Staggered-Field-Induced Hole Pairing in One-Dimensional Correlated Systems

J. Bonča, P. Prelovšek, and I. Sega
J. Stefan Institute, University of Ljubljana, 61111 Ljubljana, Slovenia

H. Q. Lin and D. K. Campbell
Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545
and Department of Physics, University of Illinois, Urbana, Illinois 61801
(Received 3 February 1992)

We examine the influence of a staggered magnetic field on states involving a few holes in the one-dimensional t-J and Hubbard models. We apply exact diagonalizations of small systems, an analytical treatment of an anisotropic model, and a high-field perturbation expansion. Our results suggest that even modest staggered fields, $h \ll t$, induce the formation of bound hole pairs in a broad range of parameters, in particular for $J/t<1$ in the t-J model and for $U/t>1$ in the Hubbard model. In the same regions, by studying the density-density correlations and the compressibility, we argue that many holes form a paired state and that phase separation does not occur.

PACS numbers: 74.65.+n, 71.10.+x, 75.10.Lp

The discovery of high-temperature superconductivity (SC) in layered copper oxides and the unusual normal-state properties of this novel class of metals have in recent years stimulated numerous theoretical investigations of low-dimensional, strongly correlated systems. Nonetheless, the central question of whether simple prototype models for *planar* correlated electronic systems, such as the two-dimensional (2D) single-band Hubbard or t-J models [1], allow for an SC ground state with paired fermions remains thus far unresolved. Since much more is known about the properties of one-dimensional (1D) models [2], it is natural to seek and study 1D analogs of the real 2D models. Unfortunately, although in 1D both the Hubbard model [3] and the supersymmetric t-J model [4] ($J/t=2$) are exactly solvable, they exhibit no evidence of superconductivity in the physically relevant repulsive-interaction regime. Instead, they belong to the universality class of Luttinger liquids [5] and exhibit long-range, power-law behavior of correlation functions, characterized by a single nontrivial exponent K_ρ [6]. The phase diagram of the 1D t-J model is well understood even away from the $J=2t$ point [7]. For instance, numerical investigations confirm Luttinger-liquid behavior up to the phase-separation instability, which appears at the critical value $J_s(n)/t$, which depends on the fermion density n.

In this Letter we argue that the appropriate 1D analogs for the true 2D system are models involving *staggered external* magnetic fields, and we show that the presence of the staggered field changes qualitatively the model properties, allowing for pairing and arguably for superconductivity. Specifically, we consider the 1D Hubbard model in a staggered field h,

$$H=-t\sum_{is}(c_{i,s}^\dagger c_{i+1,s}+\mathrm{H.c.})+U\sum_i n_{i\uparrow}n_{i\downarrow}-\tfrac{1}{2}h\sum_i(-1)^i(n_{i\uparrow}-n_{i\downarrow})\,, \qquad (1)$$

and the related 1D t-J model [1],

$$H=-t\sum_{is}(c_{i,s}^\dagger c_{i+1,s}+\mathrm{H.c.})+J\sum_i(\mathbf{S}_i\cdot\mathbf{S}_{i+1}-\tfrac{1}{4}n_in_{i+1})-h\sum_i(-1)^iS_i^z\,. \qquad (2)$$

In the strong-coupling limit $U\gg t$ the Hubbard model (1) is equivalent to model (2) with $J\sim 4t^2/U$, if we neglect the next-neighbor hopping terms which are of the same order as J. Outside the strong-coupling regime and for strong fields ($h\sim U$), the equivalence no longer holds, so we investigate both models separately.

Our motivation for introducing staggered fields in the 1D systems is related to the behavior of 2D (or higher dimensional) weakly doped magnetic insulators. Very close to half filling, in 2D, both models (likely) exhibit long-range antiferromagnetic (AFM) order: At least the AFM correlation length is large. In a 1D system, to produce the same AFM ordering, one must (in general) introduce a staggered magnetic field. Technically, the staggered field can be obtained from the original 2D system by performing a mean-field-type decoupling of the spin exchange between chains. A finite h can then simulate several phenomena found previously in 2D systems at low doping, which originate from the longer-range AFM correlations and from the spin string effects [8,9]. These include the strong enhancement of hole coherent masses, and the formation of singlet hole pairs even at $J/t<1$ [10]. Recently it has been found that finite-range AFM correlations, introduced in a 1D model via a longer-range spin exchange, also produce similar effects [11].

