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FERROMAGNETIC POLARONS IN THE ONE-DIMENSIONAL $t-t'-J$ MODEL

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It is shown that the addition of the next-nearest neighbour hopping term (t') to a t-J model on a chain prevents the spin-charge decoupling for $J/t \ll 1$ and may result in the formation of stable $S > 0$ spin polarized states. From numerical results on finite chains with a single hole, a stepwise increase of S with decreasing J is found, accompanied by a very large enhancement of the polaron mass. Qualitative agreement is found with results based on an effective spinless-fermion model. In this framework finite concentration of holes is also studied.

The one-dimensional models of strongly correlated electrons *e.g.*, the exactly solvable $d = 1$ Hubbard model and the related t-J model, have attracted considerable attention, primarily as a test-ground for some of the ideas, relevant for the HTSC.[1] Although their main feature, the spin-charge decoupling[2], is not common to $d > 1$, questions such as the possible existence of the ferromagnetically (FM) polarized state in the (2-d) t-J model for finite concentration of holes and the related problem of phase separation cannot be considered as settled. Recently it has been observed[3] that the spin-charge coupling and the FM polarized states in a t-J model on a chain can be induced by the next-nearest neighbour hopping term, the underlying physics possibly resembling the transition to the Nagaoka regime in related 2-d system.

Motivated by the above considerations we report on the study of a t-t'-J model on a chain,[4]

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

describing the nearest neighbour (t) and next-nearest neighbour (t') hopping of fermions in the presence of empty sites in the Heisenberg spin system. In dealing with the above model progress can be made by exploiting the idea of charge-spin separation[3] which for $t' = 0$ is known to persist even for $J/t > 1$, as examplified, *e.g.*, by the weak renormalization of the coherent mass of a single hole.[5] Without going into detailes[4] one can consider an effective model instead,

$$H_0 = -t\sum_{j}(a^{\dagger}_j a_{j+1} + \mathrm{H.c.}) + J\sum_{j'}\vec{S}_{j'}\cdot\vec{S}_{j'+1} + t'\sum_{j}\left[a^{\dagger}_{j+2}a_j\,(\frac{1}{2} + 2\vec{S}_{j'}\cdot\vec{S}_{j'+1}) + \mathrm{H.c.}\right]\,, \quad (2)$$

where j' counts the sites occupied with spins *only*, while operators $a^{\dagger}_j$ (a_j) correspond to spinless fermion(s). Note that the t'-term *exchanges* the two spins in the direction of hopping. Moreover, for $t' < 0$, the *ferromagnetic* alignment of the two spins is favoured. Thus, a hole polarizes its immediate surrounding, the size of the FM polaron depending on $J/|t'|$. To gain a qualitative understanding, we treat the effective model within the classical approximation for spins. A simple picture emerges in which the spinless fermion is trapped within an effective potential well of depth $\sim |t'|$ and size $\approx 2S$, generated by the FM aligned spins. A more detailed analysis shows that $S = (\pi^2 t/6J)^{1/3} - (t/6|t'|)^{1/2}$. It also follows that for each t' there exists a treshold value of $J_c/t \propto (|t'_c|/t)^{3/2}$ above which there can be no FM polaron with $S < S_c \propto \sqrt{t/|t'|}$ (for $|t'|/t \ll 1$).

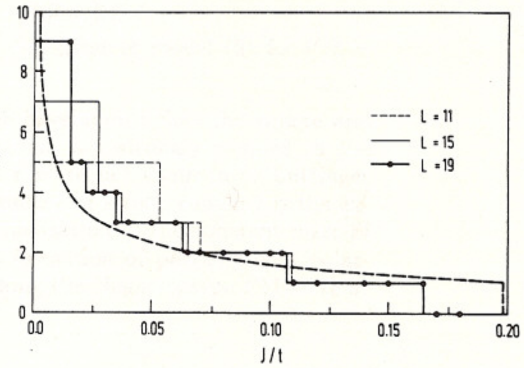

FIGURE 1
Ground state spin S *vs.* J/t for $t'/t = -0.2$ for different chain lengths. S obtained within model (2) is also shown (dashed line).

We have also exactly diagonalized the t-t'-J model on finite (cyclic) chains. In Fig. 1 the evolution of the ground state value of spin S as we decrease J/t is shown for a single hole and for different chain lengths for $t'/t = -0.2$. Note the remarkable agreement with S obtained within the effective model. The spin-charge coupling induced by the t'-term has also dramatic effects on effective quasiparticle mass. In Fig. 2 we present data for the effective coherent hopping t_c^*/t (inverse mass) for a single hole within the model (1). In the region with $S = 0$ spin and charge are coupled only weakly and $t_c^* \sim t_i^* \sim 1.0$ (t_i^* is incoherent hopping). However, decreasing J/t results in a dramatic drop in t_c^*, a feature characteristic of the classical polaronic effect[6] indicating moreover strong coupling of charge to spin, whereas t_i^* remains essentially unrenormalized.

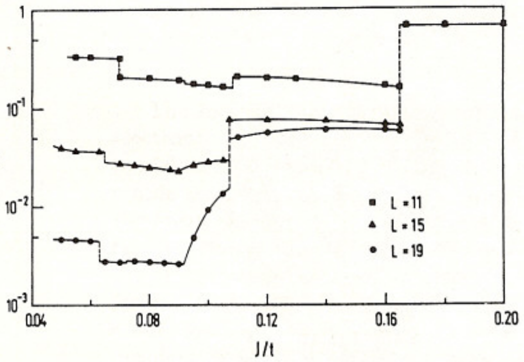

FIGURE 2

The effective hopping t_c^*/t vs. J/t for $t'/t = -0.2$. Note the logarithmic scale along the vertical axis

Finally we briefly address the problem of *many holes*. Within the effective model (but bearing in mind its limitations) we obtain the phase diagram, presented in Fig. 3 for $t'/t = -0.2$. No substantial differences are expected for smaller ratios, provided that the density of fermions n and J are scaled as $\sqrt{|t'|/t}$ and $(|t'|/t)^{3/2}$, respectively. The main features are: the AFM phase for large J/t and small n, the intermediate region FM_1 where a (periodic) array of singly occupied FM polarons is most stable, and the appearance of the phase-separated (PS) region at $J/t \ll 1$ and $n \ll 1$, which corresponds to *all* fermions being localized within a single FM distortion, extending over a fraction of the system. It goes into the FM phase on increasing n.

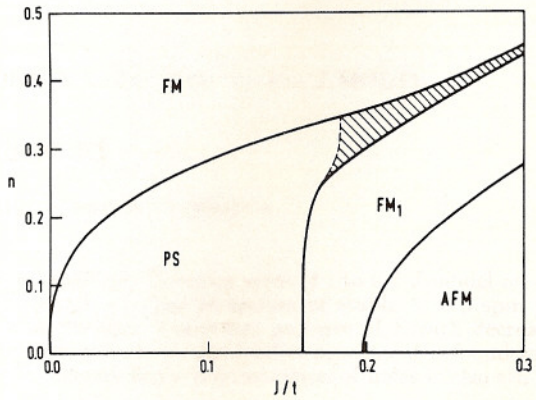

FIGURE 3

Phase diagram for the effective model (2) for $t'/t = -0.2$.

In conclusion we have shown that the charge and spin degrees of freedom are strongly coupled in the regime $J/t \ll 1$, a feature not common to Luttinger liquids. A clear signature of strong coupling is the extremely large renormalization of the coherent mass of the hole as well as formation of partially spin polarized states approaching the Nagaoka-type FM state at $J = 0$.

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