Superconductivity from Commensurate Flux Phases

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We use a renormalized mean-field theory of the t-J model to show that flux states closely related to those recently proposed by Anderson, Shastry, and Hristopoulos are stabilized, at values of $J/t \gtrsim 1$, when the flux per plaquette is commensurate with the electron density in a way simlar to that found recently for noninteracting electrons. These states (in the interacting t-J model) are characterized by a collective gauge variable which leads to superconductivity. At not too small values of J/t the state with half a flux quantum per plaquette is stable at low doping.

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From the beginning of high-T_c superconductivity,[1] Anderson[2] has proposed that it was a property of strongly correlated electrons on a square latice described by the t-J model.[3] Mean-field theories on the quantum spin liquid (QSL) of this model found a huge redundancy at half filling (i.e., one electron per site) which was lifted to give either a d-wave resonating-valence-bond (RVB) state or a $\frac{1}{2}$-flux state when holes were introduced.[4,5] Anderson,[6] Wiegmann,[7] Laughlin,[8] and others[9] proposed commensurate generalizations of the $\frac{1}{2}$-flux states of Affleck and Marston[4] and Kotliar[4] away from half filling. An explicit form was given recently by Anderson, Shastry, and Hristopoulos.[10] Very recently Hasegawa, Lederer, Rice, and Wiegmann[11] showed that the energy of noninteracting spinless electrons had an absolute minimum when the flux per plaquette, Φ (in units of hc/e), exactly equals the electron density, ν, per site.

In this Letter we use a renormalized mean-field theory[10] to calculate the energy of commensurate flux phases (CFP) and show they have special stability, at values of $J/t \gtrsim 1$ [see Eq. (1) below]. The dependence of these states on the gauge degrees of freedom has interesting consequences leading, as we will argue below, to superconductivity.

The total energy of noninteracting spinless electrons is shown in Fig. 1 versus the band filling $\nu=\frac{1}{2}-\delta$ for small values of δ, and for various values of Φ, $\Phi=\nu$, $\Phi \lesssim \nu$, and $\Phi \gtrsim \nu$. The energy at fixed ν as a function of Φ exhibits a cusp[11] at $\Phi=\nu$. Near half filling, the energy increase of the state $\Phi=\nu$ compared to the state $\Phi=\frac{1}{2}$ is significantly smaller than the increase $\propto \delta^{3/2}$ of the $\Phi=\frac{1}{2}$ phase (with a gain $\sim\delta^2$).

Consider the t-J model[3]

$$H=-t\sum_{\langle i,j\rangle,\sigma} P_d(c^\dagger_{i\sigma}c_{j\sigma}+c^\dagger_{j\sigma}c_{i\sigma})P_d+\sum_{\langle i,j\rangle} J\mathbf{S}_i\cdot\mathbf{S}_j\,, \quad (1)$$

where $c^\dagger_{i\sigma}$ creates an electron spin σ at site i. The constraint of no doubly occupied site is ensured by the projector $P_d=\prod_i(1-n_{i\uparrow}n_{i\downarrow})$. The parameters t and J describe hopping and Heisenberg coupling between nearest-neighbor sites. The lattice has L sites and $(1-2\delta)L$ electrons.

We examine as a possible ground state (GS)

$$|\Psi\rangle=P_d|\Psi_0\rangle=P_d\prod_l^{\text{occ}}\tilde{c}^\dagger_{l\uparrow}\tilde{c}^\dagger_{l\downarrow}|0\rangle\,. \quad (2a)$$

A complete orthonormal set of operators $\tilde{c}^\dagger_{l\sigma}$ is obtained from the original basis operators $c^\dagger_{i\sigma}$ by a unitary transformation

$$\tilde{c}^\dagger_{l\sigma}=\sum_i \psi_l(\mathbf{r}_i)c^\dagger_{i\sigma}\,, \quad (2b)$$

where $\{\psi_l\}$ are eigenstates of the tight-binding Hamiltonian[10]

$$H_0=-\sum_{\langle i,j\rangle,\sigma}[\exp(i\phi_{ij})c^\dagger_{i\sigma}c_{j\sigma}+\text{c.c.}]\,. \quad (3)$$

