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1993 J. Phys.: Condens. Matter 5 3565

(http://iopscience.iop.org/0953-8984/5/22/008)

J. Phys.: Condens. Matter 5 (1993) 3565–3572. Printed in the UK

The phase diagram of the 2D Holstein–t–J model near half filling

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Received 11 December 1993

Abstract. We have used an exact diagonalization technique to explore the ground-state phase diagram of the two-dimensional Holstein–t–J model near half filling. The nature of the ground state is analysed, calculating self consistently the local lattice distortions, on-site spin and charge densities, as well as the magnetic structure form factor. We demonstrate that doped holes tend to form hole-polaron or bipolaron states. Compared to that in the uncorrelated model (spinless fermions), the critical electron–phonon coupling strength for the self-trapping transition of the doped charge carriers is considerably reduced by the antiferromagnetic exchange interaction. The relevance to the cuprate superconductors is discussed.

The importance of both strong antiferromagnetic Coulomb correlations [1] and strong electron–phonon (EP) interactions [2] has become increasingly recognized as being essential in understanding the superconducting and the unusual 'normal' state properties of high-T_c materials. Recent ion channelling [3] and neutron scattering [4] experiments give evidence for large anharmonic lattice fluctuations in several of the cuprates, where the coupling of the so-called apical 'breathing' modes to the in-plane electron system leads to local (rather than global) phonon-driven charge instabilities. Photoinduced absorption measurements in $La_{2-x}Sr_xCuO_{4-\delta}$ and $YBa_2Cu_3O_{7-\delta}$ are also an indication that a self-localized structural distortion is present around the doped charge carriers [5]. Based on these experimental findings the existence of polaronic or bipolaronic electronic states was heavily debated [6], where in the cuprate superconductors the (bi)polarons were expected to be rather 'large' [7–9].

The theoretical difficulties result from the fact that at low doping level the high-T_c systems are close to an antiferromagnetic Mott insulating state [10], i.e. we are faced with the question of how the EP effects are influenced by the strong electronic correlations. Zhong and Schüttler [11, 12] pointed out that an enhanced tendency towards polaron formation can be understood as a consequence of a pre-existing self-localization of the charge carriers due to their interaction with the antiferromagnetic fluctuating Cu^{2+}-spin background. On the other hand, the EP coupling may lead to a polaronic narrowing of the effective bandwidth and might, therefore, drive the system further into the strongly correlated regime [9]. Let us emphasize at this point that the investigation of such strongly coupled EP systems is of fundamental importance, not only in connection with high-T_c copper oxides. There are other long-standing problems which have attracted renewed attention, e.g. the dynamics of the self-trapping transition [13], or the commensurate–incommensurate phase transitions in low-dimensional charge-density-wave (CDW) systems such as the MX chain compounds [14].

0953-8984/93/223565+08$07.50

In order to address some of these issues from a microscopic point of view, in this paper we will study the two-dimensional (2D) t–J model with additional Holstein-type [15] EP interaction in the adiabatic limit by means of a Lanczos diagonalization method. First exact results for the ground state of the single-hole Holstein–t–J model have recently been obtained by the authors [16] on finite lattices up to 18 effective sites at a few characteristic coupling strengths. Here, we restrict the size of the model to the tilted $\sqrt{10} \times \sqrt{10}$ lattice with periodic boundary conditions (cf. figure 1(a)) in order to map out the *complete* phase diagram of the Holstein–t–J model with *one* and *two* holes. Of course, we have checked with the 16- and 18-site lattice that the qualitative features of the following results remain unchanged.

