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Charged solitons in the Hartree-Fock approximation to the large-U Hubbard model

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Stable Hartree-Fock solutions consisting of parallel arrays of line defects in the antiferromagnetic order are found in the large-U Hubbard model, in two dimension near to half-filling. The excess holes are bound by a gain in kinetic energy of order t to form charged-soliton lines. There is a close parallel to one dimension. Quantum fluctuations are not treated but are expected to be important.

INTRODUCTION

The properties of strongly correlated electrons are topical because of the high-T_c copper-oxide superconductors.[1] The simplest model of this type is a one-band Hubbard model

$$H=t\sum_{\langle i,j\rangle,\sigma}(c_{i\sigma}^{\dagger}c_{j\sigma}+c_{j\sigma}^{\dagger}c_{i\sigma})+U\sum_{i}n_{i,\uparrow}n_{i,\downarrow}\,, \tag{1}$$

where $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$ is the number operator for particles on site i with spin σ, and U and t are the on-site Coulomb repulsion and the hopping matrix element between nearest neighbors (NN), respectively. This model is too simple to describe in detail the CuO_2 planes with d states on the Cu atoms and p states on the O atoms. The two-band model, however, can be reduced in certain limits to an effective one-band Hamiltonian $\tilde{H}$ of the t-J form[2] (written here for electrons),

$$\tilde{H}=-t\sum_{\langle i,j\rangle,\sigma}(a_{i\sigma}^{\dagger}a_{j\sigma}+a_{j\sigma}^{\dagger}a_{i\sigma})+\sum_{\langle i,j\rangle}J(\mathbf{S}_i\cdot\mathbf{S}_j-\tfrac{1}{4}n_in_j)\,, \tag{2}$$

where

$$a_{i\sigma}^{\dagger}=(1-n_{i,-\sigma})c_{i\sigma}^{\dagger}\quad\text{and}\quad n_i=\sum_{\sigma}c_{i\sigma}^{\dagger}c_{i\sigma}\,.$$

The parameters t and J describe the hopping matrix element for the charged singlet and the NN Heisenberg coupling. There is a close relationship between H and $\tilde{H}$ since it has long been known that H can be transformed into $\tilde{H}$ by means of a canonical transformation in the limit $t/U\ll 1$ and the deviation from half-filling is small [i.e., $n_h(=1-\sum_{\sigma}\langle n_{i\sigma}\rangle)\ll 1$]. In this case $J=4t^2/U$.

Recently there has been a lot of work on mean-field approximations to $\tilde{H}$. The difficult local constraint in $\tilde{H}$, which limits the occupation on any site to at most one electron, can only be approximately treated. In this paper we examine the Hubbard Hamiltonian (1) for which this problem as such does not appear. We will use a Hartree-Fock approximation and take t/U, $n_h\ll 1$. Our motivation is threefold. First, quite a lot is known about the properties in one dimension.[3,4] A comparison of our Hartree-Fock results with exact results in one dimension is instructive. Second, we were motivated by the recent Hartree-Fock calculations of Zaanen and Gunnarson using a two-band model.[5] The comparison between two- and one-band models is useful. Third, the recent discovery of incommensurate spin fluctuations in $La_{2-x}Sr_xCuO_4$ crystals[6] is a further motivation since such correlations are predicted in Hartree-Fock calculations. Our calculations were only done at a large value of U and the exact relationship to the spin-bag polarons introduced by Schrieffer, Wen, and Zhang[7] and studied in detail by Su[8] at intermediate U requires further consideration.

HARTREE-FOCK EQUATIONS

In the mean-field approximation, the U term in (1) is linearized (for holes) as

$$H_U=U\sum_{i}(\langle n_{i,\uparrow}\rangle n_{i,\downarrow}+\langle n_{i,\downarrow}\rangle n_{i,\uparrow}-\langle n_{i,\uparrow}\rangle\langle n_{i,\downarrow}\rangle)\,. \tag{3}$$

We look for a solution where the average values $\langle n_{i,\sigma}\rangle$ are spatially varying. We take the real-space supercell to be a rectangle (or a square) of L sites and minimize the energy with this constraint. We consider only supercells with an even number of holes and impose the further constraint that the up and down spin bands are degenerate. This excludes ferromagnetic polaron-type solutions which in the t-J model are unstable above $J/t\sim 0.07$.[9] If $L=2$, the Hartree-Fock (HF) ground state is the simple commensurate antiferromagnetic (AF) phase of wave vector $\mathbf{Q}_0=(\pi,\pi)$.[10] This applies to the half-filled band where the solution is simply $\langle n_{i\sigma}\rangle=\frac{1}{2}[1+\sigma m(-1)^{i_A}]$ with $i_A=2$ for the $i\in A$ sublattice and $i_A=1$ otherwise. In the limit $t/U\to 0$, $m\sim 1-2J/U$ and energy per site $E_{\rm tot}=-J$/site corresponding to a simple Néel state. The energy of a single additional hole $E_{\rm tot}(N+1)-E_{\rm tot}(N)$ has a minimum value $U-J$ in this limit. For finite n_h this phase is not stable with respect to a phase of large supercell with nonuniform spin and charge.

