Ferromagnetic polarons in a one-dimensional t-J model with next-nearest-neighbor hopping

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In a t-J model on a chain, an additional next-nearest-neighbor hopping term destroys the complete spin-charge separation at $J/t \ll 1$ and induces the formation of stable spin-polarized $S > 0$ states. The properties of a single ferromagnetic polaron are investigated by the exact diagonalization of small systems and by the approximative treatment of an effective model, describing a spinless fermion coupled to the spin background. Both methods give consistent results on the critical J_c for the polaron formation on the increase of the spin S and the polaron size with decreasing J. A very large enhancement of the polaron mass with increasing S is observed. Systems with a finite concentration of holes are also studied within the same framework. Analytical considerations indicate on the bound many-hole states and consequently on phase-separated regions in the phase diagram.

I. INTRODUCTION

One-dimensional models of strongly correlated systems have recently attracted considerable attention. The increased theoretical efforts in this direction are due to the possible relevance of one-dimensional ($d = 1$) results and related ideas[1] for strongly correlated electrons in layered copper-oxide-based superconductors.

In particular, a number of papers have been devoted to the exactly solvable $d = 1$ Hubbard model[2,3] with large Coulomb repulsion U, represented also by the t-J model. An attractive, but specific feature of the latter model at $J/t \ll 1$ is the separation of charge and spin degrees of freedom in the entire energy range,[4] which leads also to a large spin degeneracy of the ground state at $J = 0$. On the other hand, this phenomenon is not present in planar and higher-dimensional systems, at least not in some better understood regimes. The well known example is the ferromagnetically (FM) polarized ground state of a single hole added to the half-filled band in the $U = \infty$ Hubbard model, i.e., in the t-J model with $J = 0$, as shown by Nagaoka[5] for certain lattices. Apart from this statement, other aspects are less clear. The question of the possible existence of the FM state for a larger number of holes[6] and at finite hole concentrations,[7] cannot be considered as settled. Related is a recent claim of the phase separation[8] in the same regime. Even the simpler problem of a single FM polaron at finite $J > 0$ is understood only very crudely, in spite of quite numerous studies of FM polarons in magnetic semiconductors.[9,10]

Recently, it has been recognized[11] that even in a t-J model on a chain the charge-spin coupling and the FM polarized states can be induced by the next-nearest-neighbor hopping term, investigated before also in planar systems.[12,13] In the following we consider the corresponding extension of the usual t-J model,

$$H = -t\sum_{is}(c^{\dagger}_{i,s}c_{i+1,s} + \text{H.c.}) - t'\sum_{is}(c^{\dagger}_{i,s}c_{i+2,s} + \text{H.c.}) + J\sum_{i}\mathbf{S}_i \cdot \mathbf{S}_{i+1}, \tag{1.1}$$

describing the nearest-neighbor (t) and next-nearest-neighbor (t') hopping of fermions in the presence of empty sites in the Heisenberg spin system, represented by spin operators $\mathbf{S}_i = \frac{1}{2}\sum_{ss'}\boldsymbol{\sigma}_{ss'}c^{\dagger}_{is}c_{is'}$. Here, $c^{\dagger}_{is}, c_{is}$ are projected fermion operators, not allowing for a double occupation of sites.

The limiting case $t' = 0, J = 0$ represents in $d = 1$ the marginal situation where the ground state is degenerate with respect to the spin S. Any $t' \neq 0$ lifts the degeneracy and (at least for a single hole) $t' < 0$ stabilizes the fully saturated FM (Nagaoka) state with maximum S. The single-hole ground state at large $J > 0$ still has the smallest possible S. So we can follow, e.g., by the exact diagonalization of short chains, the evolution of the FM polaron on decreasing J at fixed t'. Due to restrictions on the size this has so far not been possible in the exact diagonalization studies of $d = 2$ systems.[14,15] Namely, numerical results (mainly on 4×4 lattice) show an abrupt jump from the smallest spin ($S = \frac{1}{2}$) to $S_{\max}$, which is clearly not expected in a large system. Much bigger linear extensions can be studied exactly in a $d = 1$ system, which allows for a quantitative study of FM polarons.

Our aim is also to introduce an analytical approach, based on the charge-spin separation at $t' = 0$. The latter gives even a quantitative agreement with the exact diagonalization results on single-polaron properties. In addition, the method allows the treatment of the many-hole case. We can thus discuss the hole binding and the instabilities towards the phase separation. In Sec. II we derive the effective model of spinless fermions coupled to a Heisenberg spin subsystem. The problem of a single polaron can be then adequately treated within the conventional classical spin approximation.[9,10] Within this approach we evaluate the size and the spin of the FM polaron and show that similar results are obtained even within the simplified continuum approximation. Section III is devoted to the presentation of results obtained by the exact diagonalization of chains with up to 19 sites. In Sec. IV many-hole states are studied analytically within the effective model, in particular with respect to

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the phase-separated region and other possible phases at $J/t \ll 1$.

