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Flux phases in two-dimensional tight-binding models

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Using a gauge-invariant tight-binding model on a rigid square lattice, we discuss the transition between a low-temperature flux phase in which orbital magnetic moments alternate antiferromagnetically in sign from plaquette to plaquette and a normal metallic phase. The order parameter, which may be chosen to be the magnetic flux penetrating a plaquette, goes continuously to zero at the transition. We also consider similar phases in a model with m spin colors antiferromagnetically exchange coupled.

The discovery of high-T_c superconductivity has led to increased interest in highly correlated electron and spin systems in two dimensions. In particular, Anderson[1] has suggested that the two-dimensional Hubbard model in the large-U limit on a square lattice off of half filling might have a resonating-valence-bond (RVB) ground state rather than a Néel ground state and that electron correlations in such a state might favor superconductivity. There have been many formulations[2-5] of the RVB state. In the original formulation,[6] there is no broken symmetry to distinguish it from a high-temperature paramagnetic phase. Recently, however, there have been proposals for RVB states that break time-reversal symmetry[5,7,8] and proposals for related flux states that break both time-reversal and lattice-translation symmetry.[5,9] In this paper, we will use mean-field theory to study two models that have low-temperature flux phases and high-temperature paramagnetic conducting phases. The order parameter in the flux phase is the staggered magnetic flux penetrating a lattice plaquette. It goes continuously to zero at the second-order transition to the metallic phase.

Kalmeyer and Laughlin[7] have shown that the RVB state for the spin-$\frac{1}{2}$ Heisenberg model on a triangular lattice is well described by a fractional quantum Hall (FQH) wave function. This state is characterized by a nonvanishing expectation value $\mathbf{S}_1\cdot(\mathbf{S}_2\times\mathbf{S}_3)$ for any triple spins $\mathbf{S}_1$, $\mathbf{S}_2$, and $\mathbf{S}_3$ on the lattice and thus by broken time-reversal symmetry. One of us[8] has shown that the projection onto the spin-singlet Jastrow subspace of the tight-binding Hubbard model in the limit of infinite on-site repulsions U leads to a FQH wave function again with a nonvanishing expectation value of $\mathbf{S}_1\cdot(\mathbf{S}_2\times\mathbf{S}_3)$. Affleck and Marston[9] have shown that a generalized Hubbard model with m "flavors" of electrons has a flux phase ground state in the limit of large m. In this phase, the gauge-invariant product around a lattice plaquette of the expectation value of the hopping operator,

$$\bar{\kappa}_{ij}=\sum_\sigma \bar{\kappa}_{ij}^\sigma \equiv \sum_\sigma c_{i\sigma}^\dagger c_{j\sigma}\,, \tag{1}$$

coupling the electron annihilation operator $c_{j\sigma}$ at site j to the creation operator $c_{i\sigma}^\dagger$ at site i, i.e.,

$$P=\langle\bar{\kappa}_{12}\rangle\langle\bar{\kappa}_{23}\rangle\langle\bar{\kappa}_{34}\rangle\langle\bar{\kappa}_{41}\rangle=|P|e^{-i\phi_p} \tag{2}$$

is nonzero. The gauge-invariant phase ϕ_p alternates in sign from plaquette to plaquette exactly as the spin does in the Néel state. P is complex except when $\phi_p=0$ or $\phi_p=\pi$. Thus, like the Néel state, the flux phase is invariant under time reversal followed by a lattice translation. Wen, Wilczek, and Zee[10] have pointed out that for any triple of sites 1, 2, 3,

$$\mathrm{Im}P_{123}=\mathrm{Im}\langle\bar{\kappa}_{12}\bar{\kappa}_{23}\bar{\kappa}_{31}\rangle=-\tfrac{1}{4}\langle\mathbf{S}_1\cdot(\mathbf{S}_2\times\mathbf{S}_3)\rangle\,. \tag{3}$$

This relation establishes an equivalence between flux order and spin triple order.

To date, most work on RVB-related phases has focused on ground-state properties ($T=0$). Little attention has been paid to finite temperature and the phase transition to a high-temperature disordered state that is expected to occur at nonzero temperature in systems with a broken discrete symmetry (e.g., time reversal) at low temperature. Here, we consider two models having flux phases at low temperature and paramagnetic conducting phases at high temperature. We show that ϕ_p and related parameters can be treated as traditional order parameters that vary continuously with temperature T, vanishing in mean-field theory as $|T_c-T|^{1/2}$ near a critical temperature T_c.