Electrons on a lattice in a magnetic field with flux p/q per plaquette have $\phi_{ij}=2\pi\int_i^j\mathbf{A}\cdot d\mathbf{l}$, where $\mathbf{A}$ is the vector potential. H_0 is diagonalized in the reduced zone;

$$\tilde{c}^{(n)\dagger}_{\mathbf{k}\sigma}=\sum_{\mathbf{R}}\sum_j a^{(n)}_j(\mathbf{k})c^\dagger_{\mathbf{R}+j\sigma}\exp[i\mathbf{k}\cdot(\mathbf{R}+\mathbf{r}_j)]\,, \quad (4)$$

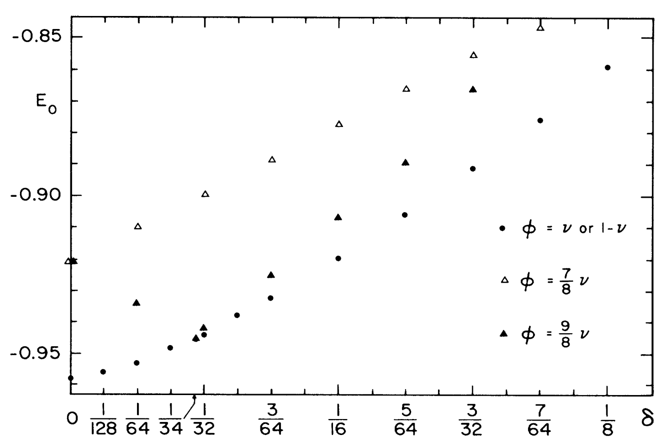

FIG. 1. Total energy of the spinless free-electron gas under magnetic field as a function of the deviation δ from half filling and for various linear relations between flux and filling $\nu=\frac{1}{2}-\delta$. The cusp in the upper curve occurs for a flux $\Phi=1-\nu$, equivalent to $\Phi=\nu$.

where $\mathbf{R}$ labels a supercell and $\mathbf{r}_j$ is within the supercell. $|a_j^{(n)}(\mathbf{k})|^2$ is the weight of the state $(\mathbf{k},\sigma)$ on the site j in the supercell and is deduced by solving the eigenstate problem,

$$\sum_j H_{ij}^0(\mathbf{k}) a_j^{(n)}(\mathbf{k}) = E_{\mathbf{k}}^{(n)} a_i^{(n)}(\mathbf{k}) ,$$

where

$$H_{ij}^0(\mathbf{k}) = -\sum_{\mathbf{R}} \exp\{i[\mathbf{k}\cdot(\mathbf{R}+\mathbf{r}_{ij})+\phi_{i\,j+\mathbf{R}}]\} .$$

The energy spectrum contains q bands (labeled by n). Because of the electromagnetic gauge invariance,

$$E(k_x+2\pi m/q, k_y+2\pi n/q) = E(k_x,k_y) ,$$

so that each band is q-fold degenerate and L/q^2 momenta are chosen in the reduced Brillouin zone of size $(2\pi/q)^2$.

The wave function (2a) is a spin singlet. Poilblanc[12] has pointed out that it is equivalent to the wave function proposed in Ref. 10 and that it can be written in a QSL form,

$$|\Psi\rangle = P_d\left[\sum_{i,j} a(\mathbf{r}_i,\mathbf{r}_j) c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger\right]^{N/2}|0\rangle ,$$

where

$$a(\mathbf{r}_i,\mathbf{r}_j) = a(\mathbf{r}_j,\mathbf{r}_i) = \sum_l^{\text{occ}} \psi_l(\mathbf{r}_i)\psi_l(\mathbf{r}_j) .$$