II. EFFECTIVE MODEL

The t-t'-J model (1.1) in its original representation is not suitable for analytical approximations. We therefore employ the idea of the charge-spin separation, valid at $t' = 0$ and $J/t \ll 1$. It has been shown[4] that the exact Bethe-ansatz wave function for the Hubbard chain at $U/t \gg 1$ can be expressed as a product of wave functions corresponding to spinless fermions and spins as in a Heisenberg spin chain, respectively. This holds as well for the t-J model at $J/t \ll 1$. Still, both degrees of freedom — charge and spin — cannot be considered as entirely decoupled due to delicate relations between spin and fermion coordinates.

At least for a single hole added to the half-filled band, we can rewrite the statement of the charge-spin separation at $t' = 0$ as an effective model

$$H_0 = -t \sum_j (a_j^\dagger a_{j+1} + \text{H.c.}) + J \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1}, \tag{2.1}$$

where j counts only occupied sites (with spins), while operators $a_j^\dagger$ (a_j) correspond to creation (annihilation) of a spinless fermion (holon) at the site j. In the following we use the convention that the hole at the site j is located between spins $j-1$ and j. There are several indications that H_0 is a satisfactory description well beyond the limiting regime $J/t \ll 1$. In particular, the coherent mass of a single hole has been shown[16] to remain nearly unrenormalized even for $J/t > 1$. In fact, the only term making the difference to the t-J model with a single hole is a superfluous spin exchange over the hole site j, which, however, leads only to very weak effects at $J/t < 1$.[17]

It is now easy to incorporate the effect of $t' \neq 0$. In addition to shifting the hole for two sites, the next-nearest-neighbor hopping also exchanges two spins in the direction of hopping. The operator performing such fermion interchange is $I = -(\frac{1}{2} + 2\mathbf{S}_j \cdot \mathbf{S}_{j+1})$,[4] so that the corresponding term becomes

$$H' = t' \sum_j \left[a_{j+2}^\dagger a_j \left(\tfrac{1}{2} + 2\mathbf{S}_j \cdot \mathbf{S}_{j+1}\right) + \text{H.c.} \right]. \tag{2.2}$$

It is evident that H' induces a coupling between spin degrees of freedom and the holon. In the following we first investigate the effective model $\tilde{H} = H_0 + H'$ for a single hole. But we expect that $\tilde{H}$ retains its meaning even for a larger number (but small concentration) of holes. The relation is, however, not as strict as for a single hole, due to improper description of configurations with two holes being close. While j still counts occupied sites, there exist configurations with neighboring holes, within our notation both located at j, not allowed in $\tilde{H}$. On the other hand, $\tilde{H}$ allows for some spurious processes for nearby holes. E.g., two fermions with indices $j, j+1$ (i.e., holes separated by an occupied site) can exchange. Still we do not expect that such processes are crucial for the discussion of the coupling between quite large FM polarons, as studied in Sec. IV.

A. Classical spin approximation

In the following we treat the effective Hamiltonian, Eqs. (2.1) and (2.2), within the simplest classical spin approximation (essentially equivalent to the Hartree approximation for spins) where spin operators are replaced by classical vectors of length $\tilde{S}$. It is plausible to assume that static spin directions will remain in a plane ($\varphi_j = 0$) so we introduce only canting angles ϑ_j. The Hamiltonian is then

$$\tilde{H} = -t \sum_j (a_j^\dagger a_{j+1} + \text{H.c.}) + J\tilde{S}^2 \sum_j \cos(\vartheta_{j+1} - \vartheta_j) + t' \sum_j (a_j^\dagger a_{j+2} + \text{H.c.}) \left[\tfrac{1}{2} + 2\tilde{S}^2 \cos(\vartheta_{j+1} - \vartheta_j) \right]. \tag{2.3}$$

It should be noted that the approximation at this level is an essential improvement over the traditional treatment[9,10] where simplifications were performed on the initial model, e.g., Eq. (1.1) in our case.

Assuming $t' < 0$ means that the FM spin configuration $\vartheta_{j+1} = \vartheta_j$ is energetically favored in the region where the condition $4|t'|\langle a_{j+2}^\dagger a_j \rangle > J$ is fulfilled. In the FM polaron the kinetic energy of the hole is reduced, whereas the creation of the polaron costs the exchange energy proportional to the length of the FM region.

