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Generalized flux states of the t-J model

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We investigate certain generalized flux phases arising in a mean-field approach to the t-J model. First, we establish that the energy of noninteracting electrons moving in a uniform magnetic field has an absolute minimum as a function of the flux at exactly one flux quantum per particle. Using this result, we show that if the hard-core nature of the hole bosons is taken into account, then the slave-boson mean-field approximation for the t-J Hamiltonian allows for a solution where both the spinons and the holons experience an average flux of one flux quantum per particle. This enables them to achieve the lowest possible energy within the manifold of spatially uniform flux states. In the case of the continuum model, this is possible only for certain fractional fillings and we speculate that the system may react to this frustration effect by phase separation.

The discovery of high-temperature superconductors has led to a revival of interest in two-dimensional strongly correlated electronic systems. A model of central interest is the t-J Hamiltonian.[1] At half-filling, it reduces to the Heisenberg model which develops long-range order at zero temperature. Away from half-filling, however, a quantum spin-liquid description has been proposed.[1] This state is a spin singlet, has no long-range magnetic order, and is characterized by a uniform charge density and limited-range antiferromagnetic correlations.[2-4] Among the suggested mean-field descriptions of the spin liquid, the flux phase of Kotliar[3] and Affleck and Marston[4] at and close to half-filling has the lowest ground-state energy for a wide range of the parameters. Besides the mean-field approaches, variational wave functions making use of the Gutzwiller projection have also been proposed[5] and studied numerically.[6,7] Finally, a large number of related works is concerned with chiral spin liquids, where excitations with fractional statistics may arise.[8] However, these states have been shown to give the lowest energy only for large values of the next-nearest-neighbor (NNN) coupling[9] and we will not consider them here. Long-range generalizations of the flux phase, including NNN coupling and beyond, have recently been studied.[10]

In line with a suggestion by Anderson,[11] Lederer and co-workers studied possible generalizations of the flux phases for different fillings.[6,7] Investigating a few doping concentrations, they found evidence that the exchange energy (J) is minimized at about one flux quantum per particle. Then, using the same trial wave function, they calculated the contribution of the kinetic term (t) to the ground-state energy and studied the competition between the t and the J terms which occurs because the former prefers zero flux.

In this work, we first study the motion of an electron in a uniform magnetic field for arbitrary fillings and fields and establish the linear proportionality between the filling factor and the optimal flux with high accuracy. Then we turn to the t-J model and represent the doping and the no-double-occupancy constraint in a slave-boson formalism. Up to multiplicative factors in the effective Hamiltonian, the mean-field approximation for the slave bosons is known to be equivalent to the Gutzwiller projection.[6,7] However, in the slave-boson approximation, the hard-core nature of the bosons is treated only on the average. We develop a method to represent this feature more satisfyingly and explore its consequences. Finally, we discuss the relation of variational approaches to mean-field techniques and the problems associated with the passage to the continuum limit.

First let us consider the motion of an electron in a fixed external magnetic field. The Hamiltonian is

$$\mathcal{H} = \sum_{\langle i,j\rangle} c_i^\dagger c_j e^{i\phi_{i,j}} + \text{H.c.}\,, \qquad (1)$$

where $\langle i,j\rangle$ refers to nearest-neighbor sites and the sum of $\phi_{i,j}$ along any closed contour gives the flux of the magnetic field through the enclosed area. The single-particle spectrum, which forms a well-known fractal, has been studied in detail by Hofstadter.[12]

We have numerically diagonalized Eq. (1) for lattices of various sizes, up to 40×40. We calculate the ground-state energy for a fixed number N of particles by summing the first N energy eigenvalues.[13] We obtained its value for 200 different filling factors and about 1000 values of the magnetic flux (see Figs. 1 and 2). Consequently, we are able to find the location of the global and local minima of the total energy with high accuracy. Figure 1 exhibits two prominent features: (i) The ground-state energy shows a sharp global minimum as a function of the flux

