are studied and of interest in the context of high T_c superconductivity [8,14–17]. Though bipolarons are spin singlet (polarons of opposite spin binding together), the existence of spin–triplet inter-site bipolarons is confirmed by studies on heavy-fermion superconductivity [18,19]. In the limit of low bipolaron density, the excitation spectra are superfluid with the bipolarons being superconducting [7]. It has been suggested that Bose–Einstein Condensation (BEC) of these bipolarons may lead to superconductivity in some high-T_c materials [20,21]. The existence of 'superlight small bipolarons', which are real-space hole pairs dressed by phonons in doped charge-transfer Mott insulators, have been suggested as the possible ground-state of high-T_c cuprates [22,23]. The interaction between the bipolarons has also been investigated using Fröhlich–Hubbard model on a discrete 1D lattice. While no bipolaron–bipolaron attraction exists in the Hubbard–Holstein model, an attraction between bipolarons exists in the extended Holstein–Hubbard model [24]. If

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the bipolarons are small and are well separated relative to their size, they may condensate to form BEC of bipolarons with the transition temperature determined by the size/effective mass of the bipolarons. Hence, the study of the properties of the bipolarons and interaction between them will be of interest to understand the possible mechanism of high-T_c superconductivity and different properties of the other strongly correlated materials.

A polaronic $t-J_p$ model, with a short-range polaronic spin-exchange J_p of phononic origin, for highly polarizable ionic lattices like cuprates and other oxides like $BaKBiO_3$ was also proposed [25]. It was argued that in the limit where bare long-range Coulomb and Fröhlich EP interactions negate each other, giving rise to the $t-J_p$ Hamiltonian. At low density, it was established that the ground state of this model to be bipolaronic singlet with a superconducting phase transition at a temperature well above $100K$ [26,27]. Thus, it can be expected that this model can extract the essential features of high T_c superconductivity and hence require further study.

Inspired on these theoretical and experimental findings, we will report the formation of different types of bipolarons based on the $t-J_p$ model which is an approximation of the realistic model considering long-range Coulomb and EP interactions in the strong coupling limit in 1D and 2D. We aim to identify and investigate the region of parameter range preferable for the formation of bipolarons of different sizes and masses, their mobility, interactions among each other and pairing correlation which might support superconductivity in high T_c cuprates.

2. Hamiltonian

The microscopic model for investigating strongly correlated real materials simply considers the direct interaction between charge carriers ($e-e$ interaction) and indirect interaction via lattice vibration (Fröhlich EP interaction). The model Hamiltonian can be written as

$$\begin{aligned} H = &-\sum_{(i,j)\sigma} T_{ij}(\tilde{c}^{\dagger}_{i\sigma}\tilde{c}_{j\sigma} + h.c.) \\ &+ \sum_{(j>i)\sigma\sigma'} V_{ij}\tilde{n}_{i\sigma}\tilde{n}_{j\sigma'} \\ &-\omega_0 \sum_{(i,j)\sigma} g_{ij}\tilde{n}_{i\sigma}(a^{\dagger}_j + a_j) \\ &+\omega_0 \sum_j a^{\dagger}_j a_j \end{aligned} \tag{1}$$

where i, j represent the position of the particles. The first term is the electron hopping term with T_{ij} as bare hopping amplitude, second term represents long range Coulomb repulsion with V_{ij} as interaction strength, third term is the coupling of an electron at site i with an ion at site j with g_{ij} as the dimensionless coupling strength and the fourth term is the phonon degrees of freedom. Here σ represents spin and we set $\hbar = 1$.

Well known Lang–Firsov transformation [28], transforms the Hamiltonian $H_{LF} = e^A H e^{-A}$ where $A = -\sum_{(i,j),\sigma}\tilde{n}_{i\sigma}g_{ij}(a_j - a^{\dagger}_j)$. This transformation displaces the simple harmonic oscillators and effectively negate the long-range interactions ($(V_{ij} - \omega_0\sum_l g_{il}g_{jl}) \sim 0$).

