RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 42, NUMBER 13 1 NOVEMBER 1990

Flux-density wave and superconducting instability of the staggered-flux phase

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(Received 22 May 1990)

We study the stability of the staggered-flux phase in the t-J model away from half filling using a systematic large-N slave-boson approach. Found, below a critical doping concentration $\delta_c = a(J/t)^2$, is a flux-density-wave instability with an incommensurability wave number $\sim\delta^{3/4}$. The instability towards a modulated-flux state is due to low-lying phase fluctuations of the valence bonds. When the doping parameter exceeds δ_c, we find a fully gapped d-wave superconducting state due to residual quasiparticle interactions.

The study of doped Mott insulators has received renewed interest following Anderson's formulation of the resonating-valence-bond (RVB) theory of high-temperature superconductivity.[1] To quantify Anderson's suggestions, it is useful to construct soluble models that contain some of the essential ingredients of the Mott phenomena. Affleck and Marston[2] extended the magnetic superexchange interaction to accommodate electrons transforming under SU(N), and carried out a $1/N$ expansion. At half filling they found an insulating state with an excitation spectrum characterized by point zeros. This state, independently discovered in a different mean-field decoupling of the t-J model,[3] is a nontrivial example of a Mott insulating state. It was later found that, on the square lattice, this state is linearly unstable against dimerization.[4] However, the analysis of Ref. 4 showed that the dimerization was due to a finite-amplitude instability. Therefore it can be avoided by adding quartic terms involving only amplitude modes to the Lagrangian, leaving the low-energy dynamics of the phase modes unperturbed. Marston and Affleck[5] argued that frustration stabilizes the flux phase against dimerization. When one dopes away from half filling the self-consistent mean-field flux is no longer given by π but by a staggered array of fluxes $\phi \simeq \pm\pi(1-\delta t/J)$. We will refer to this state as the staggered-flux phase (SFP). A different state having uniform flux different from π away from half filling, has been studied recently by variational methods.[6] This is the uniform-flux phase which displays remarkable commensurability effects at special filling factors. Important questions concern the physical properties of these states.

In this paper, we investigate the properties of the staggered-flux state by studying the leading $1/N$ corrections to the $N=\infty$ solution for small but finite density of holes. The large-N expansion is not perturbative in the hopping parameter t, or the exchange parameter J of the t-J model. It allows us to study analytically the competition between the kinetic energy t of the holes and the magnetic exchange energy J. We find that the staggered-flux phase is unstable, for $J > a\sqrt{\delta}t$, towards a modulated-flux state in which the staggered flux is modulated by slowly varying uniform flux. On the other hand, when $J < a\sqrt{\delta}t$ the SFP is stable. In this region, the residual interaction between the quasiparticles mediated by low-energy phase fluctuations gives rise to a fully gapped d-wave superconducting phase.

The generalized t-J model studied in this paper is described by the Hamiltonian

$$H = -\frac{t}{N}\sum_{\langle i,j\rangle,\sigma}(\tilde{c}_{i\sigma}^{\dagger}\tilde{c}_{j\sigma} + \text{H.c.}) + \frac{J}{N}\sum_{\substack{\langle ij\rangle \\ \sigma,\sigma'}}\tilde{c}_{i\sigma}^{\dagger}\tilde{c}_{i\sigma'}\tilde{c}_{j\sigma'}^{\dagger}\tilde{c}_{j\sigma} \tag{1}$$

subject to systems of local constraints: $\sum_\sigma \tilde{c}_{i\sigma}^{\dagger}\tilde{c}_{i\sigma} \le N/2$. The σ and σ' are flavor indices running from 1 to N. To treat a finite concentration of holes we use the slave-boson approach and introduce a boson operator b_i in the decomposition of the electron operator $\tilde{c}_{i\sigma} = b_i^{\dagger}c_{i\sigma}$. We follow the analysis of Dombre and Kotliar,[7] who investigated the optical conductivity in this model. But we focus on the static, $\omega \to 0$, $q \gg \omega$ limit of the response functions. The partition function at temperature β^{-1} is given by the functional integral