The Bloch waves of (3) are constructed in the reduced Brillouin zone [of size $(2\pi)^2/L$] as

$$\Psi_{\mathbf{k}\sigma}^{\dagger}=\sum_{\mathbf{R}}\sum_{j=1}^{L}\alpha_{j\sigma}(\mathbf{k})c_{\mathbf{R}+j\sigma}^{\dagger}\exp i\mathbf{k}\cdot(\mathbf{R}+\mathbf{r}_j)\,, \tag{4}$$

with

$$1/L\sum_{j=1}^{L}|\alpha_{j\sigma}(\mathbf{k})|^2=1\,.$$

$|\alpha_{j\sigma}(\mathbf{k})|^2$ is the weight of the state $(\mathbf{k},\sigma)$ on the site j in the supercell and is obtained by solving, for a given $(\mathbf{k},\sigma)$

state, the $L\times L$ linear system,

$$\sum_j H_{ij}^{\sigma}(\mathbf{k})\alpha_{j\sigma}(\mathbf{k}) = E_{\mathbf{k}\sigma}\alpha_{i\sigma}(\mathbf{k}) , \tag{5}$$

where

$$H_{ij}^{\sigma}(\mathbf{k}) = U\langle n_{i-\sigma}\rangle\delta_{ij} + \sum_{\mathbf{R}} \exp i\mathbf{k}\cdot(\mathbf{R}+\mathbf{r}_{ij}) t_{i,j+\mathbf{R}} .$$

The hopping integral $t_{i,j+\mathbf{R}}$ is nonzero when i and $j+\mathbf{R}$ are NN. The energy spectrum then contains L bands (labeled by l). Self-consistency is ensured by the set of coupled nonlinear equations,

$$\langle n_{i\sigma}\rangle = \sum_{l=1}^{L} \sum_{|\mathbf{k}|<k_F^{\sigma}} |\alpha_{i\sigma}^{(l)}(\mathbf{k})|^2 , \tag{6}$$

with

$$1/L \sum_{\sigma,i=1}^{L} \langle n_{i\sigma}\rangle = n .$$

One should not forget that $|\alpha_{i\sigma}(\mathbf{k})|^2$ is itself a function of all the $\langle n_{j\sigma}\rangle$. The summation in (6) is performed up to the Fermi level. n is the total hole density close to half-filling, i.e., $n=1+n_h$, $n_h=1/N_0$ ($N_0\geq 5$). N_0 is related to the order of commensurability of the superstructure.

SOLITON LINE

We investigate the simplest kinds of solutions which have many features of a one-dimensional problem. We consider the possibility for the AF background to have a series of line defects localized along the (1,0) or the (1,1) directions and we minimize the HF energy by iterating Eqs. (5) and (6). Obviously these stable solutions are *a priori* local minima of the HF energy. Although it is impossible to assert that our lowest minimum [the (1,1) soliton] is actually the absolute minimum of the class of the HF solutions, this study proves that the kinetic-energy gain per hole can be of order t within HF. On each side of the solitons, the AF order parameter has a phase difference of π. The argument that such a phase difference would spread out over large distances to minimize exchange energy does not apply in the presence of the charged soliton.[11] Since the soliton line is a line of zeros in the magnitude of the order parameter there is no inconsistency in having a π phase shift on either side of the line and no tendency to twist the order parameter. In the half-filled band, this is an excited state with a magnetic energy cost of order $J/2$ at the boundary. However, such a state becomes a lowest HF ground state as doping is introduced. The (1,0) soliton line is centered on a row of sites ($S1$) or between two neighboring rows of sites ($S2$). ($S1$) and ($S2$) are antisymmetric and symmetric, respectively, with respect to a reflection along the soliton line. The soliton line along (1,1) (called $S3$) is obtained by considering an $L\times L$ supercell, L odd, with a phase shift of π in the AF order parameter on the diagonal of the cube.