$$\begin{aligned} H_{LF} = &-\sum_{(i,j)\sigma} T_{ij}(X^{\dagger}_i X_j \tilde{c}^{\dagger}_{i\sigma}\tilde{c}_{j\sigma} + h.c.) \\ &+\omega_0 \sum_j a^{\dagger}_j a_j \end{aligned} \tag{2}$$

with $X_j = exp[-\sum_p g_{jp}(a^{\dagger}_p - a_p)]$. It has been shown [25] that in the strong coupling limit this model can be reduced to a polaronic model with a hopping term describing the motion of strongly correlated polarons and a spin-exchange between polarons on different sites. The Hamiltonian has the following form

$$\begin{aligned} H_{t-J_p} = &-\sum_{(i,j)\sigma} t_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma} + H.c.) \\ &+2\sum_{(j>i)}(J_p)_{ij}(\vec{S}_i.\vec{S}_j + \frac{1}{4}n_i n_j) \end{aligned} \tag{3}$$

where $t_{ij} = T_{ij}exp(-g^2_{ij})$ is the polaronic hopping amplitude, $(J_p)_{ij} = T^2_{ij}/2\omega_0 g^2_{ij}$ represents the spin-exchange interaction between polarons. $\vec{S}_i$ is the spin-$\frac{1}{2}$ operator defined in terms of the Pauli matrices as: $\vec{S}_i = \sum_{\sigma\sigma'} c^{\dagger}_{i\sigma}\vec{\tau}_{\sigma\sigma'}c_{j\sigma'}$ and $n_i = \sum_{i\sigma} c^{\dagger}_{i\sigma}c_{i\sigma}$ is the density operator.

All the quantities in the polaronic $t-J_p$ Hamiltonian are defined through the material parameters [25], in contrast to the input parameters in most of the previous studies of strongly correlated EP systems. The kinetic term in Eq. (3) describes the motion of fermions under a strong correlation in the presence of long-range Coulomb and EP interactions resulting in polaronic band narrowing. The second term is the spin-exchange term, with J_p describes the spin-exchange between carriers and is responsible for the two-particle bound state.

Though the $t-J_p$ hamiltonian looks similar to the well-known $t-J$ Hamiltonian [29], they have wide differences. While double occupancy is prohibited in the later model, there is no constraint in the double occupancy in the $t-J_p$ model. Also, there is a '+' sign instead of '–' sign in the last term which provides repulsion between the pairs.

3. Formulation

Our study follows the exact diagonalization (ED) method [30] on 1D and 2D lattice clusters of varying size and number of particles. Though the results obtained by the ED method are exact and approximation free, the main limitation lies in the restriction of the choice of cluster size. We present our work on an 8-,10-, 18- and 26-site cluster (Supplementary item Fig. 1) [31] for 2 particles (for both 1D and 2D) and 18-site for 4 particles system (only 1D) with periodic boundary conditions.

In this paper, we restrict the range of interaction up to nearest neighbor only and set $t_{ij} = t$ and $(J_p)_{ij} = J_p$. We first calculate the probability (correlation) of finding two polarons at a different site as [14,32]:

$$P^s_{bp}(|i-j|) = \langle\psi_0|\sum_{\sigma} n_{i,\sigma}n_{j,-\sigma}|\psi_0\rangle \tag{4}$$

$$P^t_{bp}(|i-j|) = \langle\psi_0|\sum_{\sigma} n_{i,\sigma}n_{j,\sigma}|\psi_0\rangle \tag{5}$$

where $P^s_{bp}(|i-j|)$ and $P^t_{bp}(|i-j|)$, represent the correlation between antiparallel ($S_z = 0$, singlet) and parallel ($S_z = 1$, triplet) orientation of spins between the polarons respectively. In parallel orientation of spins, $i = j$ is not considered due to Pauli exclusion principle. $|\psi_0\rangle$ is the ground state wave function.

We then estimated the size of the bipolaron by

$$R_b/a = \sum_{ij,\alpha} P^{\alpha}_{bp}(|i-j|)\times(|i-j|)/\sum_{ij,\alpha} P^{\alpha}_{bp}(|i-j|) \tag{6}$$

Here $|i-j|$ is the distance between two sites measured in the units of the lattice constant a and α stands for spin singlet (s) and spin triplet (t).

The mobile bipolarons, which may indicate the presence of superconductivity, if any, is calculated in terms of energy dispersion relation for bipolarons. For this we have used Singlet-Subspace projection method. The singlet basis is defined as:

For on-site pair ($d = 0$)

$$|0,k\rangle = \frac{1}{\sqrt{N}}\sum_j e^{ikaj}c^{\dagger}_{j\uparrow}c^{\dagger}_{j\downarrow}|0\rangle \tag{7}$$