The minimization of the total energy $\langle \tilde{H} \rangle$ consists of two steps. Representing the single spinless fermion wave function as $|\Psi\rangle = \sum_j \psi_j a_j^\dagger |0\rangle$ with ψ_j real, we get for the fermion the Schrödinger equation

$$-t(\psi_{j-1} + \psi_{j+1}) + (U_{j-1}\psi_{j-2} + U_{j+1}\psi_{j+2}) = \varepsilon_1 \psi_j, \tag{2.4}$$

with the effective potential

$$U_j = t' \left[\tfrac{1}{2} + 2\tilde{S}^2 \cos(\vartheta_{j+1} - \vartheta_j) \right]. \tag{2.5}$$

From Eq. (2.3) it is obvious that the local minimization of

$$\Delta_j = (J + 4t'\psi_{j+2}\psi_j) \cos(\vartheta_{j+1} - \vartheta_j) \tag{2.6}$$

leads to two possibilities, i.e., $\cos(\vartheta_{j+1} - \vartheta_j) = \pm 1$ for $J + 4t'\psi_{j+2}\psi_j \lessgtr 0$, corresponding to the local FM and antiferromagnetic (AFM) ordering of neighboring spins, respectively. Hence U_j can take only two values, $U_j = t'(\frac{1}{2} \pm 2\tilde{S}^2)$.

The second step is the determination of the FM polaron length. It is evident that beyond some large value of J the polaron formation is not possible. The system then consists of AFM ordered spins and a hopping fermion. In this case the ground state has the wave vector $k = 0$ (for $|t'|/t < \frac{1}{4}$) and the energy

$$E_{\mathrm{AFM}} = -\tilde{S}^2 JL - 2t - 2t'(2\tilde{S}^2 - \tfrac{1}{2}), \tag{2.7}$$

where L is the length of the system. At smaller values of J formation of the FM polaron is favorable and the energy of such configuration with respect to the reference E_{AFM} is

$$e_1 = 4\tilde{S}^2 Js + \varepsilon_1 + 2t + 2t'(2\tilde{S}^2 - \tfrac{1}{2}). \tag{2.8}$$

Here $2s$ is the length of the FM polaron, i.e., s is the number of overturned spins relative to the reference Néel state. For $S = \frac{1}{2}$ we can also interpret s as a total spin of the system, since $2sS = s$. It should be noted that we henceforth consider only configurations with even $2s$, which appear in odd chains with periodic boundary conditions, as investigated also in Sec. III by the exact diagonalization method.

By inspection of Eqs. (2.3) and (2.8) we recognize that for large values of $s \gg 1$ the kinetic energy of the fermion localized within the polaron increases $\propto t/s^2$, while the magnetic energy is enhanced $\propto Js$. Thus the total energy is minimum at $e_1 \propto (tJ^2)^{1/3}$ and the polaron size $s \propto (t/J)^{1/3}$. As expected, FM polarons are large at $J/t \ll 1$. On the other hand, according to Eq. (2.6) too large J prevents the formation of the polaron and there are restrictions on values of J and t' for which the FM polaron exists.

In order to find stable solutions we first determine numerically the eigenvalue of Eq. (2.4) for the fixed polaron length $2s$. Then we choose s so that e_1, Eq. (2.8), is minimum. Additionally one has to check that $e_1 < 0$, otherwise the FM configuration is only metastable relative to the AFM state, Eq. (2.7). In the following calculation we use $\tilde{S} = \sqrt{S(S+1)} = \sqrt{3}/2$.

In Fig. 1 we present the spin s as a function of J/t obtained numerically for fixed $t'/t = -0.2$. For $J/t \ll 1$ the predicted relation $s \propto (t/J)^{1/3}$ is followed, while for larger J/t values s descends in steps till the critical value J_c/t, beyond which the FM polaron is not stable. Figure 2 displays J_c/t as a function of $|t'|/t$. As will be shown below for the simplified model the dependence is $J_c/t \propto (|t'_c|/t)^{3/2}$. For each t' there exists also a minimal value of spin, s_c, which corresponds to the threshold value J_c/t. Results for s_c are also plotted in Fig. 2. For $|t'_c|/t \ll 1$ critical spin follows $s_c \propto \sqrt{t/|t'|}$.

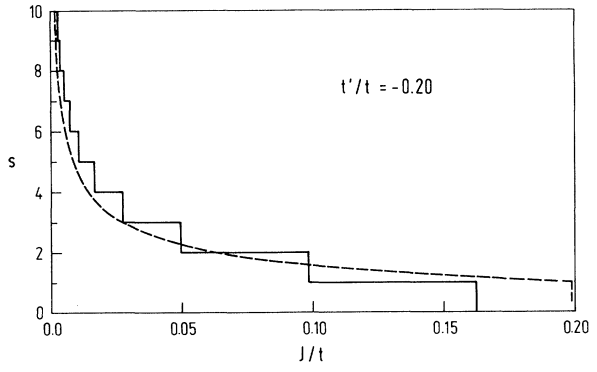

FIG. 1. Spin s vs J/t for $t'/t = -0.2$, calculated within the classical spin approximation is presented with full line. Dashed line represents the result for s within the continuum version of the model, Eq. (2.13).

