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Domain walls in a doped antiferromagnet

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Résumé. — Les effets d'une faible concentration de trous sur l'état antiferromagnétique du modèle de Hubbard bidimensionnel sont étudiés analytiquement et numériquement. On trouve qu'il est énergétiquement favorable de former des parois d'une largeur finie, avec les trous localisés dans des états liées aux parois. Pour une concentration faible mais finie de trous, un réseau régulier de parois est stable, c'est-à-dire on a un état antiferromagnétique incommensurable isolant, avec une aimantation polarisée linéairement et un vecteur d'onde variant linéairement avec la concentration des trous. Si la répulsion électron-électron croît, l'orientation préférée des parois change de parallèle à une direction du réseau à diagonale. La possibilité d'effets fluctuatifs dans la phase incommensurable ainsi que le rapport avec des expériences récentes sur La$_{2-x}$Sr$_x$CuO$_4$ sont discutés.

Abstract. — The effects of a small amount of holes on the antiferromagnetic state of the two-dimensional Hubbard model are investigated analytically and numerically. It is found that it is energetically favorable for the system to form domain walls of finite width, with the holes localized in bound states at the walls. For a small but finite concentration of holes, a regularly spaced array of domain walls is formed, i.e. one has an insulating incommensurate antiferromagnet, with a linearly polarized magnetisation pattern and a modulation wavevector proportional to the hole concentration. With increasing electron-electron repulsion, the preferred orientation of the walls changes from parallel to a lattice direction to diagonal. Possible fluctuation effects in the incommensurate phase and relations with recent experiments on La$_{2-x}$Sr$_x$CuO$_4$ are discussed.

1. Introduction.

One of the most interesting and probably also most significant physical properties of high-temperature superconductors [1, 2] is the close proximity of superconducting and insulating antiferromagnetic phases: for exactly one d-band hole per copper atom in the CuO$_2$-layers, these compounds are insulating antiferromagnets [3, 4], whereas introduction of extra holes (or electrons [5]) leads to the appearance of metallic and superconducting properties. The

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antiferromagnetism is rather straightforwardly explained by correlation effects in a half-filled band, e.g. in the well-known Hubbard model. It is then rather tempting to try to explain superconductivity, and in particular the high critical temperatures, also in terms of electronic, possibly magnetic, mechanisms [6], rather then by the usual phonon-mediated attraction. It is important to realize that the same electrons (in hybridized Cu-O orbitals) are giving rise to both the magnetic and superconducting properties. In this respect high-\(T_c\) superconductors are rather similar to organic superconductors [7], where a magnetic mechanism is indeed believed to be responsible for superconductivity [8].

It is thus of great importance to understand the effect of a small concentration of holes in an otherwise half-filled band: what are the properties of these holes (mobility etc.), what is the effect of these holes on the magnetic properties, can the coupling of the holes to magnetic degrees of freedom lead to superconductivity? In the framework of the Hubbard model, these questions have been investigated starting both from the limits of weak [9, 10] and strong [6, 11, 12, 13] electron-electron interaction (real compounds probably are in some intermediate regime). In most of these investigations, it is assumed that a small concentration of holes does not change the two-sublattice structure of the antiferromagnetic state. With increasing hole concentration the antiferromagnetic order parameter then decreases, until it eventually disappears at some critical concentration. A recent calculation for strong electron-electron repulsion finds a critical concentration of about 6\% [14]. In this picture, the doped holes then are mobile even at infinitesimally small concentrations, which strictly speaking should lead to metallic low temperature properties in this idealized (especially disorder-free) model.

An alternative possibility is suggested by one-dimensional charge-density-wave systems [15, 16]: in that case deviations from half-filling lead to the appearance of a regularly spaced array of domain walls (solitons) at which the holes are localized. Upon further increase in hole concentration this state smoothly transforms into a sine-wave incommensurate structure. In the present paper I will show that this is also what happens in the two-dimensional case relevant to high-\(T_c\) compounds, at least in the framework of the Hartree-Fock approximation (which is expected to be reliable in the weak correlation limit, see Sect. 5). In the strong-correlation limit, domain walls have been studied recently [17, 18]. The results presented here cover a wide range of correlation strengths, and will make clear the similarities and differences between different limiting cases. That the present calculation has some relevance to the experimental situation is indicated by recent experiments [19] showing incommensurate short-range antiferromagnetic order in strontium-doped \(La_2CuO_4\).

In the following section, the appearance of incommensurate antiferromagnetism will be shown using the Stoner criterion in the weak-coupling limit. In sections 3 and 4 analytical and numerical results for single domain walls of different types will be derived. Finally, in section 5, the implications of these results for the effect of doping on antiferromagnetism, quantum and thermal fluctuation effects in the incommensurate phase and some possible experimental implications will be discussed.

2. Stoner criterion.

I consider the standard Hubbard Hamiltonian

\[ H = -t \sum_{<rr'>} \left( a_{rs}^+ a_{r's}^+ + a_{rs} a_{r's} \right) + U \sum_r n_{r\uparrow} n_{r\downarrow}, \tag{2.1} \]

where \(a_{rs}\) destroys an electron at site \(r\) with spin projection \(s\), and \(\langle rr'\rangle\) indicates summation over all nearest-neighbor pairs on a square lattice. The single-particle eigenenergies of (2.1)
are $\varepsilon_k = -2t(\cos(k_x) + \cos(k_y))$. For exactly one electron per site (half-filled band) the model has a two-sublattice commensurate antiferromagnetic groundstate (here and in the following « commensurate » is understood to mean « two-sublattice antiferromagnet »). In order to understand what happens to this state when there is slightly less (or more) than one electron per site, consider the RPA-(Stoner) criterion for occurrence of a magnetic instability with modulation wavevector $k$:

$$1 - (U/2)\chi_0(k, T) = 0, \quad (2.2)$$

where $\chi_0$ is the $k$-dependent magnetic susceptibility of the noninteracting system at temperature $T$:

$$\chi_0(k, T) = \frac{1}{2\pi^2} \int d^2q \frac{f(\varepsilon_{q+k}) - f(\varepsilon_q)}{\varepsilon_q - \varepsilon_{k+q}}, \quad (2.3)$$