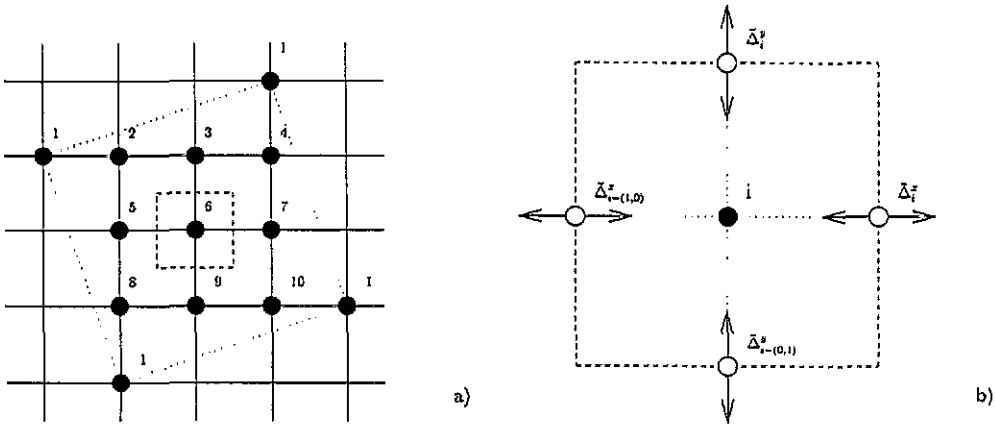

Figure 1. (a) The tilted effective ten-site cluster used in this work, where periodic boundary conditions are applied at the dotted lines. (b) Definition of the harmonic lattice distortions $\Delta_i^{x,y}$ for a single CuO_4 unit (cf. the broken square in (a)). The filled and open circles represent copper and oxygen respectively.

The Holstein–t–J system is defined by the Hamiltonian

$$\mathcal{H} = -t \sum_{\langle ij \rangle, \sigma} \left(\tilde{c}_{i,\sigma}^{\dagger} \tilde{c}_{j,\sigma} + \mathrm{HC} \right) + J \sum_{\langle ij \rangle} \left(\boldsymbol{S}_i \cdot \boldsymbol{S}_j - \frac{n_i n_j}{4} \right) - \sum_i \Delta_i n_i + \frac{1}{2\lambda} \sum_i \left(\left(\Delta_i^x \right)^2 + \left(\Delta_i^y \right)^2 \right) \tag{1}$$

where $\boldsymbol{S}_i = \frac{1}{2} \sum_{\alpha,\beta} \tilde{c}_{i,\alpha}^{\dagger} \boldsymbol{\sigma}_{\alpha\beta} \tilde{c}_{i,\beta}$, $n_i = n_{i,\uparrow} + n_{i,\downarrow}$, and $n_{i,\sigma} = \tilde{c}_{i,\sigma}^{\dagger} \tilde{c}_{i,\sigma}$. The first two terms represent the standard t–J model acting in a projected Hilbert space without double occupancy, where the operator $\tilde{c}_{i,\sigma}^{(\dagger)} = c_{i,\sigma}^{(\dagger)}(1 - n_{i,-\sigma})$ annihilates (creates) a spin σ electron in a Wannier state at site i. J measures the antiferromagnetic exchange interaction, and the transfer amplitude t is restricted to nearest-neighbour hopping processes $\langle ij \rangle$ on an effective square lattice. The third and fourth terms take into account the coupling of a single dispersionless optical phonon branch to the electronic on-site energy and the elastic energy of a harmonic lattice, respectively. Those terms are treated within the adiabatic approximation. In the context of the copper oxides, the local Holstein coordinates $\{\Delta_i\}$ correspond to bond-parallel oxygen lattice displacements according to an in-plane oxygen

breathing mode, i.e. the Δ_i can be interpreted as an internal optical degree of freedom of the effective lattice site $i = (i_x, i_y)$ (see figure 1(*b*)). In this case, one has

$$\Delta_i = \Delta_i^x - \Delta_{i-(1,0)}^x + \Delta_i^y - \Delta_{i-(0,1)}^y \tag{2}$$