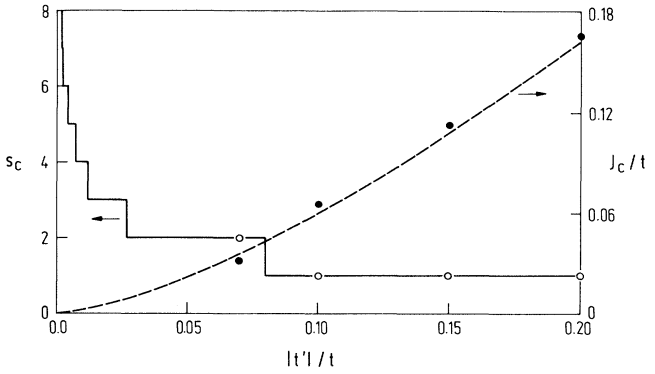

FIG. 2. Critical s_c (full line, left scale) and J_c/t (dashed line, right scale) vs $|t'|/t$ within the classical spin approximation. Dots represent results obtained by exact diagonalization of the model Eq. (1.1) on the $L = 19$ chain.

B. Continuum model

Since it is desirable to get an analytical description of the above asymptotic relations, in particular for rather delicate dependence on t', we simplify the model even further by introducing the continuum version of Eq. (2.3). We allow the fermion to move continuously along the chain coordinate x. The FM polaron is centered around the origin, from $x = -s$ to $x = s$ and $\cos(\vartheta_{j+1} - \vartheta_j) \to c(x) = \pm 1$ inside and outside the polaron, respectively. Leaving in the t' term only diagonal terms $\psi_{j+2}\psi_j \sim |\psi(x)|^2$, we get up to a constant

$$\tilde{H} = \int dx\{t\ |\partial\psi(x)/\partial x|^2 + \tilde{S}^2 c(x)[J + 4t'|\psi(x)|^2]\}. \tag{2.9}$$

The FM polaron here represents a simple square well potential of depth $8\tilde{S}^2 t'$ and of width $2s$.

The total energy, given relative to AFM, is

$$e_1 = 4\tilde{S}^2 Js + tk_1^2 + 8\tilde{S}^2 t', \tag{2.10}$$

where k_1 is the smallest positive root of the equation

$$k_1 = \sqrt{8\tilde{S}^2|t'|/t}\cos(k_1 s). \tag{2.11}$$

Energy e_1 has to be minimized with respect to s. The FM polaron will be formed if minimum energy is negative, otherwise the AFM configuration is stable. Energy Eq. (2.10) is minimum if the wave function satisfies the boundary condition

$$|\psi(s)|^2 = \frac{\cos^2(k_1 s)}{s + \left(8\tilde{S}^2|t'|/t - k_1^2\right)^{-1/2}} = \frac{J}{4|t'|}, \tag{2.12}$$

which corresponds to the minimization of Eq. (2.6) in the discrete version of the model. The solution for $1/s$ can be found from Eqs. (2.11) and (2.12) by expanding in powers of a dimensionless parameter ζ

$$\zeta = \left(\frac{J}{\pi^2 \tilde{S} t}\right)^{1/3} \left(\frac{t}{2|t'|}\right)^{1/2},$$
$$\frac{1}{s} = \left(\frac{8}{\pi^2}\frac{\tilde{S}^2 J}{t}\right)^{1/3} [1 + \zeta + \zeta^2 + O(\zeta^3)]. \quad (2.13)$$

The final result for the spin s is

$$s = \left(\frac{\pi^2}{8\tilde{S}^2}\frac{t}{J}\right)^{1/3} - \left(\frac{t}{8\tilde{S}^2|t'|}\right)^{1/2}, \quad (2.14)$$

which is correct for $\zeta \ll 1$, hence for $s \gg 1$. In Fig. 1 this result is presented (dashed line) as a function of J/t for the particular case $t'/t = -0.2$. The agreement with the solution of the discrete version of the model is very good. The main difference is in the critical J_c value, which in the case of the continuum model extends to $J_c = 0.198\,t$, instead of $J_c = 0.162\,t$ for the discrete model. The difference can be attributed to the fact that some terms of the order of t' are neglected in the continuum model. This can also explain why the agreement between the models is even better for smaller values of $|t'|/t$.

Equation (2.12) has a solution only within a certain range of J and t' values. There exists a critical J_c', for which e_1, Eq. (2.10) still has a local minimum at given value of t'. The corresponding spin is s_c'. Expressions for these critical values can be determined exactly

$$J_c'/t = c_J \tilde{S}\left(\frac{|t'|}{t}\right)^{3/2}, \quad s_c' = c_s\left(\frac{t}{\tilde{S}^2|t'|}\right)^{1/2}, \quad (2.15)$$

where $c_J = 3.29$ and $c_s = 0.19$. However, it appears that at the minimum e_1 is slightly positive and thus the solution is metastable. In fact, on increasing J a discontinuous transition to the AFM configuration happens before reaching J_c'. Nevertheless J_c' and s_c' remain good estimates for the critical values J_c and s_c. The comparison of Eqs. (2.15) with numerical solutions shows a difference mainly in constants c_J, c_s.