$$Z = \int \mathcal{D}\Delta\mathcal{D}\Delta^{\dagger}\mathcal{D}c\mathcal{D}c^{\dagger}\mathcal{D}b\mathcal{D}b^{\dagger}\mathcal{D}\lambda \exp\left(-\int_0^\beta d\tau\mathcal{L}\right),$$
$$\mathcal{L} = \sum_{j\sigma}\left[c_{j\sigma}^{\dagger}\left(\frac{\partial}{\partial\tau} - \mu_F\right)c_{j\sigma} + b_j^{\dagger}\frac{\partial}{\partial\tau}b_j + i\lambda_j\left(c_{j\sigma}^{\dagger}c_{j\sigma} + b_j^{\dagger}b_j - \frac{N}{2}\right)\right] + \frac{N}{J}\sum_{i,\mu}|\Delta_{i,i+\mu}|^2 + \mathcal{H}, \tag{2}$$
$$\mathcal{H} = -\sum_{i,\mu,\sigma}c_{i\sigma}^{\dagger}c_{i+\mu\sigma}\left(\Delta_{i,i+\mu} + \frac{2t}{N}b_{i+\mu}^{\dagger}b_i\right) + \text{c.c.},$$

where $\Delta_{i,i+\mu}$ is a complex link variable (valence bond) used to decouple the exchange term in (1), and the link index $\mu = \pm\hat{x}, \pm\hat{y}$ on a square lattice. In this paper, we restrict ourselves to a two-sublattice structure with the indices i and j running over A and both A and B sublattices, respectively. The integration over the time-independent Lagrange multipliers enforces the constraint of no double occupancy. In the large-N limit, the bosons are condensed $b_A = b_B = |b| = \sqrt{\delta N/2}$ with the absolute phase set to zero. $i\lambda_A$ and $i\lambda_B$ take the value λ_0 consistent with the Bose-condensation assumption while the chemical potential μ_F is adjusted to have $\delta/2$ holes per flavor. To set up the notation we review the large-N limit of the model.[5,7] The saddle point is described by the mean-field Hamiltonian

$$\mathcal{H}_{\rm MF} = \sum_{k\sigma} \left(c^\dagger_{Ak,\sigma}, c^\dagger_{Bk,\sigma} \right) \begin{pmatrix} \lambda_0 - \mu_F & e_k \\ e_k^* & \lambda_0 - \mu_F \end{pmatrix} \begin{pmatrix} c_{Ak,\sigma} \\ c_{Bk,\sigma} \end{pmatrix} \tag{3}$$

where

$$e_k = -2[(\Delta_x + t\delta)\cos k_x + (\Delta_y + t\delta)\cos k_y] = |e_k| e^{-2i\phi_k}.$$

We take $\Delta_{A,\pm x} = Qe^{-i\phi}$, $\Delta_{A,\pm y} = Qe^{i\phi}$ consistent with SFP ansatz. $\mathcal{H}_{\rm MF}$ can be diagonalized by a Bogoliubov transformation

$$c_{Ak,\sigma} = u_k \psi_{+,k\sigma} - v_k \psi_{-,k\sigma},$$
$$c_{Bk,\sigma} = v_k^* \psi_{+,k\sigma} + u_k^* \psi_{-,k\sigma}, \tag{4}$$

with $u_k = v_k = (1/\sqrt{2}) e^{-i\phi_k}$, leading to two quasiparticle fermion bands with dispersion

$$E_k^\pm = \pm 2[(Q\cos\phi + t\delta)^2(\cos k_x + \cos k_y)^2 + Q^2\sin^2\phi(\cos k_x - \cos k_y)^2]^{1/2}. \tag{5}$$

The MF value of Q is self-consistently determined by

$$\frac{2Q}{J} = \sum_k \cos k_x \cos(2\phi_k - \phi) f(E_k) \mathrm{sgn}(E_k),$$

where the summation is restricted to the reduced Brillouin zone and $f(E_k)$ is the Fermi-Dirac function. The spectrum (5) has two zeros at $\mathbf{k}^0_{1,2} = (\pi/2, \pm\pi/2)$. We calculated the compressibility in this phase

$$\frac{dn}{d\mu} = \frac{N\rho}{1 + 2t\rho(\epsilon_1 + \epsilon_2/\epsilon_1) - J\rho\epsilon_2} \tag{6}$$

where $\rho = \sum_k \delta(E_k - \mu_F)$ is the Fermi-level density of states and $\epsilon_1 = \mu_F/2(Q\cos\phi + t\delta)$, $\rho\epsilon_2 = \sum_k \delta(E_k - \mu_F) \times (\cos k_x + \cos k_y)^2$. We verified that at small doping the compressibility (6) is positive.