For inter-site pairing

$$|d,k\rangle = \frac{1}{\sqrt{2N}}\sum_j e^{ika(j+d/2)}(c^{\dagger}_{j\uparrow}c^{\dagger}_{j+d\downarrow} - c^{\dagger}_{j\downarrow}c^{\dagger}_{j+d\uparrow})|0\rangle \tag{8}$$

d is the spacing between two particles, $|0\rangle$ is the vacuum state. Using these basis the $t-J_p$ Hamiltonian can be represented in tri-diagonal form whose eigenvalues determine the energy dispersion $E(k)$. We have evaluated the bipolaron effective mass

$$m^*_{bi} = \hbar^2/(\frac{\partial^2 E}{\partial k^2})_{k=0} \tag{9}$$

and correlated the result with bipolaron kinetic energy by ED calculation. For linear chain

$$KE_{bi}^{1D} = -t\langle\psi_0| \sum_{(i,j),\sigma} (c_{j+1\sigma}^{\dagger} c_{j\sigma'}^{\dagger} c_{i+1\sigma} c_{i\sigma'} + h.c.)|\psi_0\rangle \tag{10}$$

where (i,j) extends up to nearest-neighbor sites.

To search for the nature of pairing of the polarons pairs and possible superconducting phase, if any, we have calculated the on-site singlet pair and neighboring site singlet pair correlation function (s-wave and d-wave in higher dimensions [33])respectively by:

$$P_s = \langle \Sigma_i^{\dagger} \Sigma_j \rangle \tag{11}$$

$$P_d = \langle \Delta_i^{\dagger} \Delta_j \rangle \tag{12}$$

with $\Sigma_i = c_{i\uparrow} c_{i\downarrow}$ and $\Delta_i = \frac{1}{\sqrt{2}}(c_{i\uparrow} c_{i+1\downarrow} - c_{i\downarrow} c_{i+1\uparrow})$. For the rest of the paper we will call on-site and NN site singlet pairing as $s-$ and $d-$ wave pairing respectively.

Finally, to observe the clustering of bipolarons (formation of bipolaron composite) in the ground state, we calculate the bipolaron–bipolaron binding energy in terms of [14,32]

$$\triangle_4 = E_0^4 - 2 \times E_0^2 \tag{13}$$

where E_0^n is the ground state energies of n polarons.

In this communication, we study EP interaction at intermediate ($t <\sim J_p$) to extreme strong coupling ($t \ll J_p$) in the framework of the $t-J_p$ model. We report the possibility of binding of two bipolarons along with the existence of superconductivity and/or Bose–Einstein Condensation. The crossover between different types of bipolarons is also investigated. We take 2, 4 particle systems, with equal up and down spins, to investigate the rich physics of the polarons and bipolarons and the interactions between them based on the $t-J_p$ model. Systems with higher particle density are not of interest as superconductivity due to bipolarons appears at low bipolaron density [7].

4. Results and discussions

4.1. Ground state energy

We first compare a few initial observations with the existing works to validate the assumptions and procedures of our work. We first observe the variation of the ground state energy (E_0) with t/J_p for the two polaron systems on 8-, 10-, 18-, 26-site linear and square lattice. The results are plotted in Figs. 1(a) and 1(b). Though larger clusters are always preferable over 18 or 26 sites, the storage of the basis state configuration, as well as computational limitations due to an exponential growth of Hilbert space, impose a serious restriction on the study of larger clusters. Results for both 1D and 2D indicate that the qualitative behavior of the ground state energy with t/J_p for different cluster sizes are similar and is in good agreement with the previous results in 1D. Moreover, the maximum variation of ground state energy of our 8-, 10- and 18-site chain with respect to 26 sites linear chain (See ESI Table 1) is 5.95%, 3.74% and 0.75% respectively. Thus it can be argued that the finite size effect of the 26-site chain will be small concerning even larger clusters. Moreover, the choice of larger clusters will require sufficiently large computational time and space. Thus our results on 26- and/or 18-site clusters are sufficient to study this system efficiently with nearly negligible finite size effect. We also obtain a highly degenerate two-particle energy level of the model, in agreement with the previous work [26]

$$E_0(t=0) = -J_p, E_1(t=0) = 0, E_2(t=0) = J_p \tag{14}$$

These values of the 2-particle energy states at $t = 0$ are independent of cluster size and geometry. Interestingly, the degeneracy of the ground state and highest energy states, corresponding to the bipolaronic spin–singlet and triplet state respectively, is equal to and twice equal to the number of sites for 1D and 2D respectively.