and $f(\varepsilon)$ is the Fermi occupation function. In the vicinity of half-filling the chemical potential $|\mu|$ is small, and then an expansion for $|\mu|, T \ll t, |q| \ll \pi$ gives

$$\chi_0(Q_0 + q, T) = \chi_0(Q_0, T) - \frac{1}{4\pi^2t} [f(\bar{\mu}, \bar{q}_+) + f(\bar{\mu}, \bar{q}_-)], \quad (2.4)$$

where $Q_0 = (\pi, \pi)$ is the wavevector of the commensurate state, $\bar{q}_\pm = t(q_x \pm q_y)/2\pi t$, $\bar{\mu} = \mu/2\pi T$, and

$$f(x, y) = \text{Re} \int_{-\pi}^{\pi} \frac{du}{\sin u} \left[ \psi \left( \frac{1}{2} + ix + iy \sin u \right) - \psi \left( \frac{1}{2} + ix \right) \right]. \quad (2.5)$$

Here $\psi$ is the digamma function. At zero temperature one has the limiting form

$$\lim_{x, y \to \infty} f(x, y) = -2 \frac{\text{Re}}{2} \arcsin^2 \left( \frac{y}{x} + i0^- \right) \quad (2.6)$$

As long as $\text{Re} [\psi"((1/2 + ix)] < 0$, i.e. as long as $|x| < x_0 = 0.30409\ldots$, $y = 0$ is a minimum of $f(x, y)$, and consequently $\chi_0$ has its maximum at $Q_0$. On the other hand, for $|x| > x_0$, the minimum of $f$ occurs at $y \neq 0$, and consequently the maximum of $\chi_0$ is at wavevectors $Q_1 = (\pi \mp \delta, \pi)$ and at the symmetry-related $Q_2 = (\pi, \pi \mp \delta)$. In the physical variables, this corresponds to $|\mu| > 2x_0\pi T$. From equation (2.6) one finds at zero temperature $\delta = \mu/t$. For sufficiently large deviation from half-filling and sufficiently weak $U$ the antiferromagnetic instability therefore occurs at an incommensurate wavevector. The phase diagram obtained from equations (2.2) and (2.4) is shown in figure 1. A more detailed analysis [20] shows that close to the transition the incommensurate phase has a sine-like (not spiral) magnetic structure, characterized by a single wavevector $Q$:

$$\langle m_z(r) \rangle = m_0 \cos (Q \cdot r), \quad (2.7)$$

where $Q = Q_1$ or $Q = Q_2$ close to the transition, i.e. the discrete lattice symmetry is also broken.

The simple one-harmonic form of the spin modulation (2.7) is only appropriate close to the transition line. Further inside the incommensurate phase, and in particular in the immediate vicinity of half-filling, higher harmonics are very important, as will be seen in the following sections.
3. Analytical results.

3.1 HARTREE-FOCK EQUATIONS. — Motivated by the observation that the magnetically ordered state is of the sine-wave type (i.e. it is not a spiral), I use the following decomposition of the local number operators:

$$n_{rs} = \langle n_{rs} \rangle + \delta_{rs} \ .$$  \hfill (3.1)

In the Hartree-Fock approximation one then neglects terms of second order in the fluctuation operators $\delta_{rs}$. Introducing the local charge and (z-direction) magnetization operators by

$$\rho_r = n_{r\uparrow} + n_{r\downarrow} \ , \quad \sigma_{zr} = n_{r\downarrow} - n_{r\uparrow} \ ,$$  \hfill (3.2)

and the corresponding averages

$$n(r) = \langle \rho_r \rangle , \quad m(r) = (-1)^{r_z} \langle \sigma_{zr} \rangle \ .$$  \hfill (3.3)

the Hartree-Fock effective single-particle Hamiltonian becomes

$$H_{HF} = -t \sum \langle \mathbf{r} \mathbf{r}' \rangle_s (a_{rs}^+ a_{rs} + a_{rs}^+ a_{rs}^\dagger)$$

$$+ \frac{U}{2} \sum \left[ n(r) \rho_r - (-1)^{r_z} m(r) \sigma_{zr} + \frac{1}{2} (m^2(r) - n^2(r)) \right] \ .$$  \hfill (3.4)

The corresponding single-particle eigenequations with spin projection $s$ are given by the eigenvalue equations

$$-t \sum_{r'} \psi_s(r') + \frac{U}{2} \left[ n(r) - (-1)^{r_z} sm(r) \right] \psi_s(r) = E \psi_s(r) \ ,$$  \hfill (3.5)

where the summation over $r'$ is over the four nearest neighbours of lattice site $r$. As usual, $n(r)$ and $m(r)$ have to be determined selfconsistently from the solutions of (3.5). One should note that the decomposition (3.1) is only appropriate for linearly polarized (e.g. sine-wave) spin structures. More complicated structures (e.g. spirals) would necessitate a different decomposition.
For exactly one particle per site the ground state is a two-sublattice commensurate antiferromagnet, with spatially constant $m$ and $n$. The finite value of $m$ couples single-particle eigenstates with wavevectors $k$ and $k + Q_0$, leading to a gap $\Delta = U m / 2$ in the spectrum of single-particle states:

$$E_{k \pm} = \pm \sqrt{\varepsilon_k^2 + \Delta^2 + U / 2}.$$  \hfill (3.6)

The gap coincides with the Fermi surface of the metallic ($m = 0$) state, so that, at $T = 0$ all occupied states have their energies lowered, leading to an energy gain of order $\Delta^2 / U$ per particle (for small $\Delta$), due to a lower exchange energy in the antiferromagnetic state (this is the well-known Peierls mechanism [21]).