The size of the supercell is closely related to the density; we have shown that the lowest energy is achieved for exactly one additional hole per site on the line. We have studied different sizes of such supercells for $J/t=0.25$; from $L=14$ (2×7) up to $L=26$ (2×13) for $S1$ and $S2$ and $L=25$ (5×5) and $L=49$ (7×7) for $S3$. The self-consistent on-site charge and spin densities are plotted in Fig. 1. The added hole density vanishes at distances of more than a few lattice spacings from the central line. The shape of the charge density is then size (L) invariant. The staggered magnetization, away from the line, also rapidly reaches the equilibrium value of $1-2J/U$ of the uniform AF phase $n_h=0$.

The holes of spin $-\sigma$ take advantage of the bottom of the self-consistent potential $U\langle n_{i,\sigma}\rangle$ until all minima are filled. On the other hand, the excess hole sits at the top of the potential losing energy of order U. A general feature of our solutions is that the excess hole can benefit from the t term in (1) by delocalizing over at least two nearest-neighbor maxima of the potential resulting from the soliton formation. If the line is located between two rows of sites ($S2$), these adjacent levels have the same energy so that the kinetic part of the Hamiltonian will introduce a splitting of $2t$ between them. With half a hole per site, the energy gain is then roughly t (per hole). If the soliton is located on the sites (like $S1$ and $S3$), the energy gain estimation is slightly more complicated; a one-dimensional HF calculation with three sites leads to an energy gain of $\sim t \gg J$ for $U\sim 12-16$.

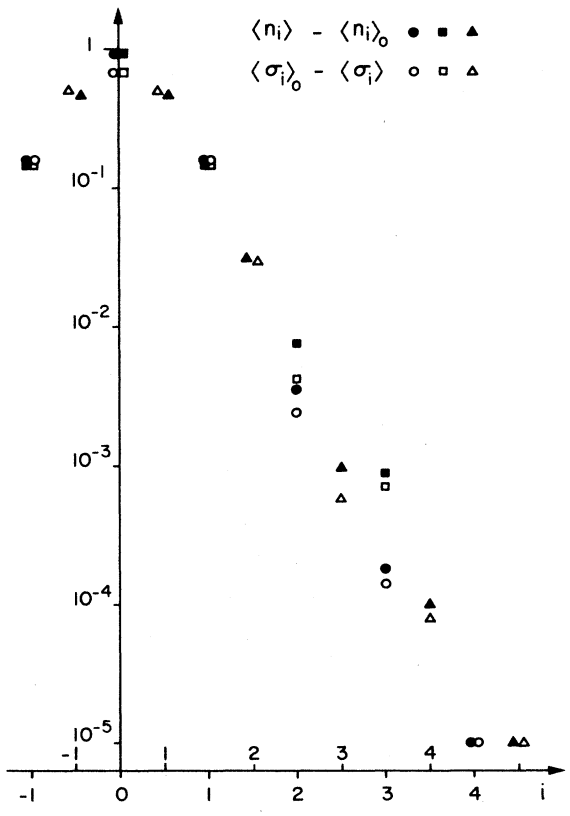

FIG. 1. Charge (filled circles) and spin (open circles) density deviations $\langle n_i\rangle-\langle n_i\rangle_0$ and $\langle\sigma_i\rangle_0-\langle\sigma_i\rangle$ from the unperturbed state ($n_h=0$) vs position i perpendicularly to the soliton line. The circles, triangles, and squares correspond to the $S1$, $S2$ (1,0) and $S3$ (1,1) solitons, respectively.

These preliminary considerations are confirmed by the numerical calculations of the energy spectra shown in Figs. 2(a) and 2(b) [for the (1,0) solitons for simplicity]. The midgap states are localized by the HF potential $U\langle n_{i\sigma}\rangle$ in the vicinity of the magnetic line. The solitons are independent since tiny energy dispersion is found perpendicularly to the line (x direction). Along y, this dispersion is usually weak (of order J) except for the upper midgap band of soliton $S1$. In this case, the HF potential at the soliton center is identical along y so that the t coupling is at a maximum. However, this does not lead to an energy gain because the band is completely filled. The actual kinetic gain always comes from the overall lowering of the midgap band due to hopping perpendicular to the line.