Further on we restrict our attention to the proposed 1D models. We show that the staggered field has a nonperturbative effect on the $h=0$ state near half filling. In particular, over a broad regime of parameters finite h induces the binding of two holes and, moreover, holes remain paired even at finite hole concentrations, i.e., pairing wins out over the phase separation. Such effects are far from obvious, since the external field does not couple to charge degrees of freedom.

To begin we analyze the t-J model in the (extreme anisotropic) Ising limit, in which we replace $\mathbf{S}_i \cdot \mathbf{S}_{i+1}$ by $S_i^z S_{i+1}^z$. In this case a single hole ($N_h = 1$), introduced into an AFM (Néel) spin background, moves in an effective potential

$$V(r) = h|r| + \tfrac{1}{2}J(1-\delta_r), \tag{3}$$

increasing with distance $|r|$ due to the string effect—here caused by the antialignment with the staggered field of the spins past which the hole has moved—while the additional term $\frac{1}{2}J$ outside the origin is due to the formation of an AFM domain wall, corresponding to a spinon. Note that the lattice distance is normalized to $r=1$. An analogous stringlike attractive interaction exists between two holes ($N_h = 2$), which at the distance $r \geq 1$ feel the potential

$$\tilde{V}(r) = h(r-1) - \tfrac{1}{2}J\delta_{r-1}. \tag{4}$$

The lowest-energy state for $N_h = 2$ does not contain spinons, so the exchange energy is not enhanced. There is even a contact ($r=1$) attractive term, since two adjacent holes break one fewer exchange bond than do two separated holes.

We can now solve the potential problems for $N_h = 1,2$ easily. Of special interest is the binding energy of the hole pair, $\epsilon_b = E_2 - 2E_1 + E_0$ [10], which can be expressed analytically in two regimes. For $J,h \ll t$ one can use the continuum approximation to the discrete problem, with the eigenfunctions corresponding to Airy functions, to find

$$\epsilon_b = 0.909(th^2)^{1/3} - J. \tag{5}$$

From Eq. (5) it follows that in weak fields ($h \ll t$) a bound pair forms for $J > J_c$ with $J_c/t \sim (h/t)^{2/3} \ll 1$. In interpreting Eq. (5) one must be aware that it applies only in the region $J,h \ll t$ and that the limit $h \to 0$ is very singular. Hence, although it is true that at fixed J increasing h decreases ϵ_b, at $h=0$ there is *no binding at all* between the holes in this parameter regime; in the $h=0$ case binding occurs *only* for $J > J_c = 4t$. This singularity can be understood physically by noting that in the anisotropic model any finite field h destroys the separation of spinons and holons on a chain. Since individual spinons and holons would have infinite energies at $h \neq 0$, it is meaningful to introduce particles only in pairs. In Eq. (5) we compare the energies of a bound holon-holon pair to two separate bound holon-spinon pairs. In the latter case, spinons cost additional energy $\sim J$, which stabilizes the holon-holon pairs at $J > J_c$. Clearly, the situation at $h=0$ is quite different, since one needs for binding an essentially different mechanism, coming only from the contact holon-holon attraction in Eq. (4).

In the strong-field case ($h \gg t$) (arbitrary J), perturbation theory yields

$$\epsilon_b = -\frac{J}{2} + \frac{2(2h-J)t^4}{(h+\frac{1}{2}J)^3(2h+\frac{1}{2}J)}. \tag{6}$$

In this regime we get $J_c/t \sim 4(t/h)^3 \ll 1$. Both approximations are consistent with the numerical solution of the potential problem in the Ising case, for which J_c/t is always less than about $\frac{1}{4}$ whatever the value of h, except at the singular point $h=0$ where $J_c/t = 4$. Importantly, for this Ising case, both the approximate and numerical solutions are carried out on an *infinite* lattice, so there are no boundary-condition or even-odd contributions.