If there is slightly less or more than one electron per site, the discussion of the last section suggests the presence of an incommensurate antiferromagnetic structure (Eq. (2.7)). This spin modulation couples single-particle eigenstates at wavevector $k$ with states at $k + Q$, with matrix element $U m_0 / 4$. With the appropriate choice of $Q$, this leads to a splitting of degeneracy of states at the Fermi surface in such a way that all or most of the occupied states (at zero temperature) have their energy lowered, whereas the unoccupied state increase their energy, leading to a gain of energy with respect to the nonmagnetic state. However, in the incommensurate case the gap is only $U m_0 / 4$, compared to $U m / 2$ in the commensurate case, and consequently the gain in exchange energy is much lower for an incommensurate modulation. Another reason favouring a commensurate over an incommensurate state is the diverging density of states at the Fermi surface for half-filling. Finally, nesting is only perfect for exactly one electron per site, and nesting enhances the energy gain due to formation of the antiferromagnetic structure.

These arguments suggest that the system can gain exchange energy by forming large regions where there is one electron per site, and put the extra holes or particles into some sort of localised states (Fig. 2). As will be seen, these localised states are situated at extended defects, namely domain walls. Of course, the gain in exchange energy is partly compensated

![Fig. 2. — The local order parameter $\Delta(x) = U m(x) / 2$ (circles) and the electron density $n(x)$ (squares) for a situation with two type I vertical walls, centered at $x = 13$ and $x = 37$, as determined from the selfconsistent solution of the Hartree-Fock equations for $U = 3t$. Full and empty symbols are results with and without the charge interaction terms, respectively. Note that inclusion of the charge interactions increases the width of the walls. Even though this seems to be a small effect here, it leads to appreciable changes in energy (compare Figs. 4 and 5).](image)
by an increase in kinetic energy, due to the localisation of carriers. Consequently, the commensurability effect is strongest for relatively large $U$ (compared to $|\mu|$) and small hole concentration, where the exchange effects are strong and the kinetic effects weak. The precise stable ground state has to be determined from the full Hartree-Fock equations (3.4), (3.5).

3.2 DIAGONAL WALL. — The symmetry of the problem suggests that domain walls will be oriented either along a diagonal or a lattice vector. For simplicity we first consider the diagonal case. Defining new variables $r_\xi = x \pm y$, for a diagonal domain wall $m(r)$ and $n(r)$ depend on $r_+$ only. The motion parallel to the domain wall then can be separated out by the ansatz

$$\psi_s(r) = e^{i p \cdot r} u_s(r_+) .$$

(3.7)

Inserting into (3.5) one obtains

$$- 2 \cos (p)[u_s(r_+ + 1) + u_s(r_+ - 1)] + \frac{U}{2} [n(r_+) - (-1)^r sm(r_+)] u_s(r_+) = Eu_s(r_+) .$$

(3.8)

For a given solution $u_s(r_+)$ of (3.8) for wavenumber $p$ and energy $E$, $(-1)^r u_s(r_+)$ is a solution of the same energy for wavenumber $p + \pi$. Noting that for any lattice site $r_+$ and $r_-$ are either both even or both odd one sees from (3.7) that the two cases actually correspond to the same wavefunction. Consequently, $p$ is restricted to the interval $(-\pi/2, \pi/2]$, and quantized in units of $2\pi / L_-$, if $L_-$ is the length over which periodic boundary conditions are applied in the $r_-$-direction. In the absence of the charge interaction ($Un(r_+)$) term, equation (3.8) is the same as that studied by Su, Schrieffer, and Heeger for soliton creation in polyacetylene [15], with a $p$-dependent bandwidth.

Now consider a domain-wall type configuration, i.e. a configuration satisfying $m(-r_+) = -m(r_+)$ and $m(+\infty) = \pm m_0$. A variational ansatz (which in one dimension is actually the exact solution [15]) would be

$$m(r_+) = m_0 \tanh \left( \frac{r_+}{\xi} \right) ,$$

(3.9)

where $\xi$ is the width of the wall. There then is, for each $p$-value, at least one bound state in the gap. This can be seen as follows: consider a finite system with $|r_+| = L_+/2$ ($L_+$ even), so that for given $s$ and $p$ there are $L_+ + 1$ solutions to (3.8). Then for each solution $u_s(r_+)$ of (3.8) with energy $E$, $(-1)^r u_s(-r_+)$ is a solution with energy $-E$, i.e. the spectrum is symmetric. As there is an odd number of states, one state with $E = 0$ has to exist. Further, if $L_+ \gg \xi$, most of the system looks nearly like a homogeneous antiferromagnet, and states with energy $|E| < \Delta_0 = U m_0 / 2$ cannot propagate. The $E = 0$ state therefore is a bound state centred on the domain wall. On the other hand, most of the spectrum is changed very little from its from (3.6), i.e. most states have energies above or below the gap. More than one bound state may exist if $\xi$ is not too small [16]. The inclusion of the charge interaction term does not change qualitatively this picture: for small $U$ the bound state level is shifted by an amount proportional to $U / \xi$, and $\xi \approx t / \Delta_0$, if $\Delta_0$ is is the gap parameter of the commensurate state. Consequently, the bound state is shifted down by approximately $(U / t) \Delta_0$ and remains in the gap. The numerical calculations of the next section show that (at least) one bound state exists for any $U$.

The existence of a bound state centered on the domain wall can stabilize a state with domain walls in a system slightly away from half-filling: at exactly half-filling half (due to spin degeneracy) of the bound states would be occupied, at energy cost $E_d$ with respect to the
ground state. Extra holes can now be created, *at no energy cost* (due to the zero energy of the bound state) by taking particles out of occupied bound states, i.e. the extra holes (or particles) would « condense » into the bound states, rather than going into extended states above or below the gap. As there are \( L /2 \) bound states for a domain wall, one for each allowed \( p \)-value, the domain wall is energetically stable if \( E_d < L \Delta_0 /2 \). To insure the stability of a domain wall the existence of a bound state is not enough: exchange energy is lost, due to the local depression of the antiferromagnetic order parameter, the continuum states suffer phase shifts, and the Coulomb energy increases, due to the accumulation of particles in localized states. All these effects are of course included if the full Hartree-Fock equations (3.4), (3.5) are used to calculate \( E_d \).