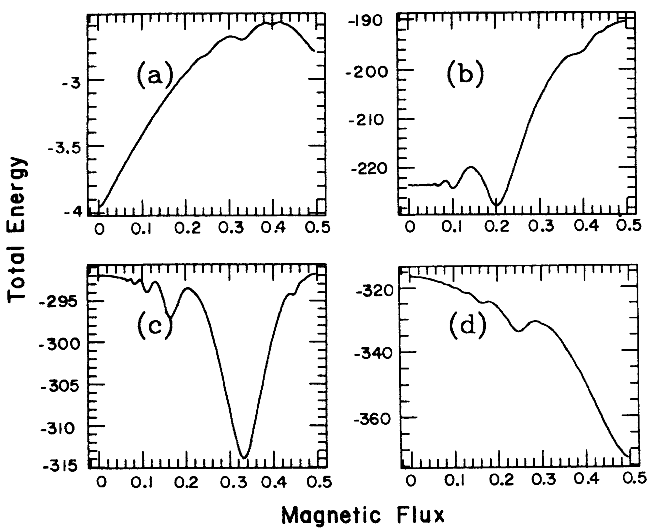

FIG. 1. Fermi-sea ground-state energy (in units of the bandwidth) vs magnetic flux per unit cell for a 20×20 square lattice. The filling factors are equal to (a) $\frac{1}{400}$, (b) $\frac{1}{5}$, (c) $\frac{1}{3}$, and (d) $\frac{1}{2}$. The minima become sharper with increasing system size.

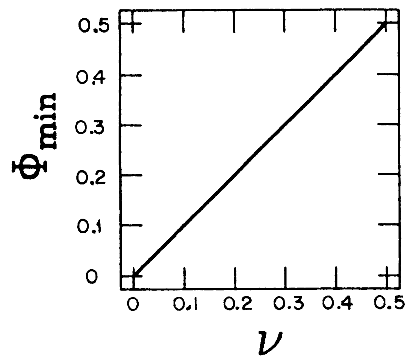

FIG. 2. Flux (in units of the flux quantum) which minimizes the kinetic energy of the Fermi sea, determined at 200 different filling factors.

exactly at plus or minus one flux quantum per particle, $\Phi=\pm\nu$ (in units of the flux quantum, modulo one flux quantum per plaquette), where ν is the electronic filling factor; (ii) a set of harmonics is observed; there are *local* energy minima at $\Phi=\nu/M_1+M_2/M_1$, where M_1 and M_2 are integers.

We suggest a physical reason for this result: Away from half-filling, the Fermi energy at one flux quantum per particle lies in the biggest gap of the spectrum, which in the continuum limit is equivalent to the first Landau gap. Thus, adiabatic manipulations should not change the qualitative features of the system. Let us imagine that we shrink the homogeneous magnetic field into infinitesimally thin vortex tubes, bound to the electrons. Then the unit flux quantum per particle turns each electron exactly into a boson, thus allowing all of them to occupy the lowest-energy state and thereby maximizing their energy gain. This type of argument is familiar from the theory of the quantum Hall effect. The analogous reasoning for the Heisenberg model is that if we treat the model in fermionic[3] and bosonic[14] mean-field approximation, the ground-state energy in the latter case is considerably lower. Thus the fermions try to lower their energy by "turning into bosons"[15] and the closest they can get to this within the bounds of the mean-field approximation is the generalized flux state with unit flux quantum per particle.

For the t-J model, we choose a spin-fermion ("spinon") and charge-boson ("holon") representation of the problem:

$$\mathcal{H}=-t\sum_{\langle i,j\rangle,\sigma}b_i^\dagger b_j c_{j,\sigma}^\dagger c_{i,\sigma}+\text{H.c.}-\frac{J}{N_s}\sum_{\langle i,j\rangle,\sigma,\sigma'}c_{i,\sigma}^\dagger c_{j,\sigma}c_{j,\sigma'}^\dagger c_{i,\sigma'}-\lambda\sum_i\left[\sum_\sigma c_{i,\sigma}^\dagger c_{i,\sigma}+b_i^\dagger b_i-1\right], \tag{2}$$