III. NUMERICAL STUDY ON FINITE CHAINS

In order to test the results of the preceding section and to find to what extent one can rely on the effective model, we now study the t-t'-J model, Eq. (1.1), by the exact diagonalization of finite chains. Here we shall be mainly concerned with the ground-state properties of the system, so that the Lanczos method is used. Using no other symmetries other than fixing the wave vector k and the z component of spin, S^z, in the one-hole case we can study chains as long as $L = 19$ sites.

From the previous studies[16] it is known that in a search for the ground-state energy E_0 and moreover for the effective mass, it is not sufficient to limit the scan over discrete values of k, i.e., $k = 2\pi l/L$. The phase factor should be introduced into the kinetic (i.e., hopping) part T of the Hamiltonian, Eq. (1.1), corresponding to the effect of a vector potential or of twisted boundary conditions.[18] The latter simply means that $t \to t\exp(\pm i\theta)$ and $t' \to t'\exp(\pm 2i\theta)$, where the sign in the exponent is taken according to the direction of the fermion motion and θ is a real angle.

We recover for $t' > 0$ a qualitatively similar behavior as for $t' = 0$.[16] As shown in Sec. II for $t' < 0$ the situation may become completely different. In our numerical studies, we choose to vary J/t at fixed $t'/t = -0.2$, although some data are obtained for $t'/t = -0.1$ as well. For convenience we mainly study odd chains of length $L \leq 19$, since they allow for a better accommodation of the AFM order (see the discussion in Ref. 16).

Starting at a sufficiently large value of J/t, the system at first persists in the $S = 0$ state. At J_c/t a crossover to the state with $S = 1$ and a different θ_0 is observed at the minimum. Further decreasing J/t results in a sequence of transitions to progressively higher values of the spin S of the ground state, until a totally polarized $S = S_{\max} = (L-1)/2$ state is reached. The resulting staircase dependence of S obtained for chains of different length (the longest being $L = 19$) is shown in Fig. 3. We note that at fixed S, θ_0 may vary continuously with J/t. This is true for states with $S = 1, 2$. For other values of S we get $\theta_0 = 0$, i.e., k is either $k = 0$ or $k = \pi$. Comparing Fig. 1 and Fig. 3 we see that the approximative treatment as displayed in Sec. II A is remarkable, taking into account the fact that higher S cannot be reproduced reliably in short chains.

Additional information on the character of the ground state may be gained from the spin-spin correlations. Of interest are the correlations

$$Z(i) = < n_0 S_i^z S_{i+1}^z >,$$
$$C(i) = < n_0 \mathbf{S}_i \cdot \mathbf{S}_{i+1} >, \quad (3.1)$$

where $n_0 = 1 - \sum_s c_{0,s}^+ c_{0,s}$. They measure the degree of

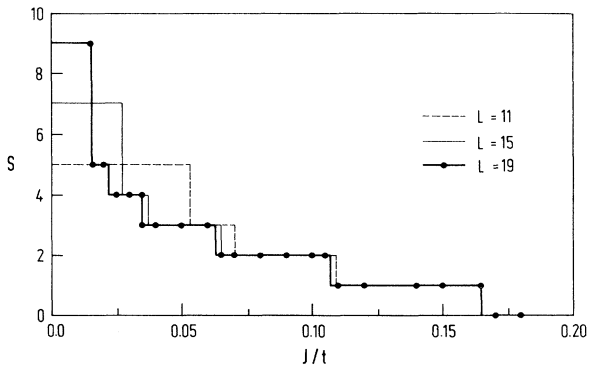

FIG. 3. Ground-state spin S for $t'/t = -0.2$ vs J/t for $L = 19$ chain. The circles correspond to actual calculations, whereas crossover points were determined by extrapolations. The staircase for $L = 11$ and 15 are also shown for comparison.

spin alignment in the vicinity of the hole. We present in Fig. 4(a) the spatial variation of $Z(i)$ and $C(i)$ for different values of J/t. From the curves it is seen that in the singlet $S = 0$ state, spins are everywhere AFM correlated. On the other hand, for $J/t < J_c/t$, where the ground state has $S > 0$, FM correlations start to build up in the vicinity of the hole. They eventually reach out over the whole investigated system for small enough J/t. In Fig. 4(b) we show the corresponding result obtained from the numerical calculation within a discrete version of the classical spin approach of Sec. II A. Correlation $C(i)$ is normalized with the classical spin $\tilde{S}^2$ and should be compared with $3\,Z(i)$ from Fig. 4(a). Again the agreement is satisfactory, in particular for larger S.