As in the case of polyacetylene one might try to solve the problem by taking the continuum limit of equations (3.4), (3.5) [22]. Neglecting again the \( U_n(r_+) \)-term, one recovers the equations of Takayama et al. [16], one for each allowed \( p \)-value, with Fermi velocity \( 2 t \cos(p) \). Taking the shape (3.9), the domain wall creation energy (compared to a state with \( m(r) = m_0 = \text{const.} \)) then becomes

\[
E_{d,\text{cont}} = \frac{L_\perp}{2 \pi} \int_{-\pi/2}^{\pi/2} dp \, E_s[\xi \Delta_0 / (4 t \cos(p))] ,
\]

where \( \Delta_0 = U m_0 /2 \) and \( E_s(r) \) is the soliton creation energy given is equations (21) and (A14) of [16]. Now a problem becomes apparent: \( E_s(r) \approx 0.17 \Delta_0 r \) for large \( r \), and consequently the integral (3.10) diverges logarithmically at \( p = \pm \pi /2 \). Thus, \( E_{d,\text{cont}} \) is much larger (in fact, infinite) than \( L_\perp \Delta_0 /2 \), the energy required to put the holes into states below the gap. Consequently, *in the continuum approximation the domain wall is unstable*. The origin of this (artificial) problem is easily found: for \( p \approx \pm \pi /2 \) the effective bandwidth \( W_{\text{eff}} = 8 t \cos(p) \) goes to zero, and consequently the premise of the continuum approximation, \( \Delta_0 \ll W_{\text{eff}} \), fails. Thus, a straightforward continuum calculation of the domain wall energy is not feasible, and I rather use numerical methods to solve equation (3.5), as will be discussed in the following section.

3.3 VERTICAL WALL. — The other high-symmetry situation is the case of a domain wall aligned vertically along the \( y \)-direction (or horizontally along \( x \)). Then \( m(r) \) and \( n(r) \) both depend on \( x \) only. The motion along \( y \) can be separated out by the ansatz

\[
\psi_s(r) = e^{ipy}[u_{s+}(x) + (-1)^y u_{s-}(x)] ,
\]

Inserting into (3.5) the following coupled eigenvalue equations follow:

\[
- t [u_{s+}(x+1) + 2 \cos(p) u_{s+}(x) + u_{s+}(x-1)] + \frac{U}{2} [n(x) u_{s+}(x) - sm(x) u_{s-}(x)] = Eu_{s+}(x) \\
- t [u_{s-}(x+1) + 2 \cos(p) u_{s-}(x) + u_{s-}(x-1)] + \frac{U}{2} [n(x) u_{s-}(x) - sm(x) u_{s+}(x)] = Eu_{s-}(x) .
\]

For a given solution \((u_{s+}(x), u_{s-}(x))\) of (3.12) for wavenumber \( p \) and energy \( E \), \((-1)^y (u_{s-}(x), u_{s+}(x))\) is a solution of the same energy for wavenumber \( p + \pi \). One sees from (3.11) that the two cases actually correspond to the same wavefunction. Consequently, \( p \) is restricted to the interval \((-\pi/2, \pi/2)\), and quantized in units of \( 2 \pi /L_y \), if \( L_y \) is the length over which periodic boundary conditions are applied in the \( y \)-direction. A
variational argument, given in detail in the appendix, shows that there are (at least) two bound states in the gap for each allowed $p$-value, and consequently a domain wall along $y$ can accommodate $L_y$ holes.

As for small $m(x)$ the antiferromagnetic order mainly couples states close to the Fermi surface ($|k_{F_y}| = \pi - |k_{F_x}|$), in a continuum approximation to (3.12) one would make the ansatz

$$u_{s \gamma}(x) = e^{i(\pi \pm p) x} v_{s \gamma}(x),$$

(3.13)

with a slowly varying $v_{s \gamma}$. Note that due to the restriction on $p$ (which here is better taken as $0 \leq p < \pi$), the plus and minus signs in (3.13) correspond to physically different solutions.

Inserting (3.13) into (3.12) and making use of the smoothness of the $v_{s \gamma}$ (i.e. neglecting derivatives higher than the first), one obtains

$$\pm 2it \sin(p) \partial_x v_{s \gamma}(x) - \frac{U}{2} sm(x) v_{s \gamma}(x) = Ev_{s \gamma}(x)$$

(3.14)

These again are exactly the equations of Takayama et al. [16], with effective overlap integral $t \sin(p)$. Due to the freedom of choosing the sign in (3.13), there now are two degenerate $E = 0$ states for each $p$ and $s$. The domain wall energy for a profile of the form (3.9) follows as

$$E_{d, \text{cont}} = \frac{L_y}{\pi} \int_0^\pi dp E_s[\xi A_0/|2t \sin(p)|].$$

(3.15)

We are faced with the same problem as in the last section: the integral diverges, and therefore in the continuum approximation the domain wall is unstable. Again the problem of a vanishing effective Fermi velocity near $p = 0$, $\pi$ is the reason, i.e. the continuum approximation breaks down. The numerical treatment of the problem is given in the next section.

3.4 RELATED MODELS. — Using well-known symmetry operations, one can try to apply the results of this and the next section to a number of other physical situations. First, consider the electron-hole transformation on the down spins:

$$a_{r\uparrow} \rightarrow c_{r\uparrow}, \quad a_{r\downarrow} \rightarrow (-1)^{x+y} c_{r\downarrow}^+.$$  

(3.16)

Under this transformation the Hamiltonian (2.1) becomes

$$H = -t \sum_{<n_r>_{s \gamma}} (c_{r_{s \gamma}}^+ c_{r_{s \gamma}^+} + c_{r_{s \gamma}^+} c_{r_{s \gamma}}) - U \sum_r n_{r\uparrow} n_{r\downarrow} - \mu \sum_r (n_{r\uparrow} - n_{r\downarrow}),$$

(3.17)

where now $n_{rs} = c_{rs}^+ c_{rs}$, and the chemical potential term, omitted in (2.1), is reinstated. Thus, we find a negative-$U$ Hubbard model in a magnetic field $B = \mu/\mu_B$ (only the Zeeman term being included). Under (3.16) one also has

$$n_{r\uparrow} \pm n_{r\downarrow} \rightarrow n_{r\uparrow} \pm n_{r\downarrow}, \quad (-1)^{x+y} a_{r\uparrow}^+ a_{r\downarrow} \rightarrow c_{r\downarrow}^+ c_{r\uparrow}^+.$$  

(3.18)

i.e. the $z$-component of the antiferromagnetic order parameter is transformed into a charge-density wave (CDW), whereas the $x$- and $y$-components transform into the real and imaginary parts of a superconducting order parameter. The spin-rotation invariance of the original model (2.1) then means that the CDW state and superconductivity are degenerate for the negative-
U Hubbard model at half-filling. Consequently, the domain wall solutions discussed here for an antiferromagnet close to half-filling also appear for the negative-U CDW in a magnetic field at half-filling. From (3.18) one would also predict a domain wall in the superconducting state in a magnetic field. However, this is not a real effect: in (3.17) the orbital effects of a magnetic field are completely neglected, and these effects suppress the superconducting state with respect to the CDW.