This is formally similar to the GS introduced by Anderson for the QSL theory.[2]

Following Gutzwiller, we renormalize the expectation values by a classical factor[5] to approximate the P_d projectors,

$$\langle c_{i\sigma}^\dagger c_{j\sigma}\rangle \sim g_t \langle c_{i\sigma}^\dagger c_{j\sigma}\rangle_0 , \quad g_t = 4\delta/(1+2\delta) ,$$
$$\langle \mathbf{S}_i\cdot\mathbf{S}_j\rangle \sim g_J \langle \mathbf{S}_i\cdot\mathbf{S}_j\rangle_0 , \quad g_J = 4/(1+2\delta)^2 , \tag{5}$$

where $\langle A\rangle$ and $\langle A\rangle_0$ are expectation values in the state $|\Psi\rangle$ and $|\Psi_0\rangle$, respectively, and 2δ is the hole doping. At half filling a d-wave projected BCS state containing both particle-hole and particle-particle pairings is equivalent to Affleck and Marston's flux state with only particle-hole pairing.[4] Furthermore, if the flux per plaquette is $\frac{1}{2}$ $(\Phi=\frac{1}{2})$ and if the gauge is defined by $|\phi_{ij}| = \pi/4$ $(\sum_\square \phi_{ij} = \pm\pi)$, the dimensionless quasiparticle spectrum is $E_{\mathbf{k}}^{(\pm)} = \pm 2(\cos k_x^2 + \cos k_y^2)^{1/2}$, and the magnetic and kinetic energies are identical, within approximation (5), to the values $-0.344J$ and $-2.71t$/hole of the d-wave projected BCS state.[5]

Assuming that $(1/2\pi)\sum_\square \phi_{ij} = p/q$ is a rational number, we construct (2a) by filling (completely or partially) some of the lowest q bands. The magnetic energy of the singlet GS is

$$\langle H_J\rangle = -\frac{3J}{8L} g_J \sum_i \sum_{\tau,\sigma} \langle \exp(i\phi_{i\,i+\tau}) c_{i\sigma}^\dagger c_{i+\tau\,\sigma}\rangle_0 \langle \exp(-i\phi_{i\,i+\tau}) c_{i+\tau\,-\sigma}^\dagger c_{i\,-\sigma}\rangle_0 . \tag{6}$$

Because of the singlet character of the state we could introduce the *same* fictitious flux and gauge for $\uparrow$ and $\downarrow$ spins corresponding to that used in $|\Psi_0\rangle$ in (2a). Because of gauge invariance

$$\langle c_{i\sigma}^\dagger c_{i+\tau\,\sigma} \exp(i\phi_{i\,i+\tau})\rangle_0 = \frac{q}{4L}\sum_{n,\mathbf{k}}^{\text{occ}} E_{\mathbf{k}}^{(n)} \tag{7}$$

independent of i, σ, and the direction to the nearest neighbor $i+\tau$. The proof is as follows: First, (7) is clearly gauge invariant since under U(1) transformations the phases arising in the wave function are absorbed by the change in $\exp(i\phi_{ij})$. If, for example, we choose the Landau gauge along x and y with different origins, it is clear that (7) should be translational and rotational invariant. The sum over occupied $\mathbf{k}$ states is performed in the reduced Brillouin zone containing L/q^2 points and n labels the filled bands. The sum (7) is over the energies of the Hofstadter problem[13] with flux p/q, up to the Fermi energy. The gauge invariance of the Hofstadter problem, i.e., the q-fold degeneracy of the bands, is responsible for the q prefactor in (7). Then, the exchange and kinetic energies per site at any flux are easily shown to be

$$\langle H_J\rangle = -\frac{3J}{16} g_J \left[\frac{q}{L}\sum_{n,\mathbf{k}}^{\text{occ}} E_{\mathbf{k}}^{(n)}\right]^2 ,$$
$$\langle H_t\rangle = 2t g_t \left[\frac{q}{L}\sum_{n,\mathbf{k}}^{\text{occ}} E_{\mathbf{k}}^{(n)}\right] \langle\langle \cos\phi_{ij}\rangle\rangle , \tag{8}$$