We now address the question of the effective quasiparticle mass. As θ dependence of $E_0(\theta)$ can be related to its variation with respect to k, we may obtain the coherent effective mass m_c^*, or the coherent hopping t_c^*, via

$$m_c^{*-1} = 2t_c^* = \frac{\partial^2 E_0(\theta)}{\partial \theta^2}\Big|_{\theta=\theta_0}. \tag{3.2}$$

One can also define the effective incoherent hopping t_i^* through

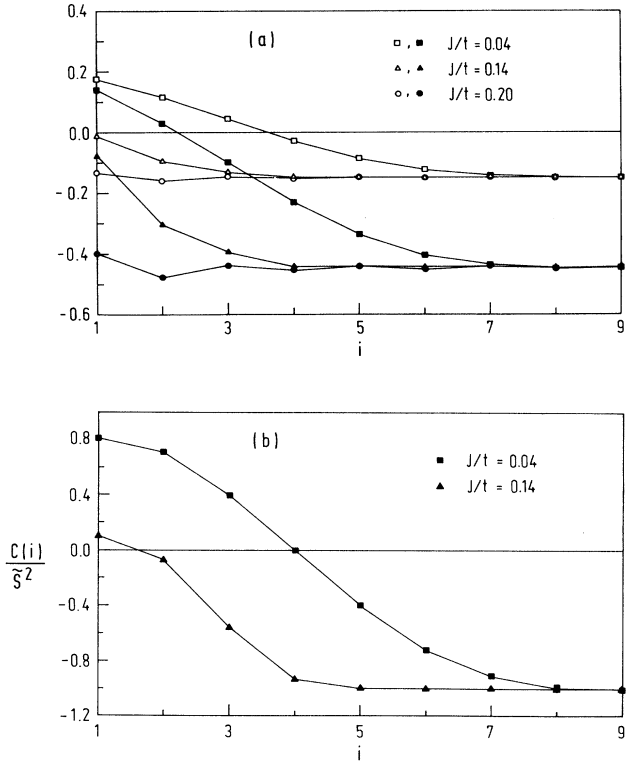

FIG. 4. (a) Correlation functions $Z(i)$ (light symbols) and $C(i)$ (heavy symbols) for different J/t and $t'/t = -0.2$. Note that for a given S, $Z(i)$ is calculated with respect to the ground state with $S^z = S$. (b) Correlation function $C(i)/\tilde{S}^2$ calculated within the classical spin approximation for $t'/t = -0.2$.

$$2t_i^* = \left\langle \frac{\partial^2 H(\theta)}{\partial \theta^2} \right\rangle_0, \tag{3.3}$$

where $< >_0$ stands for the ground-state expectation value at $\theta = \theta_0$. t_c^* and t_i^* are then simply related through the f-sum rule[16,19]

$$t_c^* = t_i^* - \int_0^\infty \sigma(\omega) d\omega, \tag{3.4}$$

$\sigma(\omega)$ being the optical conductivity. For the t-J model, where $2t_i^* =< -T >$, it has been shown analytically and by exact numerical calculations on finite chains,[16] that for one hole $t_c^* \simeq t_i^*$ up to large values of J/t. This is a direct consequence of the charge-spin separation effective over the whole energy scale.[4]

The dependence of t_c^* on J/t as calculated from Eq. (3.2) for different L is presented in Fig. 5. Pronounced finite-size effects are apparent, except for $S = 0$, the "decoupled" regime, where $t_c^* \approx t_i^* \approx t$, and for $S = 1$, for which t_c^* appears to saturate. As expected t_i^*/t remains close to 1.0 in the whole investigated region and with decreasing J/t monotonically approaches its largest value, attained in the FM state, $t_i^*\,|_{\rm FM} = t - 4t'$. On the other hand, there is a dramatic drop in t_c^* especially in the region where $S = 2$. Beyond this region t_c^* starts to increase and gradually approaches t_i^*. For smaller systems this increase is not surprising but for the largest $L = 19$ chain the $S = 3$ polaron seems still to be small enough [see Fig. 4(a)] to allow for a substantial AFM correlated region and t_c^* is expected to further decrease. As yet we do not have a satisfactory explanation for this anomaly. However, as t_c^* has not yet saturated, a possible explanation might be that the tails of the hole's wave function, which determine the effective mass, reach out over the entire system and are thus rather sensitive to its size. This is also corroborated by the fact that the ground-state wave function is smeared out over many configurations generated in the Lanczos procedure. Another explanation might be that for $S = 1, 2$, spin waves strongly scatter off the bound state of an $S = 1$ spin excitation

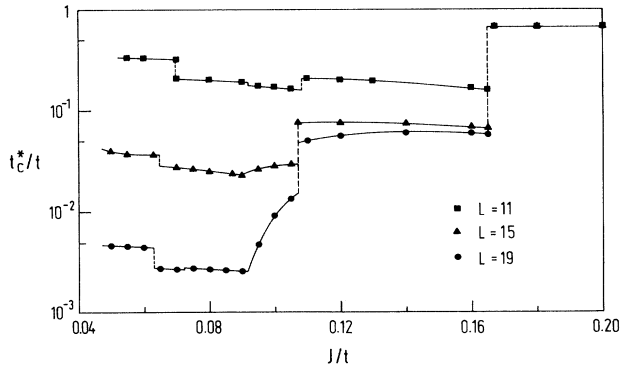

FIG. 5. The effective hopping t_c^* vs J/t and $t'/t = -0.2$ for different chain lengths L. Note the logarithmic scale along the vertical axis. For each L, regions of different ground-state values of spin S are separated by dashed vertical lines. See also Fig. 3.

and the hole (the state being a precursor to large polaron formation) and thus almost all the spectral weight leaks away into the incoherent part of the spectrum. In any case such a behavior indicates that the coupling of spin to charge is very strong and that the t-t'-J model does not behave as a Luttinger liquid[3] in the region considered.