One might also study deviations from half-filling in the negative-U Hubbard model. Then, for the CDW case the important nesting property of the Fermi surface is destroyed, whereas the degeneracy between \( k \) and \(-k\), crucial for superconductivity, is obviously conserved. Consequently, deviations from half-filling break the degeneracy between CDW and superconductivity in favour of superconductivity. Translated back, \textit{via} (3.16), to the positive-U case, this is the well-known fact the staggered magnetisation of an antiferromagnet is perpendicular to an external field.

The degeneracy between superconductivity and CDW is also broken if interaction with phonons is considered: then, the CDW can be favoured because the relevant energy cutoff is the Fermi energy, much larger than the Debye frequency which is relevant in superconductivity. The simplest model for this case is the so-called « molecular crystal model »:

\[
H = -t \sum_{<rr'>} \left( a^\dagger_{r\sigma} a_{r'\sigma} + a^\dagger_{r'\sigma} a_{r\sigma} + g \sum_r \left( n_{r\uparrow} + n_{r\downarrow} \right) u_r + \frac{K}{2} \sum_r u_r^2 \right), \tag{3.19}
\]

where \( u_r \) is a local « molecular » lattice displacement, \( K \) the corresponding force constant, and \( g \) the electron-lattice coupling. For simplicity, the unimportant lattice kinetic energy term has been omitted. In the CDW state which is stable at half-filling one has \( u_r = (-1)^{x+y} u_0 \), and an analogous modulation of the charge density. Away from half-filling, domain-wall solutions can be studied, which are governed by an equation very similar to (3.5):

\[
-t \sum_{\delta} \psi_i(r - \delta) + g u_r \psi_i(r) = E \psi_i(r). \tag{3.20}
\]

In the continuum approximation this reduces again to (3.14), however this is still a bad approximation. Therefore equation (3.20) has to be studied numerically. A preliminary investigation shows, not surprisingly, the existence and stability of domain walls away from half-filling. However, mainly due to the different spin structures of (3.5) and (3.20), the CDW case is different in some aspects from the antiferromagnet, and I will not discuss it in further detail here.


The separation of the motion parallel to the domain wall in equations (3.8) and (3.12) makes it possible to study rather large systems numerically. The main quantity of interest is the binding energy per hole, \( E_b \), i.e. the energy difference per hole between a state with domain walls \( E_1 \) and a state with constant \( m \) and with the same number \( n_h \) of holes \( E_0 \):

\[
E_b = (E_0 - E_1)/n_h. \tag{4.1}
\]

In order to extract meaningful results some care is still needed. The first method I use is to calculate \( E_0 \) and \( E_1 \) directly for fixed linear dimensions of the system. In order to be able to use periodic boundary conditions it then is necessary to consider a system that contains two equally spaced domain walls and the corresponding number of holes. This does not create any
problem provided the system is large enough so that the interaction between the two walls can be neglected. This interaction is expected to decay exponentially with a length scale \( \xi \propto \Delta_0/t \), where \( \Delta_0 \) is the gap at half-filling.

Because of the two domain walls present one has both in the diagonal and in the vertical case \( m(r + \ell) = -m(r) \), \( n(r + \ell) = n(r) \), where \( \ell = L_+/2 \) in the diagonal case and \( \ell = L_x/2 \) in the vertical case. For the diagonal case then \( u_+(r_+) \) and \( u_+(r_+ + \ell) \) are eigenfunctions of (3.8) for \( s = \uparrow \) and \( s = \downarrow \), respectively, with the same energy. Consequently, one has

\[
n(r_+) = \sum [u_+(r_+)^2 + u_+(r_+ + \ell)^2], \quad m(r_+) = \sum [u_+(r_+)^2 - u_+(r_+ + \ell)^2]. \tag{4.2}
\]

For the vertical wall \( (u_{++}, u_{+-}) \) and \( (u_{+-}, -u_{+-}) \) are solutions of (3.12) for \( s = \uparrow \) and \( s = \downarrow \) respectively, with the same energy. Thus

\[
n(x) = 2 \sum [u_{++}(x)^2 + u_{+-}(x)^2], \quad 4 \sum u_{++}(x) u_{+-}(x). \tag{4.3}
\]

In both (4.2) and (4.3) summations are over the occupied states.

Results obtained for the vertical wall (and neglecting the \( \bar{U}n \)-term in (3.12)) by solving (3.12) and (4.3) iteratively until convergence are shown in figure 3 for different values of \( U \). There clearly is a \( L_x \)-dependence of the results. A large part of this variation comes from the \( L_x \) dependence of \( E_0 \), due to the fact that not all the states below the gap are occupied. This dependence is, however, linear in \( 1/L_x \) to a very good approximation, and therefore reliable numbers can be obtained from extrapolating to \( L_x = \infty \). Alternatively, the problem can be avoided altogether using another way of calculating \( E_b \): write, for a vertical wall:

\[
E_1(L_x, L_y) = \varepsilon_0 L_x L_y + 2 \varepsilon_w L_y + O(1), \tag{4.4}
\]

where \( \varepsilon_0 \) is the Hartree-Fock ground state energy per particle at half-filling, calculated for an infinite system. Then \( \varepsilon_w \) is the energy needed to create a wall of unit length, including the energy change due to the change in particle number (note that all energies calculated are expectation values of (3.4)). As there is one hole per unit length of domain wall, and taking