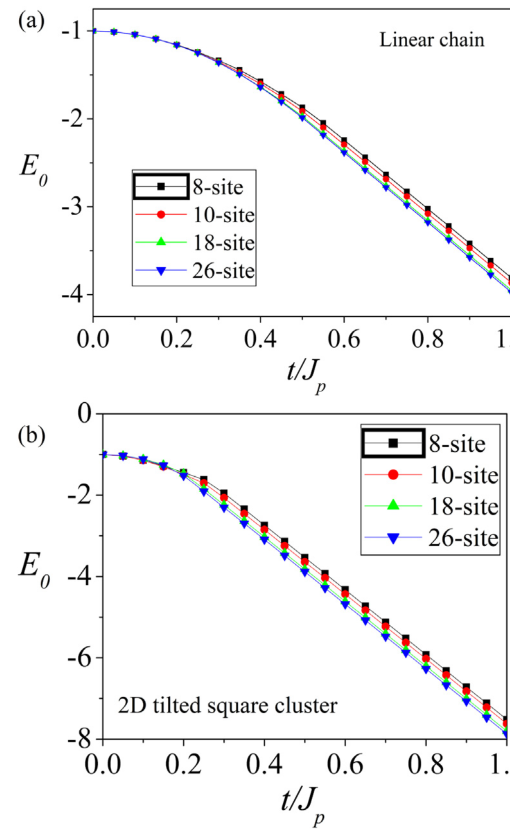

Fig. 1. Two particles ground state energy E_0 as a function of hopping for different size of the cluster. (a) linear chain and (b) tilted square cluster.

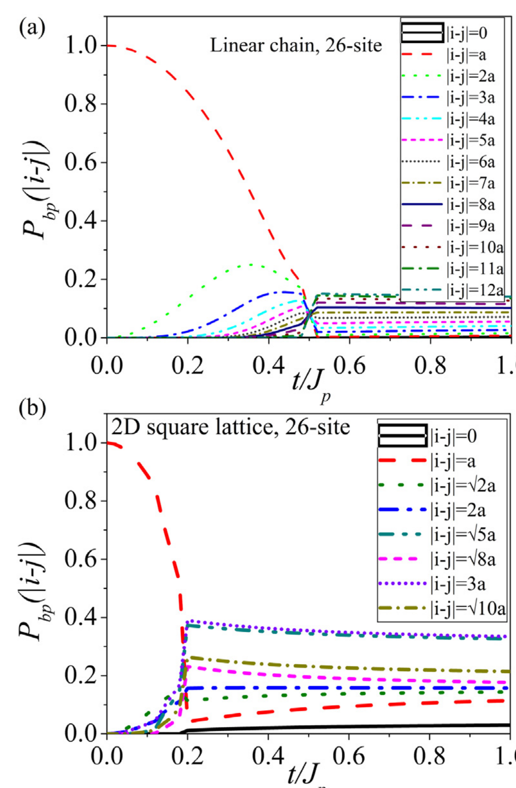

Fig. 2. Probability of finding two polarons at different distances in the ground state, in the unit of lattice constant. NN site probability is shown in bold. (a) Linear chain (b) tilted square lattice.

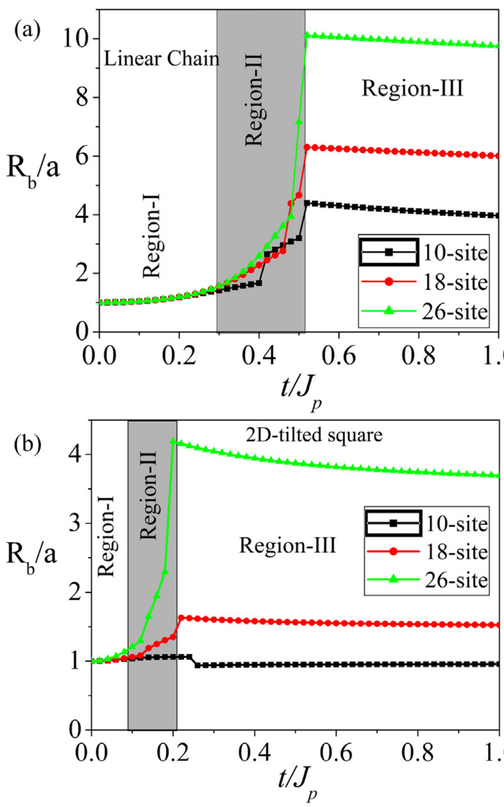

Fig. 3. Bipolaron size R_b versus t/J_p in the unit of lattice constant for three different cluster size. Three different regions corresponding to size of the bipolarons are shown. (a) Linear chain (b) 2D tilted cluster.