where we have rescaled $\alpha\bar{\Delta}_i^{x,y} = \Delta_i^{x,y}$ introducing in equation (1) the dimensionless EP coupling constant $\lambda = \alpha^2/K$ (α and K denote the bare EP interaction strength and the restoring force constant, respectively). In the numerical work all energies and interaction constants are measured in units of the hopping integral t. The model (1) could be easily extended to the inclusion of out-of-plane oxygen breathing modes [11, 12]. Based on Hartree–Fock [17], slave boson [18, 19] and quantum Monte Carlo [20] calculations, the EP coupling we adopt has been frequently used to investigate the instability of the Holstein–Hubbard model against static lattice distortions due to frozen-in phonon modes. However, the physics of the Holstein–Hubbard model is dominated by a (π, π) CDW instability (near half filling and at not too large Hubbard interaction U) [17, 19]. In contrast, the CDW state becomes suppressed in the Holstein–t–J model at least at the low doping level [9, 16]. Therefore in our model the phonon system is mainly coupled to the doped charge carriers (holes) and as a result we expect the formation of local lattice distortions, such as hole–(bi)polarons.

In order to investigate the ground-state properties of the Holstein–t–J model we adopt a modified Lanczos diagonalization technique [21] in the subspace of fixed hole number $N_h = 1$ ($N_h = 2$) and minimal total $S^z = \frac{1}{2}$ ($S^z = 0$). Starting with a random configuration $\{\Delta_i^{x,y}\}$ we calculate via the exact ground-state function $|\Psi(\{\Delta_i^{x,y}\})\rangle$ the local particle densities $\langle n_i\rangle \equiv \langle\Psi(\{\Delta_i^{x,y}\})|n_i|\Psi(\{\Delta^{x,y}\})\rangle$. According to Feynman's theorem, $\partial_{\Delta_i^{x,y}}\langle\Psi(\{\Delta_i^{x,y}\})|\mathcal{H}|\Psi(\{\Delta_i^{x,y}\})\rangle = 0$, we can solve in the next step the $2N$ self-consistency equations $\Delta_i^{x,y} = \lambda(\langle n_i\rangle - \langle n_{i+(x,y)}\rangle)$ to determine the new set of $\{\Delta_i^{x,y}\}$. For typical cases studied, less than 50 iteration loops, with 5 to 100 Lanczos steps, are necessary to obtain the lattice distortions $\{\Delta_i^{x,y}\}$ and the ground-state energy $E \equiv E(\{\Delta_i^{x,y}\})$ with a relative error less than 10^{-6}. Let us emphasize that the free variation of the effective 'on-site potentials' Δ_i in general breaks the translational symmetry of our system, i.e. for a rigorous diagonalization of the $\mathcal{H}$ matrix we have to work with an unsymmetrized basis set of many particle states.

To explore the nature of the ground state we calculate the ground-state energy E, the local expectation values of spin ($\langle S_i^z\rangle$) and charge ($\langle n_i\rangle$) density, the local lattice distortions Δ_i as well as the 'averaged' displacement $\Delta = \frac{1}{N}\sum_{i=1}^{n}|\Delta_i|$. The quantity Δ plays the role of an 'order' parameter separating hole-states with finite lattice distortion ($\Delta \neq 0$) from uniform states ($\Delta = 0$). In addition, we compute the (equal-time) spin correlation functions $\langle S_i^z S_j^z\rangle$ and the (Fourier-transformed) magnetic structure function

$$S(q, q') = \frac{1}{N}\sum_{i,j}\langle S_i^z S_j^z\rangle e^{iq\cdot(R_i - R_j)}\, e^{i(q+q')\cdot R_j} \tag{3}$$

to discuss the spin order of the system in more detail. As pointed out recently [16], the magnetic form factor, $S(Q) \equiv S(Q, -Q)$ at $Q = (\pi, \pi)$, can be used to characterize the self-trapping transition between 'delocalized' and 'localized' hole states in the Holstein–t–J model.