IV. MANY-HOLE STATES

Numerical (exact diagonalization) studies of the systems with more holes are quite limited, even for a chain. On the other hand, calculations within the effective model together with the classical spin approximation, as performed in Sec. II, are quite simple even in this case. It should be, however, repeated that at higher hole concentrations the effective model ceases to be a straightforward mapping of the initial model (1.1).

Since we are interested only in qualitative features of the many-hole system in the regime $J/t \ll 1$, we use the continuum approximation Eq. (2.9). Let us first consider *a single FM polaron containing N spinless fermions (holes)* , which has the energy per fermion

$$e_N = 4\tilde{S}^2 J\frac{s}{N} + \frac{t}{N}\sum_{m=1}^{N} k_m^2 + 8\tilde{S}^2 t' - \tfrac{1}{3}t(\pi n)^2, \qquad (4.1)$$

where k_m correspond to first N solutions of the Schrödinger equation corresponding to Eq. (2.9) and $n = N/L$ is the density of fermions. e_N and other energies henceforth are again expressed relative to the energy of the unperturbed AFM spin configuration with a finite fermion concentration,

$$e_{\mathrm{AFM}} = -\frac{\tilde{S}^2 J}{n} - 4\tilde{S}^2 t' + \tfrac{1}{3}t(\pi n)^2, \qquad (4.2)$$

representing the extension of Eq. (2.7) to finite n. The energy e_N can be calculated in the same way as for a single fermion, i.e., we first determine wave vectors k_m at fixed s and then minimize e_N with respect to the FM polarized length $(2s)$.

The solution Eq. (4.1) becomes of interest in the thermodynamic limit $L, N \gg 1$ in the regime of phase separation, where all N fermions are bound to a single FM - polarized region with a finite length $1 \ll 2s < L$. In this case the single-particle wave functions are well represented with $\psi_m(x) = s^{-1}\sin[k_m(x+s)]$, with $k_m 2s = m\pi$ and the energy per particle is

$$e_N = 4\tilde{S}^2 J\frac{s}{N} + \tfrac{1}{3}t\left(\frac{\pi N}{2s}\right)^2 + 8\tilde{S}^2 t' - \tfrac{1}{3}t(\pi n)^2. \qquad (4.3)$$

Minimizing Eq. (4.3) with respect to s/N one readily gets the spin and the energy per fermion

$$\frac{s}{N} = \left(\frac{\pi^2}{24}\frac{t}{\tilde{S}^2 J}\right)^{1/3}, \qquad (4.4)$$

$$e_N = \left(9\pi^2\tilde{S}^4 t J^2\right)^{1/3} + 8\tilde{S}^2 t' - \tfrac{1}{3}t(\pi n)^2. \qquad (4.5)$$

The above simplifications are entirely legitimate for $N \gg 1$ provided that two conditions are met: (a) all fermion states are bound within the potential, and (b) part of the system must remain AFM ordered, i.e., $2s/N < 1/n$. For concentrations n exceeding the latter condition the system clearly prefers the *fully polarized FM state*, with the energy

$$e_{\mathrm{FM}} = \frac{2\tilde{S}^2 J}{n} + 8\tilde{S}^2 t'. \qquad (4.6)$$

Another nontrivial possibility for $N \to \infty$ is the formation of *the periodic structure of FM-polarized regions.* In such a case we are clearly dealing with a Kronig-Penney model for fermions. The period of the potential is L_0 and the number of fermions per polaron ν corresponds to the number of occupied energy bands. Now the density of fermions is $n = \nu/L_0$. The minimum energy is found by varying the length of the potential wells $2s$ for fixed n and ν.