4.2. 2-particle case

We now first consider the correlation between two polarons P_{bp} $(|i-j|)$ at different sites which also measures the probability of finding two particles at different sites in the system. In Figs. 2(a) and 2(b), variation of two polarons $(p-p)$ correlation function with t/J_p for 1D and 2D systems are plotted respectively on a 26-site lattice using Eq. (4). Results clearly show that for $t/J_p = 0.0$, the probability of finding the two polarons are strictly at NN sites, which is independent of the geometry and size of the system (not shown). A strong correlation between polarons at NN sites and negligible correlation at other sites suggest the formation of inter-site singlet bipolarons with the binding energy J_p. Since the system is spin–singlet at the ground state, the formation of triplet state bipolarons is not be observed at the ground state.

For the linear chain, the probability of finding two particles at the NN site decrease gradually while it increases for NNN and other sites with an increase in hopping. In the range $0 < t/J_p < 0.5$, a small finite probability of finding the polarons at NNN and larger distant sites is observed. At t/J_p ~0.5, the probability of finding the polarons at all sites is equal and for higher t/J_p the probability of finding the polarons at different sites gets reversed. For $t/J_p \geq 0.5$, the probability of finding two-polarons at all distances is small with maximum probability occurs for the largest separation determined by lattice size. However, for the 2D tilted square cluster, the probability of finding two particles at the NN site decreases sharply with t/J_p and reaches to a very small value at $t/J_p = 0.2$. For $t/J_p > 0.2$, a small finite probability of finding the particles is observed for all sites and tends to maintain maximum separation available. For both cases, with the increase of particle hopping, the particles tend to move at distant sites from the NN site leading to the breakdown of NN site bipolarons. The magnitude of t/J_p at which small inter-site bipolarons splits into separate polarons can be marked as a critical value for the formation of small inter-site bipolarons.

In Figs. 3(a) and 3(b), we plot the average separation distance between two polarons with t/J_p for 10-, 18-, 26-site linear chain and square cluster respectively. This distance can be considered as a measure of the size of the bipolarons and is quite different from the *bipolaron radius*. At $t/J_p = 0.0$, for both 1D and 2D, the bipolaron size is small and the polarons are strictly separated by one lattice spacing consistent with Fig. 2. One can call this bipolaron as a small inter-site bipolaron. With the increase of t/J_p, the bipolaron size increases gradually and at a certain critical value, the size increases sharply to a large value depending on lattice size. With a further increase of t/J_p, the bipolaron size becomes constant. As the available linear distances between two polarons are greater in 1D, so bipolaron size is larger in 1D for large t/J_p. The calculation on a 10-, 18-, and 26-site shows the two polarons tends to maintain maximum separation depending on the system size for $t \sim J_p$. This constant value of the bipolaron size indicates the existence of large type bipolarons or nearly free polarons with little renormalization among them. Thus the size of the lattice confines the size of the large bipolarons or the separation of the polarons. The critical value of t/J_p (t/J_p ~ 0.5 and 0.2 for 1D and 2D (26-site) respectively), which marks the crossover from small inter-site bipolaron to large bipolaron is independent of the lattice size but dependent on cluster geometry. A very small variation of this critical value of t/J_p is obtained for different sizes of 2D systems which may be attributed to the varying geometries of 2D clusters. Three regions can be easily identified based on the bipolarons radius. (a) Region I, $t/J_p < 0.3$(1D) and 0.1(2D) small inter-site bipolaron of size strictly of the order of one lattice spacing. (b) Region II, $0.3 \leq t/J_p \leq 0.52$ (1D) and $0.15 \leq t/J_p \leq 0.2$ (2D) marks the transition region from small inter-site bipolaron to large bipolaron. (c) Region III, $t/J_p > 0.52$(1D) and 0.2(2D) polarons are distant apart depending on lattice size and dimension−large bipolarons or nearly free polarons. The formation of similar stable bipolarons has also been observed recently considering Coulomb repulsion and ions oscillations using a 1D continuum model [34], in contrast to our discrete model. They have shown that stable translation-invariant bipolarons exist below a certain critical strength of interactions.