Let us now present our numerical results for the ground-state phase diagram of the Holstein–t–J model. We start with the case of one hole, for which the phase diagram is shown in figure 2 in a λ versus $4/J$ diagram (because J can be related via $J = 4/U$

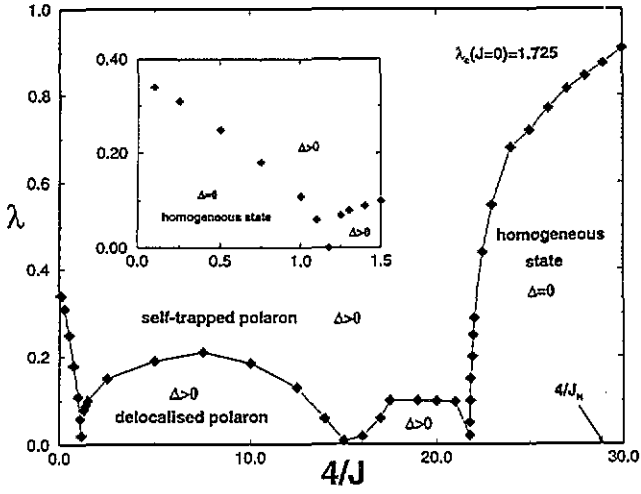

Figure 2. Phase diagram of the 2D Holstein–t–J model with one hole on an $N = \sqrt{10} \times \sqrt{10}$ lattice. The inset shows an enlargement of the region with strong antiferromagnetic exchange coupling J.

to a large-U expansion of the Hubbard model). We can distinguish two main regimes, referred to below as the self-trapped or 'localized' polaronic state and the 'delocalized' state, respectively. In the delocalized phase for small λ the occurrence of finite lattice distortions depends on the symmetry of the ground state of the pure ($\lambda = 0$) t–J model. If this ground state carries a finite momentum, the lattice is forced into a structure which is compatible with the non-trivial symmetry of the electronic wave function. Since in the physically most interesting regime of J the existence of a so-called pocket-like hole Fermi surface for the infinite system is still a matter of debate, this point is in not an academic one. The ground-state properties of the pure t–J model were studied by several authors for finite clusters up to 20 sites (cf. [21–23] and references therein). For the ten-site lattice, momentum k and total spin S of the lowest-energy state depend on the magnitude of $U = 4/J$ [24].

Obviously, the delocalized state reflects the transitions between states with non-trivial k values and an inhomogeneous electron density (here $\Delta \neq 0$ is possible) and a uniform phase, where $k = (0,0)$ or (π, π) and $\Delta = 0$. The same qualitative behaviour was found for the 16- and 18-site lattices [16], but of course, the location of the transition to the homogeneous undistorted phase is strongly finite size dependent.

In the delocalized state with finite Δ we observe at the largest possible distance *two* 'hole sites' which correspond to the translational symmetry of the ground state (see table 1). In fact, the charge density fluctuations are rather small. The spin density, on the other hand, is mainly concentrated at the hole-sites; here we find for $4/J = 0.8$ and $\lambda = 0.1$ $\langle S_i^z \rangle = 0.408$ ($i = 1,6$), whereas $\langle S_i^z \rangle = 0.023$ at the electron sites ($i \neq 1,6$). The nearest-neighbour spin correlations ($\langle S_i^z S_j^z \rangle < 0$) indicate antiferromagnetic short-range order $\forall \langle ij \rangle$. Increasing the EP coupling λ at fixed J a self-trapping transition of the hole takes place. At λ_c, $E(\lambda)$ shows a discontinuity in slope and the order parameter Δ jumps by a finite amount reflecting the fact that the distribution of $\langle n_i \rangle$, $\langle S_i^z \rangle$, and $\langle S_i^z S_j^z \rangle$ are different in both phases. As a result we found a numerical hysteresis, so one must carefully scan the $J - \lambda$ plane to find the true ground state. For large λ a strong lattice distortion can trap the hole at a *single* site. As can be seen from table 1 this leads to a substantial energy gain in $E_{\mathrm{el-ph}}$, therefore E is lowered despite the cost of elastic and kinetic energy. The variation of the $\langle n_i \rangle$ shows that the hole trapping is accompanied by the occurrence of weak charge-density oscillations on the other sites which are reminiscent of a (π, π) CDW. At the same time we observe a significant