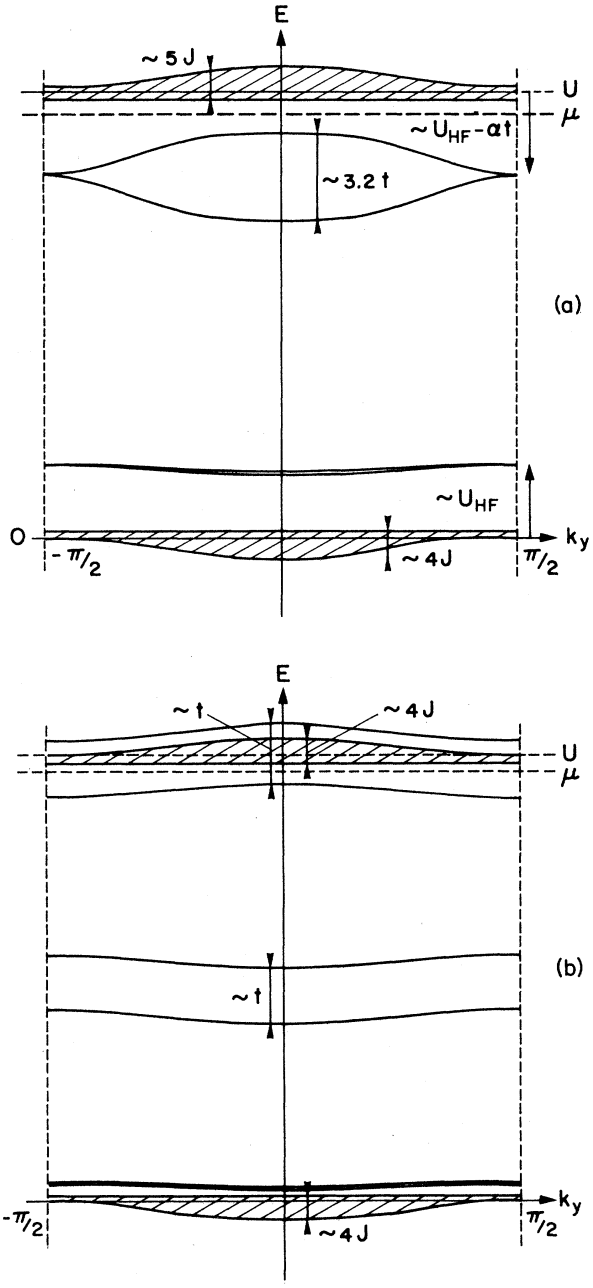

FIG. 2. Energy dispersion spectrum of the (1,0) solitons along the magnetic line: (a) $S1$ soliton, $\alpha\sim 0.5$; (b) $S2$ soliton, the midgap and the upper states are split by the hopping perpendicular to the line.

TABLE I. Numerical results of the mean-field energies for $J/t=0.25$. From the total energy per site, we extract the energy costs (after subtracting U) to add one hole to the AF uniform state. The first, second, and third columns correspond to the $S1$, $S2$, and $S3$ solitons, respectively (see text).

	Energy expectation values		
Size	$L=2\times 9$ ($n_h=\frac{1}{9}$)	$L=2\times 9$ ($n_h=\frac{1}{9}$)	$L=7\times 7$ ($n_h=\frac{1}{7}$)
E_{tot}/site	1.42992	1.42370	1.8758
E_U/U/hole	1.1406	1.1327	1.1023
ΔE_U/hole $-U$	0.124	−0.003	−0.009
ΔE_{tot}/hole $-U$	−0.923	−0.979	−1.15

The small gap in the charge excitation spectrum is of order $4J$ (compared to the AF excitation gap $U-2J$). The Fermi level lies in this gap if the line contains exactly one extra hole per site. Indeed, if one reduces the hole density (for a fixed supercell), then the top of the upper midgap band begins to empty which is energetically unfavorable. The system will then spontaneously choose a new supercell in order to keep the Fermi level pinned in the gap.

We have compared these states to the AF state at $n=1$ and computed the energy difference

$$\Delta E_{tot}/\text{hole}=E_{tot}(N+1)-E_{tot}(N)$$

to add one hole to create an incommensurate phase (see Table I). As expected, this quantity of order $U-t$ is size independent since the soliton spacing is larger than its width (of order 3 sites). The small extra kinetic-energy gain of the (1,1) compared to (1,0) lines comes from the small delocalization of the centered spin not only along x but also along y.