The low-energy excitations are closely related to the symmetry of the original Lagrangian $\mathcal{L}$ under U(1) gauge transformations $c_{j\sigma} \to c_{j\sigma} e^{i\theta_j}$, $b_j \to b_j e^{i\theta_j}$, $\lambda_j \to \lambda_j + \dot{\theta}_j$, $\Delta_{i,i+\mu} \to \Delta_{i,i+\mu} e^{i(\theta_i - \theta_{i+\mu})}$. The two-sublattice structure splits the full U(1) group of invariance into two parts; the uniform part associated with $\theta_A = \theta_B = \theta$ and the staggered part with $\theta_A = -\theta_B = \theta$. The complex order parameter Δ of SFP breaks the staggered U(1) symmetry and leaves the uniform part unbroken at half filling. We correspondingly parametrize the fluctuations in the radial gauge[8] $\Delta_{i,i+\mu} = [\Delta_{i,\mu} + R_\mu(i + \frac{1}{2}\mu)] e^{i\theta_\mu(i+\mu/2)}$; $i\lambda_j = \lambda_0 + i\lambda_j$; $b_j = b(1 + r_j)$, which are decomposed in momentum space according to

$$A_\mu^\pm(q) = \tfrac{1}{2}[\theta_\mu(q) \pm \theta_{-\mu}(q)];$$
$$\lambda^\pm(q) = \tfrac{1}{2}[\lambda_A(q) \pm \lambda_B(q)];$$
$$R_\mu^\pm(q) = \tfrac{1}{2}[R_\mu(q) \pm R_{-\mu}(q)];$$
$$r^\pm(q) = \tfrac{1}{2}[r_A(q) \pm r_B(q)].$$

The fields (A_μ^-, λ^-) correspond to the transverse and longitudinal components of the unbroken uniform U(1) symmetry and the (A_μ^+, λ^+) are related to those of the broken staggered symmetry.

We have carried out a detailed analysis of the fluctuations around the saddle point. At half filling, the fields A_μ^- are massless which decouple from the other fields. Away from half filling, they mix with charge excitations and acquire a small mass proportional to the hole concentration. The rest of the fields are strongly coupled together but their spectral weight is distributed over energies of order t or J. In this paper we concentrate on the low-energy part of the fluctuation spectrum.[9] The low-energy effective Lagrangian is given by

$$\mathcal{H} = \sum_{\alpha k\sigma} E_k^\alpha \psi^\dagger_{\alpha k,\sigma}\psi_{\alpha k,\sigma} + \sum_{\alpha,\beta} \mathcal{H}_{\alpha\beta} + N\frac{2Q^2}{J}\sum_q A_\mu(q) A_\mu(-q)$$
$$\mathcal{H}_{\alpha\beta} = -2Q\sum_{qk\sigma} A_\mu(q) v^\mu_{\alpha\beta}(q,k)\psi^\dagger_{\alpha k+q,\sigma}\psi_{\beta k,\sigma} + \text{c.c.}$$

Here we set $A_\mu \equiv A_\mu^-$, and $\mathcal{H}_{\alpha\beta}(\alpha,\beta = \pm)$ describes the coupling of quasiparticles to phase fluctuations with vertices

$$v^\mu_{--}(q,k) = \sin k_\mu \cos(\phi_k + \phi_{k+q} - \phi_\mu) = v^\mu_{++}(q,k)$$
$$v^\mu_{-+}(q,k) = i\sin k_\mu \sin(\phi_k + \phi_{k+q} - \phi_\mu), \quad \phi_{x,y} = \pm\phi.$$