Table 1. Total energy E, 'order parameter' Δ and local electron densities $\langle n_i \rangle$ for the ground state of the 2D Holstein–t–J model at $J = 0.8$. The results are given for one and two holes on a $\sqrt{10} \times \sqrt{10}$ lattice with periodic boundary conditions at characteristic electron–phonon coupling strengths λ. The electron, electron–phonon lattice contributions to the ground-state energy are denoted by E_{el}, E_{el-ph} and E_{ph}, respectively.

	$N_h = 1$		$N_h = 2$		
	$\lambda = 0.1$	$\lambda = 0.8$	$\lambda = 0.1$	$\lambda = 0.4$	$\lambda = 0.8$
E	−9.636475	−10.215938	−9.943565	−10.085228	−10.862362
E_{el}	−9.617787	− 9.121160	−9.934587	− 9.776897	− 8.586801
E_{el-ph}	−0.037374	− 2.189556	−0.017956	− 0.616663	− 4.551123
E_{ph}	0.018687	1.094778	0.008978	0.308331	2.275561
Δ	0.034583	0.528328	0.029358	0.238035	1.079392
$\langle n_i \rangle$ $i =$ 1	0.727084	0.141692	0.726424	0.382280	0.125380
2	0.943229	0.967205	0.848930	0.878186	0.968655
3	0.943229	0.997542	0.848930	0.787186	0.968655
4	0.943229	0.967205	0.726424	0.382280	0.968655
5	0.943229	0.997542	0.848930	0.878186	0.968655
6	0.727084	0.999321	0.726424	0.983162	0.125380
7	0.943229	0.997542	0.848930	0.878186	0.968655
8	0.943229	0.967205	0.848930	0.878186	0.968655
9	0.943229	0.997542	0.726424	0.983162	0.968655
10	0.943229	0.967205	0.848930	0.878186	0.968655

change in the local spin correlations $\langle S_i^z S_j^z \rangle$. Whereas the local moment on the hole site is coupled ferromagnetically to nearest-neighbour moments indicating the formation of a small ferromagnetic polaron, the antiferromagnetic correlations in the spin background become strongly enhanced. Note that now $|\langle S^z_{\text{el-sites}} \rangle| \gg |\langle S^z_{\text{h-site}} \rangle|$.

To discuss the effect of the electronic correlations on the self-trapping transition, we have considered the case of spinless fermions ($S^z = S^z_{\max}$) as well. For the one-hole case this can be mimicked by setting $J = 0$ (Nagaoka limit). Here we obtain a much larger critical λ, where the transition values $\lambda_c = 1.725$ ($N = 10$) (cf. $\lambda_c = 1.750$ ($N = 18$), 1.751 ($N = 20$) [16]) indicate a rather small finite size dependence. In addition, it is interesting to note that the hole (or equivalently one electron) is not perfectly localized even at very large λ. Away from the hole site, a small 'rest' of the hole (electron) density oscillates even in this limit in a way which corresponds to a (π, π) CDW [16].