![Fig. 3. — The binding energy normalized by \( \Delta_0 \) as a function of \( 1/L_x \) for a diagonal wall of type I, neglecting the charge interaction term, for \( U = 2t \) (circles), \( U = 3t \) (triangles), \( U = 5t \) (squares), and \( U = 10t \) (pentagons). The dimension of the systems are \( L_+ \times L_- = L_+ \times 48 \).](image-url)
one particle out of the homogeneous antiferromagnetic state costs energy $\Delta - (U/2)$, the binding energy is

$$E_b = \Delta - (U/2) - \varepsilon_w.$$  \hfill (4.5)

Here $\Delta$ is the gap parameter of the infinite system. For a diagonal wall, there is only one hole for two $L_-$-units, and therefore instead of (4.4) one has

$$E_1(L_+, L_-) = \frac{1}{2} \varepsilon_0 L_+ L_- + \varepsilon_w L_- + O(1).$$ \hfill (4.6)

The correctness of the expansions (4.4), (4.6) can be checked rather easily by increasing the linear dimensions of the systems studied. Comparing with results obtained from the first method via a $1/L$-extrapolation as in figure 3, the calculated binding energies are accurate to about three decimal places. For the lowest $U$-values studied ($U \approx 10 t$) rather large systems, up to $192 \times 96$, were needed, however for $U \approx 10 t$ it was more than sufficient to consider $24 \times 24$.

In figure 4 the numerical results for the binding energy per hole are shown, normalized by $\Delta_0$. For easy comparison with the one-dimensional case [15, 16], the charge interaction term ($U_n(x)$) in (3.8) and (3.12) is neglected for the moment. One sees that for small $U (U < 4.5 t)$ the vertical wall is energetically stable, in agreement with the position of the maxima of $\chi_0(k, T)$ found in section 2. At small $U$ one has $E_b \approx 0.34 \Delta_0$, which is not much smaller than the binding energy in the one-dimensional charge-density wave case, where one has $E_b = (1 - 2/\pi) \Delta_0 = 0.36 \Delta_0$. For the diagonal wall the binding energy is considerably smaller. This again shows the problems with the continuum approximation: from (3.10) and (3.15) both cases should have given the same value. At $U \approx 4.5 t$ there is a transition, and for stronger $U$ the diagonal wall is stable.

For both the diagonal and vertical case I have considered two possibilities: for a type I wall the zero of $m(x)$ is on a lattice site, whereas for type II the zero is halfway in between. The symmetry arguments concerning the single-particle spectra given in section 3 only apply to
type I, whereas for type II the spectra are changed. In particular, for a diagonal wall of type II, the spins next to the wall are either all $\uparrow$ or all $\downarrow$. Therefore, in this case single-particle energies for $\uparrow$ and $\downarrow$ are different. Nevertheless, bound states exist in all cases. The energy difference between types I and II is the barrier against translation of the domain wall (Peierls barrier). As expected, for small $U$, when the walls are fairly thick, this barrier is very small and cannot be resolved numerically. For stronger $U$ type I is always strongly preferred, with the binding energy tending to $\Delta_0/2$ for large $U$.

The fact that $E_b \to \Delta_0/2$ for large $U$ in figure 4 is obviously an artefact, due to the neglect of the charge interaction terms: for large $U$ one has $\Delta_0 = U/2$, but taking particles out of the half-filled situation (where in the Hartree-Fock ground state there is nearly no double occupancy of sites), one cannot gain an energy of order $U$. The results from solving the full equations (3.8) and (3.12) selfconsistently are shown in figures 5 and 6. Again, for small $U$ the vertical wall is stable, whereas for $U > U_c \approx 3.7 t$ the diagonal wall is preferred. For large $U$ the binding energy is of order $t$.

![Figure 5](image1.png)

Fig. 5. — The same as figure 4, but including the charge interaction.

![Figure 6](image2.png)

Fig. 6. — The same as figure 5, but normalized by $t$ rather than by $\Delta_0$, so that the behaviour at large $U$ is more apparent.
Contrary to the results shown in figure 4, the Peierls barrier in the present case is rather small over a large range of $U$-values. This can be understood as follows: in (3.8) and (3.12) the $U_n$-term acts as an attractive potential near the domain walls, because the holes are localised at the domain walls, and therefore $U_n$ is much smaller at the domain wall than far away from it (see Fig. 2). In general, a shallow but wide potential well will lead to stronger binding than a deep but narrow well. This then favours the type II situation, because the wavefunction of the localised states is spread out over at least two lattice sites, rather than only one for type I. For sufficiently large $U$ this effect is enough to favour type II over type I.

5. Discussion and conclusion.

In the present paper I have investigated the effect of a small amount of holes on the antiferromagnetic ground state of the two-dimensional Hubbard model with a half-filled band, using the Hartree-Fock approximation. It is well-known that for exactly half-filling there is an insulating two-sublattice antiferromagnet, with a gap $2 \Delta_0$ in the electronic spectrum. As shown in the preceding sections, going away from half-filling domain wall type structures, i.e. situations where on one side of a straight line sublattice A is mostly occupied by $\uparrow$-spins and sublattice B is mostly occupied by $\downarrow$-spins, whereas on the other side of the line the roles of the two sublattices are interchanged (Fig. 2) are energetically favorable. A domain wall of length $L$ leads to the appearance of $L$ (or $L/2$ for a diagonal wall) bound states in the gap. Holes then gain energy by « condensing » into these bound states, rather than going into extended states below the gap (in this last case the antiferromagnetic order would remain unaffected). This picture is quite analogous to « soliton doping » in one-dimensional charge-density wave systems [15, 16], even though the unusual spin-charge relations of one-dimensional solitons have no direct analogue for the present case where domain walls (« solitons ») are extended objects. As shown in section 3, contrary to the one-dimensional case continuum approximations [22] lead to unstable domain walls, and the problem seems to require numerical solution even for small $U$. I then find that the binding energy per hole, i.e. the energy gain due to the formation of a wall and its associated bound states, is of order $0.3 \Delta_0$ for small $U$ (Fig. 5), and of order $t$ for large $U$ (Fig. 6). With increasing $U$ there is a transition from the « vertical » to the « diagonal » wall at $U_c \approx 3.7 t$. The diagonal wall has been found to be stable at large $U$ by Poilblanc and Rice [17].