Integrating out the fermions, we obtain the effective Lagrangian for the gauge field

$$\mathcal{L}_{\rm eff} = -\frac{N}{2}\sum_q [\Pi^{\rm inter}_{\mu\nu}(q) + \Pi^{\rm intra}_{\mu\nu}(q)] A_\mu(q) A_\nu(-q), \tag{7}$$

where the $\Pi^{\rm inter}_{\mu\nu}$ and $\Pi^{\rm intra}_{\mu\nu}$ are the interband and intraband polarization bubbles given by

$$\Pi^{\rm inter}_{\mu\nu}(q) = 4Q^2\sum_k \frac{v^\mu_{-+}(q,k)v^\nu_{+-}(q,k)}{E^+_{k+q} - E^-_k} f(E_k^-) + \frac{2Q^2}{J}\delta_{\mu\nu}, \tag{8}$$

$$\Pi^{\rm intra}_{\mu\nu}(q) = -2Q^2\sum_k v^\mu_{--}(q,k)v^\nu_{--}(q,k) \times \frac{f(E^-_{k+q}) - f(E^-_k)}{E^-_{k+q} - E^-_k}. \tag{9}$$

At half filling the lower subband is full, and the gauge field is massless. Away from half filling, the finite hole concentration breaks the gauge symmetry and the gauge field acquires a small mass proportional to the hole concentration due to the Anderson-Higgs mechanism. The gauge-field polarization operator in Eq. (7) has the form $\Pi_{\mu\nu} = \Pi^{\rm inter}_{\mu\nu} + \Pi^{\rm intra}_{\mu\nu}$,

$$\Pi_{\mu\nu}(q) = \frac{1}{e^2(q)}(q^2\delta_{\mu\nu} - q_\mu q_\nu) + \omega_2\delta_{\mu\nu}. \tag{10}$$

The mass was calculated from $\Pi^{\text{intra}}(0) = -\omega_1 = -Q\sqrt{\delta/\pi}$ and $\Pi^{\text{inter}}(0) = \omega_1 + \omega_2$, $\omega_2 = \sqrt{2}Qt\delta/J$. These parameters determine the optical-absorption spectrum of the SFP.[7] We calculated numerically the inverse of the renormalized "charge" $e^2(q)$ and it is plotted in Fig. 1. There are two contributions. The contribution from the interband polarization is constant and positive for $q \ll 2k_F$ and is proportional to $1/q$ for $q \gg 2k_F$. This large-q behavior was noticed in Refs. 10 and 11. The intraband polarization is a *negative* constant at $q \ll 2k_F$ and rapidly approaches zero for $q > 2k_F$. For $q < 2k_F$ the intraband contribution dominates. The renormalized charge is approximately given by the expression[12] $1/e^2 = -Q/32\pi k_F$, and $E_F = -2Qk_F = -4Q\sqrt{\pi\delta}$ is the Fermi energy. The gauge-field propagator is obtained for $q < 2k_F$

$$D_{\mu\nu}(q) = \langle A_\mu(q) A_\nu(-q) \rangle = |e^2| \frac{\delta_{\mu\nu} - q_\mu q_\nu/\tilde{\omega}_2}{-q^2 + \tilde{\omega}_2} . \tag{11}$$

The instability of the model is signaled by the appearance of a pole in the propagator at $q^2 = \tilde{\omega}_2 = \omega_2 |e^2| < (2k_F)^2$. We thus established the instability of the SFP when

$$\frac{J}{t} > \alpha\sqrt{\delta} , \tag{12}$$

where $\alpha \sim 4\sqrt{2\pi} \sim 10$. For $\delta = 0.01$, this criteria corresponds to a critical value $(J/t)_c \simeq 1$. For a fixed ratio J/t,