The resulting phase diagram is presented in Fig. 6, shown for $t'/t = -0.2$. No qualitative or even quantitative differences are expected for smaller ratios, provided that in the diagram n and J are scaled as $\sqrt{|t'|/t}$ and $(|t'|/t)^{3/2}$, respectively. Starting in the regime of large J/t and small n, stable solutions correspond to the AFM spin configuration, Eq. (4.2), with a finite concentration of mobile spinless fermions. In the region, denoted by FM_1, at lower J/t the periodic array of singly occupied ($\nu = 1$) FM polarons is the most stable. It is characteristic that this regime can be reached from the AFM one also by increasing n at fixed J/t. At larger n the FM_1 region becomes unstable towards the fully polarized FM solution (with a narrow intermediate phase), representing the ground state with the maximum spin $S = S_{\max}$. Most intriguing is the appearance of the phase-separated (PS) region at low enough $J/t \ll 1$ and $n \ll 1$. In our treatment this corresponds to Eq. (4.3) with all fermions

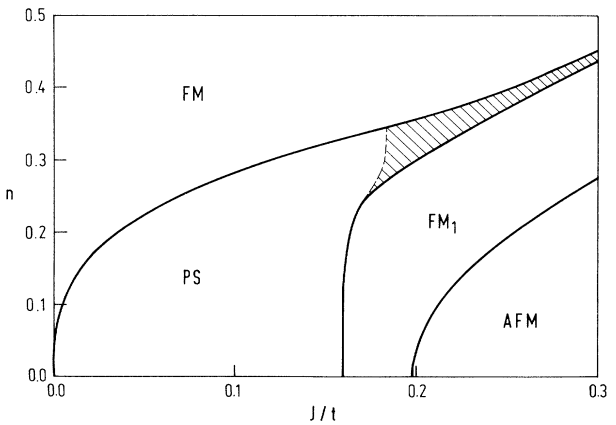

FIG. 6. Phase diagram for the continuum model at $t'/t = -0.2$. For explanation see the text.

localized within a single FM distortion, extending only through a part of the system while the rest remains an undoped AFM. Again this solution transforms to the FM phase on increasing n, when the size of the polaron reaches the system size $2s = L$. Besides these simple phases there exists an intermediate region at higher $n \gtrsim 0.3$ and $J/t \gtrsim 0.16t$ (for particular $t'/t = -0.2$), with a more complex behavior. We find here the minimum energy for periodic arrays of FM polarons with several fermions per polaron $\nu = 2, 3$, etc. Also the phase-separated solutions change in this regime into the FM region and the *doped* AFM region.

It is not straightforward to speculate what our results would imply for the true ground state of the system. For the AFM region a better treatment (e.g., without the classical spin approximation) would yield the paramagnetic, i.e., singlet $S = 0$, ground state with the characteristic Luttinger-liquid behavior.[3] For the region FM_1 (as well as for FM_ν) there are essentially two different posibilities for the physical fixed point to which this regime would correspond: (a) FM regions combine to a partially polarized $S > 0$ state, (b) the FM polarons still form a singlet state, but with changed local spin correlations relative to the AFM solution. Most interesting is the possibility of the phase-separated (PS) regime. We expect that the true ground state in this regime would also exhibit phase-separation[8] and a partial polarization $0 < S < S_{\max}$.

Recent numerical investigations[20] of the t-t'-J model on a finite chain are to some extent in agreement with our findings. The FM phase extends at larger hole doping n to much larger J/t (up to $J/t = 0.7$ at $t'/t = -0.2$). It seems that at particular t'/t no ground states with intermediate spins $0 < S < S_{\max}$ were found, which would indicate on the phase-separated region. However, it is clear that our approximations overestimate the PS regime, so possibly PS cannot be reached in a small size system. Omitted terms could also lead to an additional hole-hole repulsive interaction, still we do not believe that this can qualitatively change our conclusions.

V. CONCLUSIONS

It is clear from the preceding analysis that the t-t'-J model with $t' < 0$ allows for the ground states which do not follow the Luttinger-liquid behavior, as is the case for $t' = 0$.[3,4] We have shown that the charge and the spin degrees of freedom are strongly coupled in the regime $J/t \ll 1$ introducing partially spin-polarized states which approach the Nagaoka-type FM state at $J = 0$, at least for the single-hole case studied predominantly in this paper. A clear signature of strong coupling is the extremely large renormalization of the coherent mass of the hole, resembling more the classical (electron-phonon) polaronic effects than the "spin-string" induced enhancement $m_c^* \propto t/J$ evident in the planar t-J model.[14,15]

It is quite promising that the effective model of a spinless fermion coupled to the spin subsystem, treated in a simple classical spin approximation, provides even quantitatively satisfactory results. This is another indication that within the FM polaron the hole moves as a fermion within the static spin background, analogous to the adiabatic picture of standard polarons.

Unfortunately the mapping on the effective model remains only approximate in the many-hole situation. Since the omitted terms can change somewhat the effective hole-hole interaction, the phase diagram presented in Sec. IV cannot be considered as settled. Still it is intriguing that $t' < 0$ induces the possibilty of two different phase-separated regions in the phase diagram. While it is clear that such a region exists at $J/t \gg 1$,[8] the phase separation seems to be possible also near the FM phase for $n \ll 1$ and $J/t \ll 1$. Such separation has been speculated already in a $d = 2$ t-J model[8] at $J/t \ll 1$. This again confirms our initial idea, that $t' < 0$ induces in a $d = 1$ system some features of the planar t-J model.

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