DISCUSSION

Our HF results show periodic arrays of line defects or line solitons along the (1,1) direction similar to the Zaanen-Gunnarson results for the two-band model. Taking the Fourier transforms of the charge- and spin-density distributions we obtain a set of δ functions (Fig. 3). In an array of (1,1) solitons, the $\mathbf{Q}_0$ magnetic order is modulated by a periodicity $2A$, $A=N_0/\sqrt{2}$ being the soliton spacing, so that the strongest spin-density wave (SDW) peak is at $\tilde{\mathbf{Q}}_0(Q_0-\pi/A)=(1-n_h)\mathbf{Q}_0$. The charge-density modulation corresponding to the A spacing gives a peak at $2\pi/A\tilde{\mathbf{Q}}_0=2n_h\mathbf{Q}_0$.

The energy cost to distort the soliton line is small and the Hamiltonian contains large matrix elements $\sim t$ to move each hole. The key question is whether the array of parallel soliton lines remains or whether the fluctuations

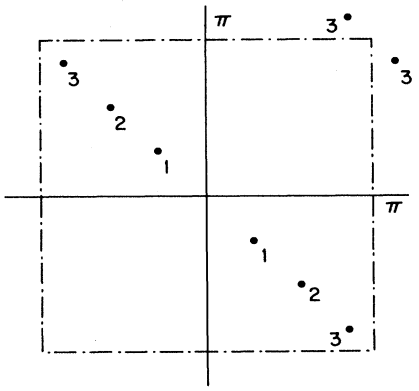

FIG. 3. Reciprocal lattice vectors for the (1,1) soliton. For the spin density (charge density), the weights are 1.0 (0.48), 0.22 (0.71), and 0.06 (1.0) at the $\mathbf{Q}_3=\mathbf{Q}_0-1/N_0\mathbf{Q}_0$ [where $N_0=1/(n-1)=7$], $\mathbf{Q}_2=2\mathbf{Q}_1$ and $\mathbf{Q}_1=2/N_0\mathbf{Q}_0$, and wave vectors, respectively ($J/t=0.25$).

due to the hole kinetic energy etc., will destroy long-range order. An alternative way of posing the question is to note that these HF solutions gain a kinetic energy $\sim -1.15t$ per added hole, but this is above the energy $\sim -3.48t$ which is possible for a hole to gain in the retraceable path approximation[12] ($J=0$). Zero-point fluctuations should be very important. It should be noted however that the discrepancy is actually smaller if one compares $E_{\rm tot}(N+1)-E_{\rm tot}(N)$ in our solution ($\sim -1.15t$) to the same quantity obtained by exact diagonalization *for the same finite value of* J/t;[9,13] in HF, adding a hole does not cost significant magnetic energy.

It is useful to look at the analogous limit in one dimension where many exact results are known. For repulsive interactions, away from half-filling, the problem is known to scale onto the Tomonaga line.[4] In the limit of strong repulsive interactions, in the Tomonaga model, there are divergences at $2k_F$ and $4k_F$ in SDW and charge-density wave (CDW) response functions, respectively (for example, see Ref. 4);

$$\chi(2k_F,\omega)\sim(\omega/E_F)^{-1+1/\gamma_\sigma},$$
$$N(4k_F,\omega)\sim(\omega/E_F)^{-2+1/\gamma_\sigma}, \tag{7}$$

where ω is the frequency, k_F is the Fermi wave vector, and the exponent $\gamma_\sigma=(1+\tilde{U}/4\pi t)^{1/2}$. We denote the scaled repulsion as $\tilde{U}$. If we use the weak-coupling form then $\tilde{U}=U/2$. Thus χ and N approach universal values in the limit $\tilde{U}/4\pi t\rightarrow\infty$. In one dimension the zero-point fluctuations destroy long-range order but divergencies remain in the response functions.

The primary wave vectors for SDW and CDW order $(1-n_h)\mathbf{Q}_0$ and $2n_h\mathbf{Q}_0$ are analogous to $2k_F$ and $4k_F$ in one dimension. The question of whether divergencies remain in two dimensions at these wave vectors we cannot answer. Nonetheless it would be worthwhile to look for them in experiments. The report of incommensurate short-range order in certain $La_{2-x}Sr_xCuO_4$ samples is encouraging.[6] It may be possible to see a $4k_F$ divergence by x rays, for example, although a charge localization in the copper oxides on a single Cu site should mainly show up as a modulation of the Cu-O distances in the plane rather than the Cu-Cu distances which may make it more difficult to observe. Finally, the influence of such incommensurate fluctuations, if they exist, on possible superconducting states is an open question. It is interesting to note in this connection that Bonča, Prelovšek, and Sega[9] found evidence for hole-hole pairing preferentially along (1,1) axes, a similar orientation to the soliton lines.

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