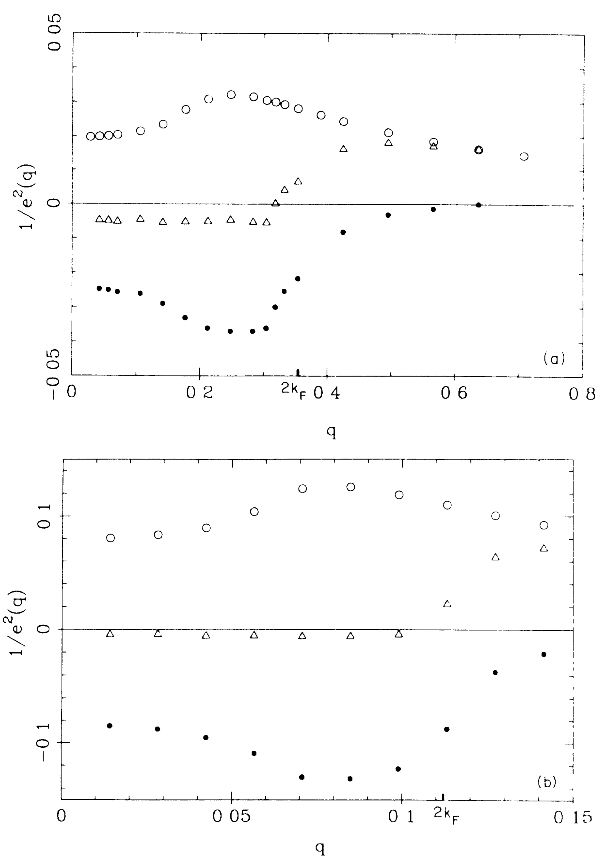

FIG. 1. Contributions to the inverse renormalized charge (open triangles) in Eq. (10) from interband (open circles) and intraband (solid circles) polarization bubbles. (a) $J/t = 1$, and the hole concentration $\delta = 0.01$. (b) $J/t = 0.5$ and $\delta = 0.001$.

the SFP is stable only if the hole density exceeds $\delta_c \sim (J/t\alpha)^2$.

When $J \gg t\sqrt{\delta}$ the system prefers to reduce energy by spontaneously generating additional uniform flux. A mean-field theory of this effect can be constructed by letting the gauge bosons $A_\mu(q)$ condense in a state of finite momentum $\mathbf{q}_0 \sim (0, \delta^{3/4})$, $A_\mu = (2A_0 \cos q_0 y, 0)$. Since A_μ corresponds to the uniform part of the U(1) symmetry on the two-sublattice structure, $A_0 \neq 0$ gives rise to a plaquette flux $4|A_0 q_0| \sin(q_0 y)$. The condition for a nontrivial solution of A_0 is precisely given by Eq. (12). We hence identify the $J/t > \alpha\sqrt{\delta}$ instability with the onset of flux-density-wave formation. The state is characterized by a modulated flux $\Phi = \pm 4\phi_0 + 4A_0 q_0 \sin(q_0 y)$ with an incommensurate wave-number proportional to $\delta^{3/4}$. The appearance of the incommensurate flux phase at low hole density is a result of the competition between hopping and exchange energies. This phase has close analogies to the incommensurate magnetic structures found in the Hubbard model.[13]

The SFP is stable when $J < \alpha t\sqrt{\delta}$. As the concentration of holes increases, the flux decreases and a transition to a Fermi-liquid state takes place at a finite value of $\beta t\delta/J$.[14] The parameter β turns out to be close to α so there is a region of hole concentration $(\beta\delta < J/t < \alpha\sqrt{\delta})$ in which the staggered-flux state is stable. In this phase the excitations are the fermionic quasiparticles (4) with a small Fermi surface consisting of two small circles centered at $\mathbf{k}^0_{1,2} = (\pi/2, \pm\pi/2)$. They interact via the exchange of the gauge field (11). This effect is of order $1/N$, and we can treat this interaction in the BCS weak coupling framework. The residual interaction between the quasiparticles is given by

$$V_{\text{eff}}(k,k',q) = -v^\mu_{--}(q,k) D_{\mu\nu}(q) v^\nu_{--}(q,k') .$$

We will show that this interaction is attractive for frequencies $\omega \le \omega_0 \approx (\tilde{\omega}_2 - 4k_F^2)^{1/2}$. The gap equation for the superconducting order parameter $\Delta_k^{\text{SC}} = e^2 \sum_{k'} V_{\text{eff}} \times (k,k',k'-k) \langle \psi^\dagger_{k'\uparrow} \psi^\dagger_{-k'\downarrow} \rangle$ has the usual form

$$\Delta_k^{\text{SC}} = -\frac{1}{N} \sum_{k'} V_{kk'} \frac{\Delta_{k'}^{\text{SC}}}{[(E_{k'} - E_F)^2 + |\Delta_{k'}|^2]^{1/2}} .$$

Quasiparticles on different sections of the Fermi surface do not interact to leading order in δ. It is, therefore, convenient to work in the shifted zone by transforming $\mathbf{k} \to \mathbf{k} + \mathbf{k}^0_{1,2}$. The effective interaction $V_{kk'}$ has a simple form on the Fermi circles

$$V_{kk'} = \frac{4|e^2| Q^2}{-2k_F^2[1 - \cos(\theta - \theta')] + \tilde{\omega}_2} ,$$

where θ and θ' denote the angles that k and k' make with the x axis.