Mobile bipolarons are one of the important parameters for the existence of superconductivity [35]. In Fig. 4(a), we plot the energy dispersion of bipolaron for different t/J_p. Effective mass is calculated from the graphical analysis of Fig. 4(a) and using Eq. (9). Bipolaron to polaron effective mass as a function of the ratio t/J_p is shown in Fig. 4(b). It is immediate from the graph that $m^*_{bi} \sim 2m^*_p$ in the region $t/J_p \sim 0.3$. The variation of bipolaron kinetic energy with t/J_p (Fig. 4(c)) in 1D shows that kinetic energy of the bipolarons follow a nearly parabolic form in the range $0 < t/J_p < 0.5$, with a maximum at $t/J_p = 0.3$. For $t/J_p \geq 0.5$ the kinetic energy of the bipolarons are negligible. At small t/J_p, the contribution to the polaron hopping amplitude is mainly due to the motion of the polaron pairs (bipolarons), while for large t/J_p, the contribution arises only from single-particle hopping processes. As long as the inter-site bipolarons exist ($t/J_p \leq 0.52$), they move in the lattice independently and indicate conductivity. Strong bipolaron hopping kinetic energy at the vicinity of $t/J_p \sim 0.3$ and $m^*_{bi} \sim 2m^*_p$ in that region signals small, light and mobile bipolarons, suggests the existence of a possible superconducting phase around $t/J_p \sim 0.3$.

At region I, due to the extreme strong EP coupling ($t \ll J_p$), the bare hopping is largely reduced by strong exchange interaction and helps the formation of two-particle bound states, resulting in the formation of NN bipolarons. With the increase of motion of the polarons, the polarons at NN positions tend to move at distant sites which correspond to the increase in correlation at larger distances and hence, an increase in bipolaron size. This corresponds to Region II. In other words, it can be argued that region II hopping leads to coherent propagation of static configuration. However, for large t/J_p, the polarons are separated at a

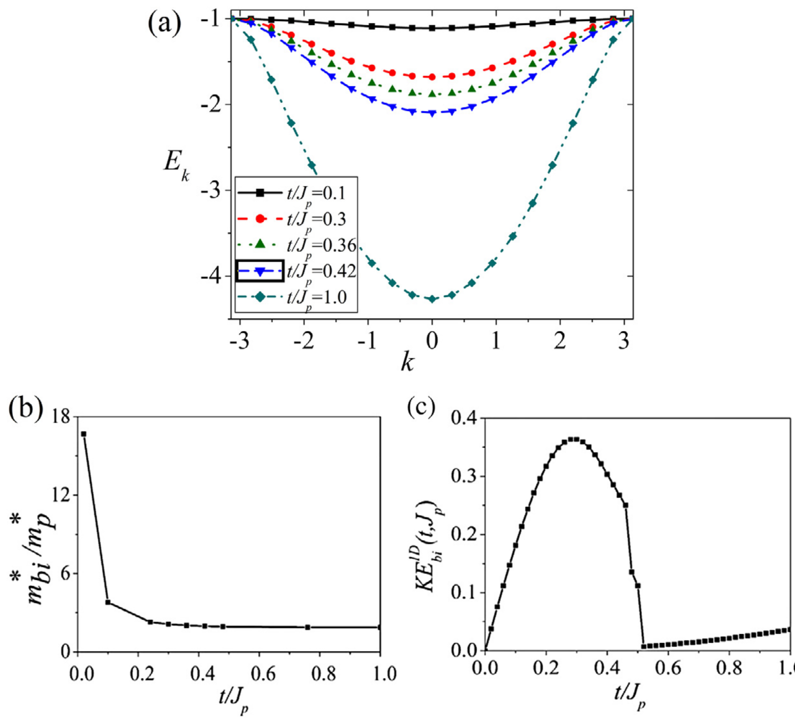

Fig. 4. (a) Energy dispersion for bipolaron in linear chain ($L = 18$) for different values of t/J_p. (b) Ratio of bipolaron to polaron effective mass as function of the ratio t/J_p (c) NN bipolaron kinetic energy w.r.t. t/J_p.

maximum permissible distance depending on the lattice size, leading to the constant size. Contrary to the results of the 18- and 26-site cluster, the bipolaron size decreases slightly above the critical value for a 2D 10 site cluster. This result may be due to the confinement of the polarons in a very small region, which largely affects the results. Moreover, small bipolarons are perfectly mobile for small t/J_p in both the geometry.

4.3. 4-particle case

We now present results for 4-particles in an 18-site lattice linear chain only. Since the linear dimension of a square is very small, even for an 18-, 26-site cluster, results for four-particles may not be reliable enough and hence are not presented. At $t/J_p = 0.0$, the ground state is exactly $-2J_p$ i.e. twice the ground state energy for 2-particle systems, in agreement with analytical results.