The isotropic t-J model can also be investigated analytically in the $h,J \gg t$ regime by extending the above perturbation expansion to include the anisotropy parameter $\gamma = J_\perp/J$. It is easy to see that the leading correction is $\delta\epsilon_b \propto \gamma J t^2/h^2 > 0$, which in the regime $J < 4t^2/h$ is of the same order as the correction term already considered in Eq. (6). To study the full model in the most interesting regime ($h,J \ll t$), we use exact diagonalization of small clusters. Here we present results for a chain of $N = 16$ sites with periodic boundary conditions, and $h = J/2$. The latter choice has a particular physical meaning since, in a mean-field treatment of a 2D t-J model on a square lattice, one finds $h = 2J\langle S_z \rangle$, with $\langle S_z \rangle \sim 0.3$ for an ordered 2D AFM. We calculate numerically the binding energy ϵ_b by comparing energies for $N_h = 0,1,2$. We find that ϵ_b follows Eq. (5) qualitatively and even quantitatively for $J/t < 0.6$. For instance, in the present case we get $J_c/t \sim 0.3$.

In small systems our simulations suggest that a more reliable test for binding than ϵ_b is the behavior of the hole density-density correlations $g(r)$,

$$g(r) = N\langle n_{h,i} n_{h,i+r} \rangle, \tag{7}$$

where $n_{h,i} = 1 - n_i$, since we find that $g(r)$ is less sensitive to the boundary conditions and the system size than ϵ_b, which requires a comparison of results for systems with different N_h and even different total spin S_z. In the case of $N_h = 2$, results for $g(r)$, shown in Fig. 1 for various J/t, clearly confirm the formation of a bound pair at $J/t \gtrsim 0.3$. Note that for $h=0$ and $J < t$, $g(r)$ should be that of two spinless fermions $\propto \sin^2(\pi r/N)$, due to effective charge-spin decoupling [2,5,12]. As seen in Fig. 1 we find similar behavior for $h > 0$ but $J < J_c$. The most pronounced influence of $h > 0$ remains, however, the rapid decrease of the binding threshold, since at $h=0$ bind-

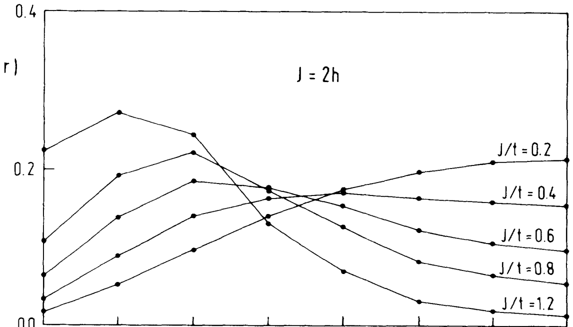

FIG. 1. Hole density-density correlations $g(r)$ for the t-J model in a staggered field $h = J/2$ vs distance r for two holes at different ratios J/t. Results are for the chain with $N = 16$ sites.

ing in the isotropic t-J model appears only at $J_c/t \sim 3.5$ [7,13]. Turning to the issue of phase separation and the nature of the multihole states, we start by noting that in the standard 1D t-J model ($h=0$) at low hole doping $n_h \ll 1$ the onset of hole binding at $J_c/t \sim 3.5$ seems to coincide with the phase separation (PS) transition [7], without an intermediate phase with paired holes. While the situation in the 2D t-J model appears quite open in this respect [13,14], our 1D model with $h>0$ clearly shows that the bound pair formation for $N_h=2$ extends to hole pairing at $N_h=2N_p \geq 4$, at least in certain regimes.