where $\langle\langle\cos\phi_{ij}\rangle\rangle$ is the average over all the bonds of $\cos\phi_{ij}$. As expected, this depends on the gauge, being $\frac{1}{2}$ in the Landau gauge and 0 in the symmetric gauge, for example. This is simply a consequence of the U(1)-symmetry breaking of the kinetic term $[c_{i\sigma}\to c_{i\sigma} \times \exp(i\alpha_i)]$. In this approach, the flux p/q is to be considered as a variational parameter as well as the gauge. For half filling and half flux, with the gauge discussed above, i.e., $|\phi_{ij}| = \pi/4$, $\langle\langle\cos\phi_{ij}\rangle\rangle = 1/\sqrt{2}$. Equation (8) establishes for the first time a direct connection between the GS energy of the correlated electron system at arbitrary fractional filling away from half filling and the total energy of the noninteracting spinless electron gas on a lattice in a uniform magnetic field.[11] The occurrence of cusplike minima in $E_0(\Phi) = (q/L)\sum_{n,\mathbf{k}}^{\text{occ}} E_{\mathbf{k}}^{(n)}$ at $\Phi = \nu$ has interesting consequences, since it occurs in both energy terms $\langle H_J\rangle$ and $\langle H_t\rangle$.

The stability of the CFP depends on the behavior of $K(\Phi) = \max\langle\langle\cos\phi_{ij}\rangle\rangle$ with gauge as a function of the flux $\Phi = p/q$. Optimization with respect to $\nabla\xi$ on $\langle\langle\cos(\phi_{ij}+\xi_i-\xi_j)\rangle\rangle$ for a set of rational Φ (Fig. 2) shows an absolute maximum at $\Phi=0$ $(K=1)$ and a local maximum at $\Phi=\frac{1}{2}$ $(K=1/\sqrt{2})$. Related studies[14] suggest that $K(\Phi)$ has cusps at rational Φ but smaller cusps should be smoothed out by various perturbations (e.g., lattice imperfections). $\langle H_t\rangle$, for $\nu=\frac{1}{2}-\delta$ as a function of Φ, has a minimum for $\Phi=0$, very likely a local cusp-

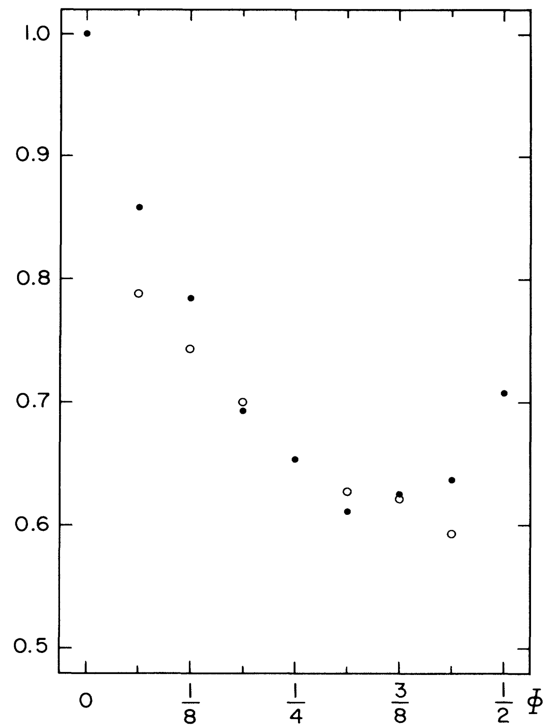

FIG. 2. Lower bounds of $K(\Phi = p/q) = \max\{\langle\langle \cos\phi_{ij}\rangle\rangle\}$. In the infinite manifold of local gauges, periodic ϕ_{ij} gauges have been chosen on a $\sqrt{q}\times\sqrt{q}$ supercell (solid circles) and a $2\times q$ supercell (open circles).