Figs. 5(a) and 5(b) shows the probability of finding two polarons. Fig. 5(a) clearly indicate that for all $t/J_p \leq 0.4$, maximum probability of finding two anti-parallel polarons are at $|i-j| = a$, small finite probabilities for $|i-j| = 4a, 5a, 6a$. The correlation at $|i-j| = a$ decrease with t/J_p. At $t \sim J_p$, the antiparallel correlation at all distances is finite and is nearly equal, which shows that the polarons to be uniformly distributed in the lattice. However, for parallel spin a small but dominating correlation is observed for $|i-j| = 4a, 5a, 6a$ for $t \ll J_p$. A strong correlation at NN sites for anti-parallel spin confirms the formation of only NN site singlet bipolarons. No triplet NN site bipolarons are formed. The long-distance correlations for an 18-site linear chain can be better explained with Figs. 6(a) and 6(b), where we have shown a schematic diagram for the most probable distribution of the polarons in the chain for small t/J_p. Though other configurations are possible they are less probable and hence not shown here. Dominating NN site correlation with small correlation at other $|i-j| = 4a, 5a, 6a$ suggest the formation of two singlet NN site bipolarons separated by a large distance.

We now study the nature of pairing of the NN site bipolarons by calculating on-site and inter-site singlet pair correlation function (s-wave and d-wave for 2D and we use this notation by brevity) pairing

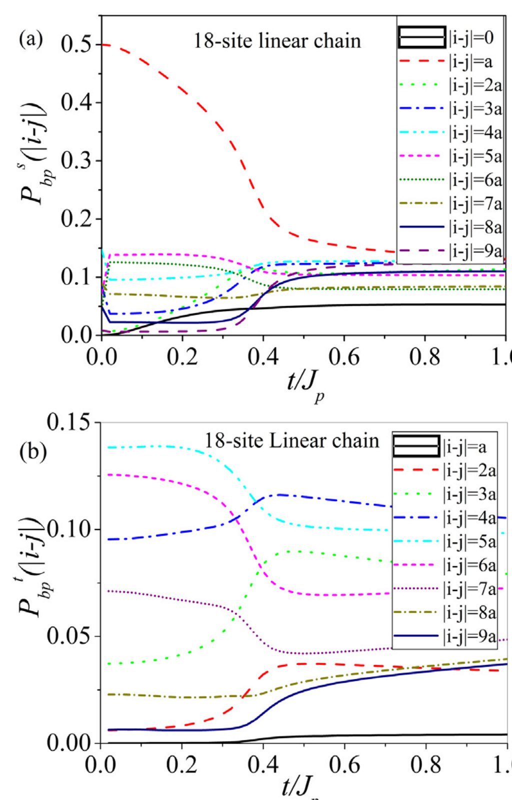

Fig. 5. Probabilities of finding two polarons at different lattice distance for different hopping strength in 18-site, 4 polarons. (a) Anti-parallel spin (b) parallel spin.

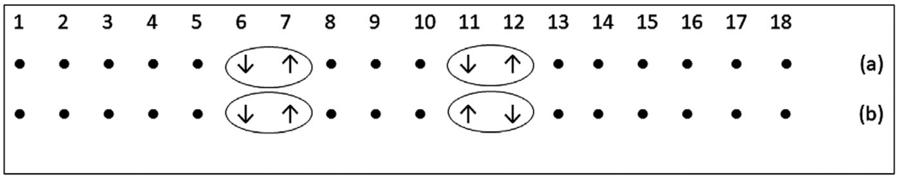

Fig. 6. Schematic probable polaronic positions based on correlation function in 1D (a) and (b). Another similar set can be identified by replacing ↑ by ↓ and vice versa.

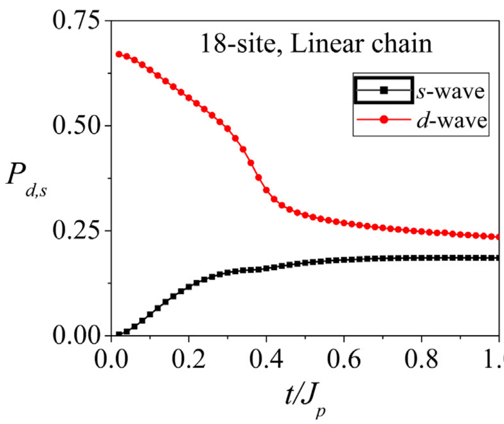

Fig. 7. s-wave and d-wave pairing correlation function versus t/J_p for 18-site linear chain with four polarons.

correlations and is shown in Fig. 7. Results indicate that for linear chain and $t \ll J_p$, the $d-$wave correlation is dominant with a negligible s-wave correlation. With an increase of polaron mobility d-wave pairing correlation decreases whereas s-wave correlation increases. At $t \sim J_p$, both d- and s-wave pairing correlation are finite with d-wave dominating most. Clearly, at the region of existence of NN-site singlet bipolarons ($t/J_p \leq 0.5$), the pairing is strongly in the $d-$ wave channel. The presence of the pairing of polarons in the d-wave channel suggests the existence of a superconducting phase.