Both models we consider have gauge-invariant couplings to the magnetic field. As a result, there is always a physical *magnetic* flux ϕ with the same sign as ϕ_p penetrating each plaquette. Thus, our flux phases are in fact orbital antiferromagnets that should be observable, if they exist, via neutron scattering. However, because magnetic moments are spread over entire plaquettes rather than localized on electrons, the magnetic form factor will die off rapidly at large wave vector, and the scattering intensity into high-order Bragg peaks will be small. In addition, as we shall see, the absolute value of plaquette magnetic moments will be small so that the scattering intensity into the brightest Bragg peak will also be small. The phase ϕ_p and the magnetic flux ϕ are dynamically coupled and their relative value is fixed in equilibrium.

The simplest model exhibiting a flux phase is a gauge-invariant tight-binding model on a square lattice. We call this the t-ϕ model. Its Hamiltonian H is the sum of a hopping Hamiltonian $H_{\rm hop}$ and a magnetic Hamiltonian H_m. We take

$$H_{\rm hop}=-\sum_{\langle i,j\rangle,\sigma}(t_{ji}c_{i\sigma}^\dagger c_{j\sigma}+t_{ij}c_{j\sigma}^\dagger c_{i\sigma})\,, \tag{4}$$

where the sum is over nearest-neighbor bonds $\langle ij \rangle$, $t_{ij} = te^{i\phi_{ij}}$, and $\phi_{ij} = -\phi_{ji} = (e/\hbar c)\int_i^j \mathbf{A}\cdot d\boldsymbol{l}$, where $\mathbf{A}$ is the vector potential which we treat as a classical variable. Also

$$H_m = \tfrac{1}{2} C \sum_p \left(\sum_{\langle i,j \rangle \in p} \phi_{ij} \right)^2 , \tag{5}$$

where the sum is over all plaquettes p. The scale of energy in cgs units is set by $C = (4\pi\mu_0)^{-1}(e^2 l/a^2)\alpha^{-2}$, where a is the lattice constant of the two-dimensional lattice in the xy plane, l is the distance the magnetic field penetrates in the z direction, $\alpha = \frac{1}{137}$ is the fine-structure constant, and μ_0 is the magnetic permeability of the medium in which the lattice is embedded. The equilibrium state of this model is clearly conducting when the ϕ_{ij} is zero and there are less than two electrons per site.

When there is one electron per site (half filling), this model has a Peierls instability favoring a doubling of the unit-cell size which can be accomplished (in the absence of coupling to other degrees of freedom such as lattice distortions) by the antiferromagnetic array of fluxes shown in Fig. 1. A natural order parameter for this phase is the staggered magnetic flux $\phi = \sum_{\langle i,j \rangle \in p} \phi_{ij}$ measured in units of the quantum of flux $\Phi_0 = hc/e$. To carry out explicit calculations, we take the unit cells at $\mathbf{R}$ to contain two sites and introduce the corresponding electron operators $c_{\mathbf{R},1,\sigma}$ and $c_{\mathbf{R},2,\sigma}$. In terms of their spatial Fourier transforms we have

$$H_{\rm hop} = -\sum_{\mathbf{q},\sigma} [c^\dagger_{\mathbf{q},1,\sigma} v(\mathbf{q}) c_{\mathbf{q},2,\sigma} + \text{c.c.}] , \tag{6}$$

where the sums are over the Brillouin zone $|q_x| + |q_y| \le \pi/a$ and

$$v(\mathbf{q}) = t_1 e^{iq_x a} + t_2^* e^{iq_y a} + t_3^* e^{iq_x a} + t_4 e^{iq_y a} , \tag{7}$$

where t_1, t_2, t_3, and t_4 are the complex hopping amplitudes around a plaquette as shown in Fig. 1. We choose a gauge in which the phase ϕ is equally distributed on all bonds so that $t_1 = t_2 = t_3^* = t_4^* = te^{-i\phi/4}$. The spectrum of

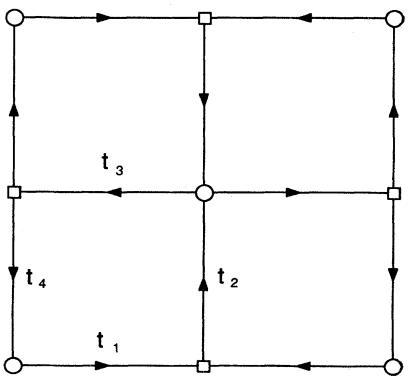

FIG. 1. Array of currents which give rise to an antiferromagnetic flux lattice. Each unit cell contains two sites, No. 1 indicated by a circle and No. 2 by a square.