like minimum at $\frac{1}{2}$, and a kinklike singularity at $\Phi = \nu$. (There is no computational evidence that this point should correspond to an actual local minimum.) Therefore, at fractional filling, the total energy $\langle H_J\rangle + \langle H_t\rangle$ has a cusplike minimum at $\Phi = \nu$, or at $\Phi = \frac{1}{2}$, if J/t is not too small. Whether $\Phi = \nu$ is an absolute minimum or not depends on the balance between the exchange term, which always favors $\Phi = \nu$, and the kinetic term which favors $\Phi = 0$ or $\frac{1}{2}$. At small δ the competition between $\Phi = \nu$ and $\Phi = \frac{1}{2}$ depends essentially on the ratio J/t. The singularity of $\langle\langle \cos\phi\rangle\rangle$ at $\Phi = \frac{1}{2}$, if confirmed, provides a mechanism for the stability of the $\Phi = \frac{1}{2}$ flux phase on a finite range around $\delta = 0$.

An important result we have obtained is that the CFP $\Phi = \nu = \frac{3}{8}$ are more stable than $\Phi = \frac{1}{2}$ and $\Phi = 0$ for $(J/t)_1 \gtrsim 1.07$ and $(J/t)_2 \gtrsim 3.0$, respectively (for the CFP $\Phi = \nu = \frac{7}{16}$ the corresponding J/t are 1.8 and 0.88). Because of the uncertainty in the calculation of K, these values are upper bounds and may be decreased by improvements on K. The critical value $(J/t)_2$ for $\delta \to 0$ is $\sim \delta$. Since $(J/t)_1$ is increasing when $\delta \to 0$, we expect a plateau around $\nu = \frac{1}{2}$ at $\Phi = \frac{1}{2}$.[15]

In fact, in our optimization of K it is favorable to choose flux distributions where the total flux in a supercell is made of $q-p$ plaquettes each with flux Φ (or $-\Phi$) and p plaquettes with flux $\Phi - 1$ (or $1-\Phi$). The two choices are related by time-reversal symmetry. So the total flux per supercell is zero.

Until now we have only discussed fictitious magnetic fluxes. We now proceed to discuss the effect of real external magnetic fields $\mathbf{H}_{\rm ext}$ on our GS. We argue that the CFP phases are superconducting states and exhibit a Meissner effect. Consider an external potential $\mathbf{A}_{\rm ext} + \nabla\beta_{\rm ext}$, where $\beta_{\rm ext}$ is any regular function, applied to the CFP at $\Phi = \nu$. Again we consider Φ as a variational parameter, the optimum value of which may depend $\mathbf{H}_{\rm ext}$. $\langle H_J\rangle$ as a function of the fictitious Φ in the wave function (2a) is obviously unchanged. The kinetic term is changed to

$$E_0(\Phi)\langle\langle \cos(\phi_{ij} + \varphi_{ij} + \nabla\beta_{\rm ext} + \nabla\xi)\rangle\rangle ,$$

where $\varphi_{ij} = 2\pi \int_i^j \mathbf{A}_{\rm ext}\cdot d\mathbf{l}$, and we have introduced the gauge term $\nabla\xi$ of the fictitious field. Assuming that $K(\Phi)$ is varying smoothly, then, due to the cusp in the exchange term, the total energy is minimized at small external field at $\Phi = \nu$, the same flux per plaquette as in the absence of $\mathbf{H}_{\rm ext}$ (electromagnetic gauge invariance is obviously fulfilled). So the total flux per supercell stays zero and this gives a Meissner screening due to the rigidity of the wave function.