The straight wall is expected to be stable against deformations: bending it (or making a corner in the wall) leads to changes in the local antiferromagnetic order which will cost some energy, and a crossing between two domain walls will reduce the total number of bound states by (at least) one unit, again leading to less binding energy. These points are supported both by Ginzburg-Landau type arguments [20] and by strong-coupling calculations [18].

The numerical results for the binding energy of a single hole found here can be compared to the binding energy $E_{b,\text{pol}}$ of a magnetic polaron, i.e. a hole (or electron) accompanied by a local deformation of the magnetic structure. For $U = 2 t$ and $U = 5 t$ Su and Chen [23] find $E_{b,\text{pol}} \approx 0.046 t$ and $E_{b,\text{pol}} \approx 0.23 t$, respectively, whereas the domain wall solution gives $E_b \approx 0.095 t$ and $E_b \approx 0.41 t$, respectively. Thus, at least for the limited domain of $U$-values where a comparison is currently possible, the domain wall solution is clearly favoured.

The results presented here were all obtained in the Hartree-Fock approximation. In principle, even for weak coupling, this is not without problems: both electron-hole and electron-electron ladder diagrams are divergent and a simple RPA ladder summation does not necessarily sum all leading divergent diagrams. In the Hubbard model, however, more complete treatments show that these effects give rise only to very small modifications [9, 24].
Spin-wave corrections to Hartree-Fock energies are also expected to be small: their phase space is roughly $\xi_0^{-2}$, with the zero-temperature correlation length $\xi_0 \approx t/\Delta_0$, i.e. the spin-wave phase space and therefore the corresponding corrections to the energy go to zero for weak coupling. More interesting are fluctuations of the domain wall position. Using the well-known relation between quantum fluctuations in $d$ dimensions and thermal fluctuations in $d + 1$ dimensions, a «quantum roughening transition» of an isolated domain wall is conceivable. Even if a rough phase exists at $T = 0$, I do not expect it to change energetics much: the binding energy per hole is essentially determined by processes on length scales of a few lattice constants, whereas roughening only affects correlations at extremely long scales. On the other hand, for a rough wall, the Peierls barrier would be absent, i.e. the wall would be mobile. One should however note that for the physically interesting case of a regularly spaced array of domain walls (see below) no roughening transition exists, not even at nonzero temperature [25].

A finite temperature orientational fluctuations destroy magnetic long-range order [26], with a magnetic correlation length $\xi_{\text{mag}}$ growing exponentially; $\xi_{\text{mag}} \propto \exp (T_0/T)$. For small $U$ the magnetic order becomes extremely long-ranged at temperatures not much below the mean-field (Stoner) critical temperature [27], with $T_0 \approx t$. At length scales shorter than $\xi_{\text{mag}}$ the present problem then is essentially equivalent to two-dimensional incommensurate «floating» phases [28]. In particular, the Bragg peaks would be replaced by power-law peaks with temperature dependent exponents, or even by finite width Lorentzians if the incommensurate phase «melts» [28].

For strong coupling I find $E_b \approx t$. This is considerably less binding energy than found from the hole kinetic energy in an antiferromagnetic background [13] ($E_b \approx 3t$) or from a Nagaoka-type spin-polaron ($E_b = 4t$ for $U \to \infty$) [29]. It is however clear that for large $U$ the Hartree-Fock approximation completely neglects hole delocalisation on a local scale and thus makes an error of order $t$ (probably an underestimate of $E_b$). A more complete calculation would be needed to decide the stability of the domain wall for large $U$. Also, for large $U$, a spiral phase (which does not localise many holes in a narrow region) may well be stable [31].

The existence of a stable domain wall in an antiferromagnet is clearly due to the presence of holes: in an undoped antiferromagnet, imposing e.g. antiperiodic boundary conditions for $x \to \pm \infty$, the minimum energy solution is a continuous rotation of the spins, with energy cost $1/L^2 \to 0$ in the thermodynamic limit ($L$ is the linear dimension of the system). On the other hand, any domain wall of finite thickness would require a finite amount of energy. The stability of the domain wall in the presence of holes is due to the formation of bound states and the energy gained by the electrons due to the occupation of the bound state. This more than compensates the loss in exchange energy, as shown by the positive binding energies found in section 4. Also, note that a slowly varying twist of the staggered magnetisation will not lead to bound states.

To obtain a stable vertical domain wall in a system of linear dimensions $L_x \times L_y$, one has to introduce $L_y$ holes. Even though this is a large number for a large system, the concentration of holes is still infinitesimal: $1/L_x$ (similar arguments hold for the diagonal wall). The physically interesting situation is clearly a small but finite concentration. One then would introduce enough domain walls so that all holes can condense into bound states. By analogy with the one-dimensional situation, the walls can be expected to be equally spaced. For the case of vertical domain walls, one has $N_w = L_x n_h$ walls, where $n_h$ is the average number of holes per site. Consequently, the modulation wavevector of the antiferromagnetic structure (i.e. the position of the principal magnetic Bragg peak) is $Q_1 = \pi (1 \pm n_h, 1)$, i.e. there is an «incommensurate antiferromagnetic structure» with a doping-dependent modulation wavevector.
This is the stable situation for $U < U_c \approx 3.7 \, t$. On the other hand, for $U > U_c$ the diagonal wall is stable. Then, for a wall of length $L_\perp$ there are $L_\perp/2$ bound states, and therefore the antiferromagnetic Bragg peaks appear at $Q_3 = \pi (1 \pm n_h, 1 \pm n_h)$. In both cases the magnetic polarization vector lies entirely in one plane, and of course structures obtained from $Q_1, Q_3$ by a rotation of $\pi/2$ are energetically equivalent, i.e. the discrete rotation symmetry of the lattice is broken.