In fact we can adduce several physical arguments for the existence of a paired ground state at $N_p \geq 2$. It is easiest to understand the anisotropic case, $\gamma=0$. In a chain with periodic boundary conditions, even N, and $N_h=2N_p \ll N$, the ground state is achieved by forming N_p separate pairs, bound by the interaction $\tilde{V}(r)$ in Eq. (4). Among neighboring pairs there is no stringlike potential, the only interaction being a contact attraction $-\frac{1}{2}J\delta_{r-1}$, which is driving also the PS transition. However, since for $t \gg J$ the pairs are quite mobile, this term cannot bind pairs (taking into account hard-core pair repulsion) for $J,h \ll t$. Hence pairs behave as free, hard-core bosons. An estimate can be performed also for the regime $h \gg t$, $J > J_c$. Here holes form tightly bound pairs with the pair radius $r \sim 1$. Such pairs move with the effective hopping $\tilde{t}=t^2/(h+J/2)$. In such a system the contact attraction leads to the phase separation at $J_s = 4\tilde{t} \gg J_c \propto t^4/h^3$, as seen from Eq. (6). Thus for $h \gg t$ we expect a broad range $J_c < J < J_s$ in which the paired state exists.

To investigate systems with more holes in the isotropic t-J model we rely mostly on exact diagonalization results for $N=16$ sites. Following previous work [7], we determine the onset of PS in our finite system by monitoring the vanishing of the inverse compressibility $\kappa^{-1} \propto \Delta = E_4 - 2E_2 + E_0$ [7]. Along the particular line $h=J/2$ we find that Δ falls monotonically from $\Delta/t=0.35$ at $J/t=0.2$ to $\Delta=0$ at $J_s/t \sim 2.0$. An independent test for PS is the behavior of hole density-density correlations: Namely, for $N_h \ll N$, on expects $g(r)$ to fall off with distance $r > N_h$ (in 1D) in the PS regime, since holes form a cluster. In Fig. 2 we present correlations $g(r)$ for $N_h=4$ for a large field $h=2t$, in order to make effects more evident. The results in Fig. 2 for large $J=2t > J_s$ clearly confirm the clustering effect in the PS region. On the other hand, below the PS threshold, $J<J_s$, the $g(r)$ curves are entirely consistent with the pairing picture. Here, the falloff of $g(r)$ at short distances $r \gtrsim 1$ marks the small radius of a single pair, while at larger r the behavior follows quantitatively the result for two free hard-core bosons. Note also that there are no essential differences between two curves with different $J<J_s$. The same physical picture is confirmed by four-point hole density correlations.

Turning now to the Hubbard model, we recall that the

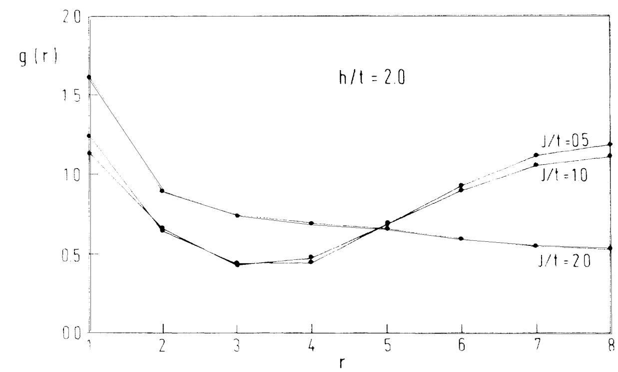

FIG. 2. Same as in Fig. 1, but for $N_h=4$ and at fixed staggered field $h/t=2$.