Finally, we plot the binding energy of two bipolarons Δ_4 in Fig. 8(a), which is an important probe to determine the formation of bipolaron pairs — a bipolaron composite. Here we have calculated E_0^2 and E_0^4 on an 18-site chain, such that the boundary condition for both E_0^n's remains the same. Results show for small to an intermediate value of t/J_p the bipolaron–bipolarons binding energy is negative, suggesting pair formation of the bipolarons – bipolaron composite for an 18-site linear chain. Also, it is evident that Δ_4 is much smaller than the bipolaron binding energy J_p. As the small bipolarons move there is a small overlapping between them, leading to a small attractive interaction forming bipolaron composite. This attraction may lead to Bose–Einstein Condensation at low temperature which may eventually lead to superconductivity. In the 1D continuum model [34], similar existence of superconducting phase due to Bose–Einstein condensation of translation-invariant bipolarons was reported. The schematic diagram for the bonding and antibonding of bipolaron pairs is shown in Figs. 8(b) and 8(c). Since two parallel polarons at neighboring sites do not exist as evident from the $p-p$ correlation function, it leads to antibonding and is repulsive. However, an attraction may exist between two bipolarons if they have the configuration shown in figure 8(b) due to virtual pairing via antiparallel alignment of the NN site polarons (shown in dashed oval). This leads to a negative bipolaron-bipolaron binding energy, forming bipolaron composite. With the increase of mobility of polarons, the polarons are far apart with a breakdown of bipolarons and bipolaron pairs.

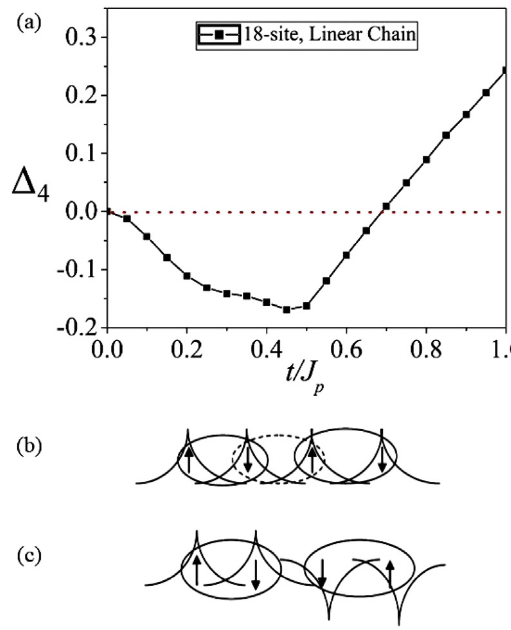

Fig. 8. Binding energy of two bipolarons versus t/J_p (b) Bonding between two bipolarons (c) Anti-bonding between two bipolarons.

5. Conclusion

In conclusion, our study of the $t-J_p$ model identifies the parameter ranges for the formation of small and large bipolarons in both 1D and 2D. The transition from small inter-site to large bipolarons or nearly free polarons are identifiable. For the two-particle system, the ground state is a bipolaronic singlet. For a small (t/J_p) polarons predominantly occupy the nearest-neighbor position for all particle density and all geometry. With the increase in the t/J_p ratio they tend to be separated at the maximum distance determined by the dimension of the lattice. The crossover from small to large bipolaron is independent of system size but depends on the cluster geometry. From the bipolaron effective mass and the kinetic energy calculation, we can conclude that at small $t/J_p(\sim 0.3)$, light and small bipolarons are perfectly mobile but for greater polaronic hopping amplitude small bipolarons breakup and the motion is a single particle process. The mobile bipolarons and their pairing in the $d-$wave channel suggest the existence of a superconducting phase. The most stable superconducting phase may emerge at the vicinity of $t/J_p \sim 0.3$. We have shown that there is the formation of bipolarons composite in the parameter range $0 < t/J_p < 0.5$ with small binding energy. This small attraction between bipolarons may lead to Bose–Einstein Condensation at low temperature which may eventually lead to superconductivity.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.physb.2019.411881.

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