$H_{\rm hop}$ consists of two branches for each spin with energies

$$\begin{aligned} \varepsilon_s(\mathbf{q},\phi) &= s\varepsilon(\mathbf{q},\phi) \\ &= 2ts\,|\, e^{-i\phi/4}\cos q_x a + e^{i\phi/4}\cos q_y a\,| , \end{aligned} \tag{8}$$

where $s = \pm 1$ and $\varepsilon(\mathbf{q},\phi) = |v(\mathbf{q})|$. This spectrum has some remarkable properties. When $\phi = 0$, $\varepsilon(\mathbf{q},0) = 0$ along the edges of the Brillouin zone defined by $|q_x| + |q_y| = \pi/a$. For all nonzero ϕ, $\varepsilon(\mathbf{q}_c,\phi) = 0$ at four points, $\mathbf{q}_c[\pm\pi/(2a), \pm\pi/(2a)]$, on the Brillouin-zone boundary, implying that at half filling, the Fermi surface consists of four points. There is a Dirac energy dispersion in the neighborhood of these points with

$$\begin{aligned} \varepsilon(\mathbf{q}_c + \mathbf{k},\phi) &= c(\phi,\theta)\,|\mathbf{k}| \\ &= 2ta\sqrt{1+\cos(\phi/2)\sin(2\theta)}\,|\mathbf{k}| , \end{aligned} \tag{9}$$

where θ is the angle $\mathbf{k}$ makes with the x axis. This leads to a linear density of states near zero energy of the form $D(\varepsilon) = |\varepsilon|/(2\pi t^2 a^2 |\sin\phi/2|)$. Thermodynamics at low temperature will be dominated by this linear term in $D(\varepsilon)$. Thus the specific heat is proportional to T^2 and the compressibility, paramagnetic, and diamagnetic susceptibilities proportional to T. As $T \to T_c^-$, the domain in ε where $D(\varepsilon) \sim |\varepsilon|$ vanishes, and there are no unphysical singularities associated with the vanishing of ϕ as $T \to T_c$. It is worth noting that when $\phi = \pi$, $\varepsilon_s(\mathbf{q},\phi)$ has the same $\mathbf{q}$ dependence as the gap function for $s+id$-wave superconductor discussed by Kotliar[4] in an RVB model for superconductivity.

To study the phase transition from the metallic state with $\phi = 0$ to the flux phase with ϕ nonzero, we consider the free energy per site $f = \frac{1}{2} C\phi^2 + f_{\rm hop}(\phi)$, where

$$f = -\frac{2}{\beta N}\sum_{\mathbf{q},s} \ln(1 + \exp\{-\beta[s\varepsilon(\mathbf{q},\phi) - \mu]\}) , \tag{10}$$

where $\beta = 1/T$ and μ is the chemical potential. The overall factor of 2 in this expression arises from the spin sum. We now restrict our attention to systems with one electron per site for which $\mu = 0$ for all temperature. In this case, the equilibrium equation of state obtained by minimizing f with respect to ϕ is $C\phi = -\partial f_{\rm hop}/\partial\phi$ or

$$C\phi = -\frac{2}{\beta N}\sum_{\mathbf{q}} t\cos q_x a \cos q_y a \frac{\tanh\frac{1}{2}\beta\varepsilon(\mathbf{q},\phi)}{\varepsilon(\mathbf{q},\phi)} \sin\phi/2 . \tag{11}$$

The transition temperature T_c, determined by the first appearance of a nonzero solution to this equation, is given by

$$\begin{aligned} T_c &= t\exp\{-2\pi[C/(2t)]^{1/2}\} \\ &= t\exp\{-2\pi\alpha^{-1}[(e^2 l/a^2)/8\pi t]^{1/2}\} , \end{aligned} \tag{12}$$

or $T_c \approx te^{-60}$ for $a = l \approx 10^{-7}$ cm and $t \approx 10$ eV. This extremely small transition temperature is a result of the very large magnetic energy associated with the creation of current loops 10 Å on a side. Thus, ϕ will always be small even at zero temperature, even though the absolute minimum of $f_{\rm hop}(\phi)$ occurs at $\phi = \pi$.