1D repulsive version at $h=0$ shows Luttinger-liquid behavior [2,5] in the whole phase diagram, so there is no pair formation at arbitrary U/t. Also, in the 2D Hubbard model the evidence for the pair formation is much less conclusive [15] than in the t-J model. Even with $h>0$ in the 1D model, it still remains challenging to prove the existence of bound pairs. One approach is the analytical evaluation of the ground state for $N_h=2$ via perturbation series in t/h—hence limited to the region $t/h \ll 1$—but for arbitrary U. The calculation is complicated by the degeneracy of the zeroth-order ground state and by the vanishing of the binding within the order $t(t/h)^2$. After a tedious calculation which will be presented in more detail elsewhere, we find for the inverse radius μ of the pair

$$\mu = \frac{Ut^2(24h^2 - U^2)}{h^3(h+U)(2h+U)}, \tag{8}$$

where Eq. (8) naturally applies only for the regime $\mu > 0$, where the pair is bound. In this regime the binding energy of the pair can then be expressed as

$$\epsilon_b = -\frac{2t^2}{h+U}\mu^2. \tag{9}$$

Equation (8) has the interesting consequence that for $h \gg t$ any finite repulsion $U>0$ induces pair binding but that the region of U in which the pair is bound is limited to $0 < U < U_c = \sqrt{24}h$.

In the regime $h<t$, which is of greater physical interest, we perform exact diagonalization of a 1D system with $N=14$ sites. The results for ϵ_b are we believe obscured by finite-size effects, since we find substantial $\epsilon_b > 0$ even for $h=0$ and $\epsilon_b \sim 0$ for $h>0$. The evidence from the hole density-density correlations $g(r)$, Eq. (7), where the hole density in the Hubbard model is defined as $n_{h,i} = (1-n_{i\uparrow})(1-n_{i\downarrow})$, seems clearer. Results for $g(r)$ in a system with $N_h=2$ at fixed $U/t=8$ and various fields h/t are presented in Fig. 3. While $g(r)$ for $h=0$ is compatible (as in the t-J model) with $g(r)$ for two noninteracting spinless fermions, the binding becomes evident even for weak fields $h/t \gtrsim 0.2$. As expected, in this strong-coupling regime $U/t \gg 1$ $g(r)$ qualitatively agrees

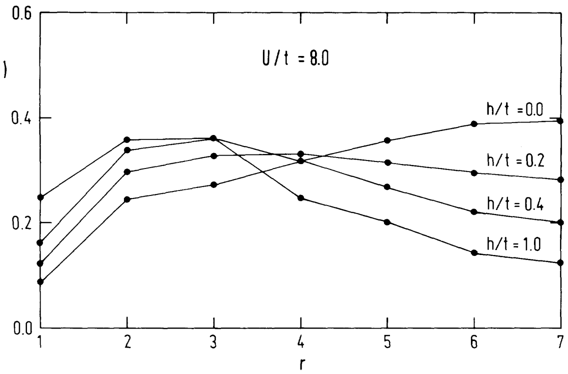

FIG. 3. Hole density-density correlations $g(r)$ vs r for two holes in the Hubbard model with $U/t=8$ and for different values h/t. Results are for the chain length $N=14$.

with that in the t-J model. Moreover, we find that $g(r)$ depends only weakly on U/t. In particular, our results for $U/t=4$ (not presented here) indicate that the maximum in $g(r)$ remains at $r=3$ for $h/t=0.4, 1.0$. On decreasing U/t the local density fluctuations increase the value of $g(r)$ and the maxima become less pronounced. In contrast to the t-J model, the transition to the unbound holes happens to be abrupt (via a level crossing) in a small system, and appears, e.g., at $U_c/t \gtrsim 8$ at $h=t$.

Within the 1D Hubbard model the interpretation of numerical results for more holes is less straightforward than for the t-J model discussed above. There seems to be no indication for the existence of the phase separation within the model at arbitrary h. This is consistent with the situation in 1D at $h=0$ [3], which is believed to be valid also for higher dimensions, although for 2D systems some evidence for possible inhomogeneous hole configurations and phase separation is coming from the results obtained within the Hartree-Fock approximation [16]. In our case we find the parameter $\Delta \propto \kappa^{-1}$ definitely positive for all cases, although decreasing with h. Also $g(r)$ for $N_h=4$ (not presented here) shows some variations with h. When compared to data in Fig. 2 these are quite subtle, which is more plausible due to the substantial pair radius $r \gtrsim 3$ for the system size ($N=14$) investigated here. Still, for finite $h>0$ the tendency is for $g(r)$ to increase at $r \sim 1$ and to decrease at intermediate $r \sim N/4$, consistent with the evidence for pairing presented in Fig. 2 for the t-J model. Our difficulties in establishing the pairing in the Hubbard model arise from the fact that pairs are not entirely localized in any limit, as evident also from the perturbation expression (8).