In the discussion given here, the effects of the long-range part $(e^2/r)$ of the Coulomb energy are completely neglected (as implied by the use of the Hubbard model). Inclusion of these effects would destabilize an isolated wall [30], due to the accumulation of charge in a relatively small part of space. For extremely small hole concentration then a Wigner-crystal type structure is more likely, and the domain wall structure would only appear at finite concentration.

In the present picture, at small hole concentrations carriers remain localized at the domain walls, and there is no single-particle conduction. One might think of a collective (tunneling through the Peierls barriers) motion of the domain walls. As the walls carry charge, this would lead to electric conduction. However, a domain wall is an extended object, and tunneling probabilities therefore would be exceedingly small (unless the quantum roughening mentioned above occurs). Moreover, even extremely small inhomogeneities would pin the walls. For all practical purposes, the incommensurate state is therefore an insulator [32]. However, with increasing hole concentration walls start to overlap, forming eventually a sine-like spin-density wave. The crossover between the two regimes should occur at $n_h \approx 1/\xi_0 \approx \Delta_0/t$. As discussed in more detail in [20], one has a transition into a state of coexisting antiferromagnetic order and mobile hole-like carriers. If on the other hand, as suggested previously, the holes go into the extended states below the gap and leave the antiferromagnetic order unchanged, one immediately creates mobile carriers. The interaction of one such carrier with the antiferromagnetic background has been investigated rather intensely [11, 12, 13, 10]. The results presented here suggest that this is an oversimplification of the behaviour of an antiferromagnet at small doping, even though more detailed investigations are needed, especially for strong $U$.

In an experiment, the incommensurate antiferromagnetic phase postulated here (and in [20]) would obviously manifest itself by magnetic Bragg peaks away from $(\pi, \pi)$. Experimentally incommensurate peaks are indeed observed [19], however they are of finite width. This may well be explained by the fact that the domain walls discussed here are charged, and therefore easily gain energy by getting pinned to charged impurities (this has also been noted in [18]). The array of domain walls then would be rather irregular, leading to finite width peaks. Even in that case, however, some of the more general features of the present theory will still hold : linear polarization of the magnetization (i.e. no spiral), linear variation of the « Bragg » peak position with hole concentration, and the position of the incommensurate peaks. These points could all be tested experimentally. One might also speculate whether the spin-glass phase of doped La$_2$CuO$_4$ is related to a very disordered array of domain walls. Finally, the finite-temperature domain wall fluctuation effects mentioned above may play a role in real compound : the magnetic interlayer coupling is known to be extremely weak, so that the incommensurate state would still have many of the features of the purely two-dimensional model.

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Appendix A. Existence of bound states of equation (3.12).

Neglecting the charge interaction \((U_n(x)\)-) term in (3.12), and introducing the « local gap » \(\Delta(x) = U_m(x)/2\) and the linear operator

\[
Lf(x) = -t [f(x + 1) + 2 \cos (p) f(x) + f(x - 1)],
\]

equations (3.12) become

\[
Lu_{s_+}(x) - s\Delta(x) u_{s_-}(x) = Eu_{s_+}(x) \\
- Lu_{s_-}(x) - s\Delta(x) u_{s_+}(x) = Eu_{s_-}(x).
\]

For any domain wall type solution one has \(\Delta(-x) = -\Delta(x)\). Then, if \((u_{s_+}(x), u_{s_-}(x))\) is a solution of (A.2) with energy \(E\), one finds straightforwardly that \((u_{s_-}(-x), u_{s_+}(-x))\) is a solution with energy \(-E\), i.e. the spectrum of (A.2) is symmetric.

For simplicity, now consider only the case \(s = +\), and introduce

\[
v_{\pm}(x) = u_{s_+}(x) \pm i u_{s_-}(x).
\]

Then (A.2) becomes

\[
(L \pm i\Delta) v_{\pm}(x) = Ev_{\pm}(x).
\]

Multiplying the equation for \(v_-\) from the left by \((L + i\Delta)\) and vice versa, I finally obtain an effective « Schrödinger equation »:

\[
\tilde{H}_{\pm} v_{\pm} = E^2 v_{\pm}, \quad \tilde{H}_{\pm} = L^2 + \Delta^2 \pm i [L, \Delta].
\]

For a domain wall one has \(\Delta(\pm \infty) = \pm \Delta_0\), and consequently any solution to (A.5) with \(E^2 < \Delta_0^2\) cannot propagate and has to be localized at the domain walls. To show the existence of such solutions I use the variational ansatz

\[
v_{\pm}(x) = N \cos \left[ (\pi - p) x \right] e^{-\alpha |x|},
\]

where \(N\) is a normalisation constant. For \(\alpha > 0\) this is a bound state wavefunction. For small \(\alpha\) one has

\[
\sum_i v_{\pm}(x) L^2 v_{\pm}(x) = K\alpha^2, \quad N^2 = 2\alpha,
\]

with a positive constant \(K\). For a real wavefunction like (A.6) the commutator term in \(\tilde{H}_{\pm}\) does not contribute.

To obtain the desired result now consider a « sharp » domain wall : \(\Delta(x) = \Delta_0 \text{sign}(x)\) if \(x \neq 0\), \(\Delta(0) = 0\). Then the potential energy is, again for small \(\alpha\)

\[
\sum_i v_{\pm}(x) \Delta(x)^2 v_{\pm}(x) = \Delta_0^2(1 - 2\alpha).
\]

Taking (A.7) and (A.8) together, it is obvious that the total energy is minimized for \(\alpha > 0\), i.e. bound states with \(E^2 < \Delta_0^2\) do exist. From the symmetry of the spectrum therefore at least two bound states with energies \(\pm E\) exist for any \(p\). Taking a smoother function for \(\Delta(x)\) only increases the potential energy gain in (A.8). The numerical results show that the existence of a bound state is not affected by the inclusion of the charge interaction term (though the symmetry of the spectrum is lost).
References


    preprint ITP-88-174.

    HIRSCH J. E. et al., ibid. 153 (1988) 549;


    SACHDEV S., Yale preprint.


    structure are given by


[32] For a detailed discussion of these effects see : FRIEDEL J., in « Low-Dimensional Conductors and