Though the magnetic flux is the most natural order parameter for the flux phase of the t-ϕ model, other gauge-invariant order parameters are equally acceptable. These

can be constructed from averages of the gauge-invariant hopping operator

$$\kappa_{ij}^{\sigma} = c_{i\sigma}^{\dagger} c_{j\sigma} e^{i\phi_{ij}} = \bar{\kappa}_{ij}^{\sigma} e^{i\phi_{ji}}, \tag{13}$$

where i and j can be any sites on the lattice. Of particular interest is the hopping operator for nearest-neighbor sites. Let

$$\hat{K} = K - iL = \langle \kappa_{12}^{\sigma} \rangle . \tag{14}$$

Then,

$$\hat{K} = |P|^{1/4} e^{-i(\varphi+\varphi_p)/4} . \tag{15}$$

The current (measured in energy units) between two sites i and j is

$$I_{ij} = -2t \, \mathrm{Im} \sum_{\sigma} \langle \kappa_{ij}^{\sigma} \rangle = \langle -\partial H_{\mathrm{hop}} / \partial \phi_{ij} \rangle . \tag{16}$$

In the flux phase depicted in Fig. 1, there is a current in every bond with magnitude $I = -2\partial f_{\mathrm{hop}}/\partial\phi$. Thus,

$$\tfrac{1}{2} I = 2tL = 2t\,|P|^{1/4} \sin(\phi+\phi_p)/4 = -\frac{\partial f_{\mathrm{hop}}}{\partial \phi} = C\phi . \tag{17}$$

This is the lattice version of the magnetic Maxwell equation, $\nabla \times \mathbf{B} = (4\pi/c)\mathbf{J}$. It provides an equilibrium relation between the magnetic flux ϕ and the plaquette phase ϕ_p. Thus, ϕ, ϕ_p, I, or L are all equally good measures of the flux order. If the sites 1 and 2 in one unit cell and 3 adjacent to 2 are vertices of a right triangle comprising half a plaquette, we find $\mathrm{Im}P_{123} = \mathrm{Im}[8\langle \kappa_{31}^{\sigma} \rangle \hat{K}^2 e^{i\phi/2} + 2\langle \kappa_{31}^{\sigma} \rangle \times \hat{K}^{*2} e^{-i\phi/2}]$. One can choose a gauge in which $\langle \kappa_{31}^{\sigma} \rangle$ is real and equal to $\langle \kappa_{13}^{\sigma} \rangle$. In this case, $\langle \kappa_{31}^{\sigma} \rangle$ is zero at half filling and when $\phi = \pi$ at all fillings. Thus, $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \times \mathbf{S}_3 \rangle$ is another order parameter for our flux phase only off of half filling and when $\phi \neq \pi$, in which case, it alternates in sign like ϕ and ϕ_p.

The simple t-ϕ model we just considered elucidates most of the important qualitative features of flux phases. Unfortunately, it has a vanishingly small transition temperature. More realistic transition temperatures are realized in the t-J model of Affleck and Marston[9] in which there are m spin colors and an exchange term,

$$H_{\mathrm{ex}} = J \sum_{\langle i,j \rangle} \sum_{\sigma,\eta} (c_{i\sigma}^{\dagger} c_{i\eta} c_{j\eta}^{\dagger} c_{j\sigma} - c_{i\sigma}^{\dagger} c_{i\sigma} c_{j\eta}^{\dagger} c_{j\eta}) , \tag{18}$$

added to the Hamiltonian. This term favors the spontaneous generation of current loops for sufficiently large m. Here we consider the t-J-ϕ model in which H_{ex} is added to the gauge-invariant model of Eqs. (4) and (5). We can treat the transition to the flux phase in mean-field (MF) theory using standard decoupling procedures in which the complete Hamiltonian is replaced by the effective Hamiltonian,

$$H_{\mathrm{MF}} = J \sum_{\langle i,j \rangle, \sigma \neq \eta} \langle \kappa_{ji}^{\eta} \rangle \langle \kappa_{ij}^{\sigma} \rangle - \sum_{\langle i,j \rangle, \sigma} (T_{ji} c_{i\sigma}^{\dagger} c_{j\sigma} + T_{ij} c_{j\sigma}^{\dagger} c_{i\sigma}) , \tag{19}$$