In conclusion we note that our analytical and numerical results reveal that a staggered field in both the t-J and Hubbard models appears to induce the pairing of holes. There are some qualitative differences in the behavior between the two models, in particular at large fields $h \gg t$ where the t-J model reveals a much stronger pair binding. This discrepancy can likely be reconciled by taking into account the next-nearest-neighbor hopping term [9], which is of the order of J. Our observation of pairing in a 1D model with $h>0$ is of relevance for 2D systems with pronounced AFM correlations, so we feel that our observation of pairing resurrects some hope that a paired ground state exists in repulsive, purely electronic 2D models. It should be stressed, however, that our results apply directly only to 1D models with the long-range AFM ordering (induced by $h>0$). Finite-range AFM correlations seem not to be sufficient to enable a stable pairing in 1D, while in higher dimensions the latter possibility is not excluded.

This work was supported in part by DOE Grant No. JF971, approved by the U.S.-Yugoslav Joint Board, and by the U.S. DOE. We thank Vic Emergy for useful comments.

[1] P. W. Anderson, Science **235**, 1196 (1987).
[2] V. J. Emery, in *Highly Conducting One-Dimensional Solids*, edited by J. T. Devreese *et al.* (Plenum, New York, 1979), p. 247; J. Sólyom, Adv. Phys. **28**, 201 (1979).
[3] E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. **20**, 1445 (1968).
[4] P.-A. Bares and G. Blatter, Phys. Rev. Lett. **64**, 2567 (1990); B. Sutherland, Phys. Rev. B **12**, 3795 (1975).
[5] F. D. M. Haldane, Phys. Rev. Lett. **45**, 1358 (1980); J. Phys. C **14**, 2585 (1981).
[6] H. J. Schulz, Phys. Rev. Lett. **64**, 2831 (1990).
[7] M. Ogata, M. Luchini, S. Sorella, and F. F. Assaad, Phys. Rev. Lett. **66**, 2388 (1991).
[8] W. F. Brinkman and T. M. Rice, Phys. Rev. B **2**, 1324 (1970).
[9] S. A. Trugman, Phys. Rev. B **37**, 1597 (1988); B. I. Shraiman and E. D. Siggia, Phys. Rev. Lett. **60**, 740 (1988).
[10] J. Bonča, P. Prelovšek, and I. Sega, Phys. Rev. B **39**, 7074 (1989).
[11] J. Bonča and P. Prelovšek, Phys. Rev. B (to be published); P. Prelovšek, J. Bonča, and I. Sega, in *Proceedings of the International Conference on Materials and Mechanisms of Superconductivity and High-Temperature Superconductors, Kanazawa* [Physica (Amsterdam) **185-189C**, 1499 (1991)].
[12] M. Ogato and H. Shiba, Phys. Rev. B **41**, 2326 (1990).
[13] V. J. Emery, S. A. Kivelson, and H. Q. Lin, Phys. Rev. Lett. **64**, 475 (1990).
[14] W. O. Putikka, M. U. Luchini, and T. M. Rice, Phys. Rev. Lett. **68**, 538 (1992).
[15] G. Fano, F. Ortolani, and A. Parola, Phys. Rev. B **42**, 6877 (1990); H. Q. Lin, Phys. Rev. B **44**, 7151 (1991).
[16] D. Poilblanc and T. M. Rice, Phys. Rev. B **39**, 9749 (1989); J. Zaanen and O. Gunnarsson, Phys. Rev. B **40**, 7391 (1989); J. A. Vergés, E. Louis, P. S. Lomdahl, F. Guinea, and A. R. Bishop, Phys. Rev. B **43**, 6099 (1991).