$\langle H_J\rangle$ is invariant under a simultaneous gauge transformation on the $\uparrow$ and $\downarrow$ spin-wave functions but $\langle H_t\rangle$ is not. A wave function

$$|\Psi_S\rangle = \exp\left[i\sum_{j,\sigma_j} S_\sigma(\mathbf{r}_j,\sigma_j)\right]|\Psi\rangle$$

corresponds to a uniform current-carrying state in the x direction when $\nabla_x S_\sigma = q_x$. $\langle H_t\rangle$ is modified to

$$\langle H_t(S_\sigma)\rangle \propto \sum_{\langle i,j\rangle,\sigma} \cos\left(\phi_{ij} + \int_i^j \mathbf{S}_\sigma\cdot d\mathbf{l}\right).$$

If S_σ is a slowly varying function on the scale of the lattice, we can expand around the optimum value of the phase ϕ_{ij} and

$$\langle H_t(S_\sigma)\rangle - \langle H_t(0)\rangle \sim |\langle H_t\rangle| \sum_\sigma \int (\nabla S_\sigma)^2 d\mathbf{r} .$$

However, only gauge changes which leave the singlet character of the wave function unchanged are allowed so $S_\uparrow = S_\downarrow$. These states carry a uniform current $\propto q_x$. Note that since the CFP have a spatially uniform charge, and since the Hofstadter spectrum has a gap, then this collective excitation will not be pinned nor will it decay in a ring geometry except by a topological excitation. Thus the CFP are capable of carrying a persistant current.

Consider a slowly varying $\mathbf{A}_{\rm ext}$ so that $\nabla S_\sigma \to \nabla S_\sigma - 2\pi\mathbf{A}_{\rm ext}$. To discuss flux quantization in a ring geometry we must examine the boundary condition. If we impose the London condition $S_\sigma(\mathbf{r}+L_x) = S_\sigma(\mathbf{r}) + 2m\pi$ (i.e., $q_x = 2m\pi/L_x$), where L_x is the ring circumference and m is an integer, then we find only the

London flux quantization giving a flux quantum of hc/e. However, other excited states are possible. Following the discussion of de Gennes[16] for a BCS superconductor, we consider one-particle states with antiperiodic boundary conditions on the ring and apply a gauge transformation with $S_\sigma(\mathbf{r}+L_x)=S_\sigma(\mathbf{r})+(2m+1)\pi$. This gives fully periodic wave functions and leads us to the Onsager flux quantum $hc/2e$. In defining an order parameter the requirement that it should be single valued around the ring shows that the proper choice for its phase will be $S(\mathbf{r})=\sum_\sigma S_\sigma(\mathbf{r})=2S_\uparrow(\mathbf{r})$. Substituting in $|\Psi_S\rangle$, we arrive at a Ginzburg-Landau-type energy expansion

$$\langle H_t(S,\mathbf{A}_{\text{ext}})\rangle-\langle H_t(0)\rangle\propto\int(\nabla S-4\pi\mathbf{A}_{\text{ext}})^2d\mathbf{r}\,.$$

This means that the GS has a broken electromagnetic global gauge symmetry. The magnitude of the order parameter will be $\propto|\langle c_{i\sigma}^\dagger c_{j\sigma}\rangle|^{1/2}$ (or $\propto\delta^{1/2}$). This form of the energy can be used to derive an Abrikosov theory of type-II superconductivity.

In conclusion, we have estimated the energy of the correlated electron gas on a lattice in the CFP represented by a Gutzwiller-projected determinant of Hofstadter single-electron wave functions. We find that CFP at $\Phi=\nu$ can be stabilized, in mean field, for reasonable δ, for values of $J/t\gtrsim1$. We find that the total energy has a cusp as a function of the flux per plaquette; this behavior suggests that CFP are *bona fide* superconducting GS of correlated electrons represented by the t-J model. At intermediate values of $J/t\lesssim1$ the state with $\Phi=\frac{1}{2}$ is stable over a range of values of δ. The form of the mean-field theory is unusual because of the cusp in the energy. The corrections to the critical values of J/t for CFP from possible additional terms in the Hamiltonian and beyond mean field remains to be investigated.

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