where $T_{ij} = [t + (m-1)J\hat{K}] e^{i\phi_{ij}} = T_{ji}^{*}$ is the gauge-covariant effective nearest-neighbor hopping. The average $\hat{K}$ of the nearest-neighbor hopping operator is to be self-consistently determined. The spectrum for this model is identical to that of the t-ϕ model with t_1 and t_3 in Eq. (7) replaced by

$$T = [t + (m-1)JK + i(m-1)JL] e^{-i\phi/4} \tag{20}$$

and t_2 and t_4 replaced by T^{*}. The equation determining $\hat{K}$ is then

$$\hat{K} = \frac{1}{N} \sum_{\mathbf{q}} v^{*}(\mathbf{q},\phi) e^{-i\phi/4} \tanh \tfrac{1}{2} \beta \varepsilon(\mathbf{q},\phi)/\epsilon(\mathbf{q},\phi) , \tag{21}$$

which when used in conjunction with the Maxwell equation [Eq. (17)] relating ϕ to L determines $\hat{K} = K + iL$ and ϕ. Because $C \gg t$, ϕ will always be much less than L, and the magnetic flux can be set to zero in Eq. (20) with negligible error. Thus K and L are determined (except for very small J) entirely by the t-J model with a transition temperature T_c of order $t \exp(-\pi\sqrt{t/4J})$. The magnetic flux is, however, fixed by Eq. (17). These equations imply that both ϕ and L vanish as $|T_c - T|^{1/2}$ as $T \to T_c^{-}$, whereas K is nonzero for all T and varies smoothly near T_c. Note that $K \neq 0$ in the high-temperature phase, which is thus a metal. From the numerical solution to Eq. (21), we find that K is larger than L for all temperatures, indicating that the phase ϕ_p of the t-J model never attains the value π favored by f_{hop}.

So far we have not included the on-site Hubbard repulsion U in our model. At half filling, this favors a spin-density-wave (SDW) state at small U that becomes the Néel state at large U. In the t-U-ϕ model obtained by adding the Hubbard repulsion to the t-ϕ model, there is, in mean-field theory, a line of first-order phase transitions in the T-U plane separating the flux and SDW phases at very small U and low T. This line terminates in a mean-field bicritical point. When J is turned on, the critical value of U at which there is a transition from the flux to the SDW phase grows with J for $m > 2$. These results will be discussed in more detail elsewhere.

The flux phase is characterized by nonzero currents in each bond. Elementary excitations in which the sign of the current in a subset of bonds is reversed are allowed, provided the total current entering every site remains zero. If the different spin colors are ignored, there are six permitted configurations of currents in bonds intersecting a given site. Thus, the symmetry of the flux phase is similar to that of the ordered phase of the six-vertex model,[11] which has a nonzero transition temperature. We therefore expect that our flux models will also have a finite transition temperature, though the coupling to the magnetic field and the presence of many spin colors may lead to interesting modifications of the exact results[11] of the six-vertex model. The SDW phase, on the other hand, has O_3 symmetry and a transition to the ordered phase only at zero temperature. We have not yet worked out the implications of these observations.

The transition from the normal metal to the flux phase presented here is not the only mechanism which can lead to a nonvanishing value of $\mathrm{Im}P_{123}$. An important alternative scenario is one in which $\hat{K}$ for a single bond remains real and nonzero for all temperatures, but in which the correlated product P_{123} develops an imaginary part in a broken symmetry phase. Such a state, of which the FQH

states of Refs. 7 and 8 are examples, exhibits directed correlated exchanges of fermions around a ring without an effective single-particle current and is likely to provide an appropriate description of correlation effects in the large-U limit. More exotic possibilities, such as the transition from a dimer phase to a flux phase discussed in Ref. 9 may also occur. In any case, it would be of interest to consider the temperature dependence of the phase of P_{123} in these condensed states. We regard it as likely that, as in the small-U version of this theory, the phase of the loop correlation function exhibits a nontrivial dependence on temperature in the condensed state.

Our analysis has concentrated on tight-binding models at half filling at $U=0$. The real challenge is, of course, to extend these ideas to the large-U Hubbard model off the half-filled band. Whether the ground state of the many-body system is well characterized as a flux phase in this limit remains to be established. However, if the flux phases are stable in this limit, their properties should be similar to those of the low-U states discussed here, just as the properties of the large-U Néel state are already manifest in the low-U SDW state.

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