The phase diagram for the two-hole case is displayed in figure 3. First let us report the results at $\lambda = 0$. Here, for $4/J \leqslant 19.88$, the lowest energy state is $S = 0$ and fivefold degenerate, the momentum being one of the star of $\boldsymbol{k} = (0, 0), (2\pi/5, 4\pi/5)$. In the region $4/J \geqslant 19.88$, the ground state is taken over by a state with $S = 0$ and $\boldsymbol{k} = (0,0)$. At finite EP coupling, we can distinguish again between a phase where holes are delocalized, and a self-trapped state. Depending on the relative strengths of exchange interaction and EP coupling, the holes will be trapped, for large enough λ, as two single polarons or as one bipolaron. In the context of the Holstein–t–J model (remember that double occupancy is strictly forbidden), we use the term 'bipolaron' for the state where the two holes are 'located' at adjacent sites sharing the same lattice distortion. There is a naive argument suggesting that different types of self-trapped states will exist: two separate immobile polarons lose the antiferromagnetic exchange energy $2J$ on four bonds each, but can gain maximal trapping energy ($\sim E_{el-ph}$). On the other hand, two holes on neighbouring sites lose the exchange energy on only seven bonds together; however, one displacement (e.g. $\Delta^x_{i-(1,0)}$) does not

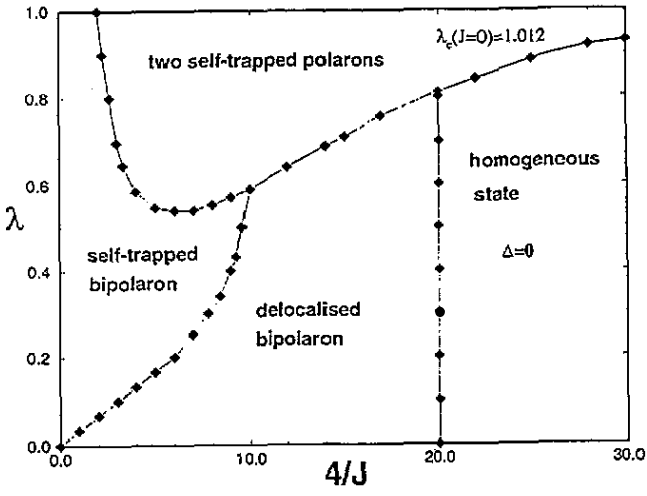

Figure 3. Ground-state phase diagram of the Holstein–t–J model with two doped holes.

contribute to $E_{\mathrm{el-ph}}$ now. The net result, including the effect of delocalization energy, gives the phase boundary shown in figure 3. In the delocalized regime, we obtain at intermediate values of J a state with finite Δ, referred to as a 'delocalized' bipolaron. Here the hole density is mainly concentrated at four sites, where two sites are always nearest neighbours. The particle densities are given for the different regimes in table 1. The transitions between delocalized and localized states are of first order. At $J = 0$, the self-trapping transition occurs at $\lambda_c = 1.01$, where the polaronic state carries maximal total spin $S = S_{\max}$. For any finite value of J, however, the ground state has $S = 0$.

Of special interest may be question of whether the EP coupling enhances the binding energy between the holes. We have therefore calculated the two-hole binding energy defined as usual by $E_B^2(\lambda) = E_2 + E_0 - 2E_1$ (the lower indices denote the hole-numbers). With the exception of a small extreme region ($J \gg 1 \gg \lambda$, where the one-hole state becomes homogeneous), the hole binding in the Holstein–t–J model was weakened as λ increases; e.g. at $4/J = 5$, we found $E_B^2(0) = -0.5378$, $E_B^2(0.05) = -0.5245$, $E_B^2(0.2) = -0.48979$, and $E_B^2(0.8) = -0.2707$. Of course, to make reasonable predictions concerning the tendency towards hole-pairing, one has to take into account the phonon dynamics.