We have found two solutions to the gap equation on a single circle

$$\Delta_1^{\text{SC}}(\theta) = \gamma_1 e^{i\theta} \Delta_0^{\text{SC}}; \quad \Delta_2^{\text{SC}}(\theta) = \gamma_2 e^{-i\theta} \Delta_0^{\text{SC}} , \tag{13}$$

where $\Delta_0^{\text{SC}} = 2\omega_0 e^{-l}$; $l = 8\pi N(t\sqrt{\delta}/J)^2$. The γ_1 and γ_2 are arbitrary phases. Besides this degeneracy within one Fermi circle, there is an additional degeneracy which corresponds to the relative phase of the gap functions on the two Fermi circles. All these states have a full gap and break time-reversal invariance. It is instructive to relate the pair amplitude of the SFP quasiparticles to the order parameter of the original electrons $\langle \tilde{c}^\dagger_{i\uparrow}\tilde{c}^\dagger_{j\downarrow}\rangle = b^2\sum_k \times e^{ik(i-j)}\langle c^\dagger_{k\uparrow}c^\dagger_{-k\downarrow}\rangle$. Using Eq. (4), we find $\langle c^\dagger_{A,k\uparrow}c^\dagger_{B,-k\downarrow}\rangle = \xi^*_k$ and $\langle c^\dagger_{A,k\uparrow}c^\dagger_{A,-k\downarrow}\rangle = -e^{i2\phi_k}\xi^*_k$ with $\xi^*_k \equiv \langle \psi^\dagger_{k\uparrow}\psi^\dagger_{-k\downarrow}\rangle$. Since ξ^* is nonzero only near the Fermi circles, the Fourier transform involves an angular average over the circles. This leads to $\langle \tilde{c}^\dagger_{i\uparrow}\tilde{c}^\dagger_{j\downarrow}\rangle = 0$ when i and j are on the opposite sublattices. To study the symmetry of the same sublattice pairing, we use the expansion $e^{i(2\phi_k-\phi)} \sim \exp(i\theta_1)$, $\exp(-i\theta_2)$ which is valid near the 1 (centered at $\mathbf{k}^0_1$) and 2 (centered at $\mathbf{k}^0_2$) Fermi circles, respectively. We note that from Eq. (13), an order parameter with d-wave symmetry is obtained if one chooses the gap function $\Delta^{SC} = \gamma_1 e^{-i\theta}$ on circle 1 and $\Delta^{SC} = -\gamma_1 e^{i\theta}$ on circle 2. This solution automatically satisfies $\langle \tilde{c}^\dagger_{i\uparrow}\tilde{c}^\dagger_{i\downarrow}\rangle = 0$. This d-wave pairing state, however, is very different from the d-wave RVB state[15,16] and differs little from the conventional s-wave pairing in that it opens a full gap in the quasiparticle spectrum, like a conventional s-wave state.

In conclusion, we used the large-N approach to study the physics of the staggered-flux phase. To leading order in $1/N$, we find an instability towards incommensurate flux structure when $J > 10\sqrt{\delta}t$. The most unstable wave vector is proportional to $\delta^{3/4}$. When $J < 10\sqrt{\delta}t$ a staggered array is the most stable configuration of the flux. However, the residual interaction between quasiparticles mediated by the low-energy phase fluctuations of the valence bonds leads to a fully gapped d-wave superconducting phase with singlet pairs on the same sublattices. The emergence of incommensurate magnetic structures as one dopes a Mott insulator seems to be very general. It is known to happen in ordered structures.[13,17] In this paper we showed that this effect also takes place when one dopes one of the possible phases of the disordered spin liquid. Indeed, using similar techniques, we also found an incommensurate flux-density-wave instability for the doped uniform RVB phase in some range of hole concentrations.[18]

We thank E. Abrahams for helpful discussions. The work at Rutgers is supported by National Science Foundation Grant No. DMR8915895.

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