It is very instructive to investigate the behaviour of the magnetic structure factor $S(\boldsymbol{Q})$, which for the pure t–J model exhibits a pronounced peak structure in the vicinity of the antiferromagnetic wave vector $\boldsymbol{Q} = (\pi, \pi)$ [25]. In our finite-cluster calculation we are restricted to the allowed discrete $\boldsymbol{q}$ vectors of the $\sqrt{10} \times \sqrt{10}$ lattice. In addition, the lack of full translational invariance means that $S(\boldsymbol{q}, \boldsymbol{q}')$ will in general depend on two momenta. Thus, we are only able to study the case $\boldsymbol{Q} = (\pi, \pi)$. Our results, presented in figure 4 for $S(\pi, \pi)$ and $E(\lambda)$, clearly indicate a different nature of the hole states in the various phases. Increasing λ at fixed $4/J = 5$, the smooth variation of $S(\pi, \pi)$ in the delocalized 'phase' is followed by a jump-like enhancement at the self-trapping transition and a much stronger variation in the bipolaronic state. At still larger EP coupling strength a further first-order transition to the self-trapped polaronic state takes place. Obviously, the hole-trapping favours an antiferromagnetic ordering of the spin background and vice versa. As mentioned above, depending on the ratio of J/λ a ground state with two well-separated small polarons or with a self-trapped bipolaron (i.e. a 'hole-cluster') gives the lowest energy (cf. table 1). This result should be contrasted with the situation for the Holstein–Hubbard model [12], where strong EP coupling favours *on-site* bipolaronic CDW order.

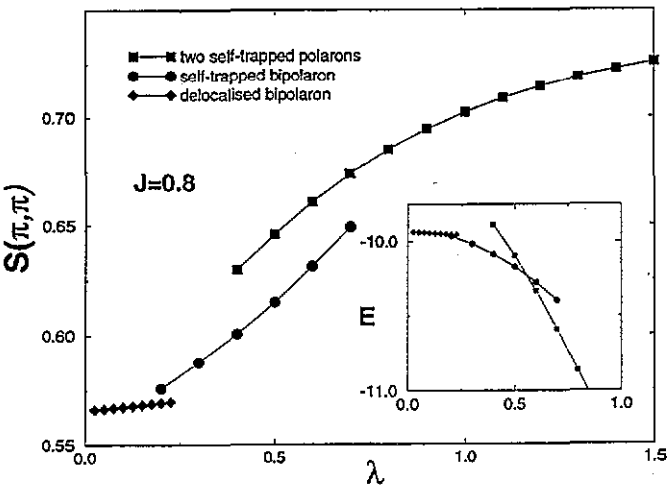

Figure 4. Magnetic structure factor $S(\pi, \pi)$ and ground-state energy E (inset) as a function of electron–phonon coupling strength λ at $J = 0.8$. For further explanation see text.

Summarizing, this paper aims to address the physics of electron–phonon coupling in strongly correlated electron systems via exact Lanczos diagonalization of the adiabatic Holstein–t–J model on a finite lattice near half filling. We have calculated for the first time the complete ground-state phase diagram as a function of EP coupling and antiferromagnetic exchange interaction strength. The Holstein–t–J model exhibits two competing ground states. For weak EP interaction one observes a rather 'delocalized' nature of the doped holes. Here the ground state reflects the symmetry of the pure t–J model (but note that a finite Δ is possible). In contrast in the strong-coupling regime large local lattice distortions cause mainly 'localized' (self-trapped) hole states, i.e. in this limit the electronic properties are dominated by lattice effects. However, our results for spin and charge densities or for the magnetic structure factor indicate a subtle interplay between electron–electron and EP interactions. In accordance with previous findings for the nearly half-filled Holstein–Hubbard model [12], we demonstrated that antiferromagnetic spin correlations can strongly enhance the probability for hole-polaron or bipolaron formation. The physical reason for this tendency is the reduced effective quasiparticle-bandwidth for the charge carriers in the t–J model (i.e. a pre-existing self-localization). As a result, compared to the (uncorrelated) case of spinless fermions, the critical EP coupling strength for the first-order self-trapping transition becomes substantially weakened by the electronic spin interaction. In agreement with recent experimental [3–5] and theoretical evidence [6, 7, 9, 11, 12], our findings point towards the importance of polaronic effects at least in the normal phase of the doped cuprates.

Acknowledgments

We would like to acknowledge useful discussions with M Deeg, D Ihle, H-B Schüttler and V Waas.

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