where N_s is the number of spinon species and the term with the Lagrange multiplier λ ensures the one-particle-per-site constraint. A typical procedure[2] now would be to assume a mean field for the holons to give simply a renormalized hopping matrix element and then to treat the exchange term by means of another mean field. However, this approach reflects the hard-core nature of the bosons only on average. For an improvement on that point we represent the bosons by fermions (fermion holon operators $h,h^\dagger$) with a vortex tube carrying one flux quantum attached to each.[16,17] In this approach no two like particles can occupy the same site simultaneously, so it recognizes the local character of the constraint and treats it more symmetrically with respect to holons and spinons. There is a constraint relating the flux of the statistical gauge potential through a plaquette of the dual lattice to an odd integer q times the hole density at the corresponding site of the original lattice:[17] $\sum_{j,\text{plaq}}\hat{A}_{i,j}=q2\pi h_i^\dagger h_i$. We make a "mean-field" approximation by replacing the vortex tubes of the statistical gauge field $\hat{A}_{i,j}$ by a homogeneous gauge field $A_{i,j}$.[17] The t and J terms are now each four-fermion interactions. We decouple them via a Hubbard-Stratonovich transformation. The resulting Hamiltonian describes two types of fermions, propagating in (different) gauge fields:

$$\mathcal{H}=\sum_{i,j}\Bigg(-t\{|Q_{i,j}|\exp[i(\Phi_{i,j}+A_{i,j})]h_i^\dagger h_j+\text{H.c.}\}-\frac{J}{N_s}\sum_\sigma[|Q_{i,j}|\exp(i\Phi_{i,j})c_{i,\sigma}^\dagger c_{j,\sigma}+\text{H.c.}]$$

$$+\frac{J}{N_s}|Q_{i,j}|^2+N_s\frac{t^2}{J}h_i^\dagger h_j h_j^\dagger h_i\Bigg)+\mathcal{H}(\text{constraint}), \tag{3}$$

where $\Phi_{i,j}$ is the phase associated with the auxiliary field $Q_{i,j}$. The four-holon interaction term gives approximately a constant shift $\sim N_s \delta^2 t^2/J$, where δ=doping, to the energy because of the constraint. This may be neglected in the limit $t\delta/J \ll 1$. We now employ a variational approach, analogous to the one in Ref. 7. We look for the minimum of the action in the space of functionals which is restricted by the requirement that the effective hopping amplitudes $|Q_{i,j}|$ correspond to an isotropic hopping probability and the phases to a uniform gauge flux Φ. As demonstrated in the first part of this paper, the optimal flux for fermions propagating in a magnetic field is one flux quantum per particle. The relevance of this result to the present problem was first stressed by Anderson.[11] In the arising mean-field Hamiltonian we have two types of fermions which propagate in simply related magnetic fields with only one variational parameter Φ. The number of holons and spinons is different, therefore the optimization of their energy terms with respect to the flux seems to lead to conflicting requirements for Φ. However, if one takes into consideration that the energy is periodic with periodicity of one flux quantum per plaquette and that the statistics-changing flux per holon can be any odd multiple of the flux quantum, then the following equations are obtained for the total optimal flux for spinons and holons, respectively: $\Phi_c N_c = \pm N_c + p_1 N_L$ and $\Phi_c N_c + qN_h = \pm N_h + p_2 N_L$, where p_1, p_2 are integers, $2\pi\Phi_c$ is the optimal flux per spinon, and N_h and N_c are the numbers of holons and spinons of a given type, respectively. Direct inspection shows that both fluxes can assume the value of one flux quantum per particle simultaneously for all rational filling factors, $\delta = N_h/N_L$, which are the ratio of odd integers. Thus we find that the hard-core nature of the holons does lead to an important result; namely, both types of excitation may be associated with an accompanying gauge field such that the lowest energy is obtained within the mean-field scheme. Since the Fermi energy now lies in the biggest gap for the doped systems, we can imagine again an adiabatic transformation of the gauge fields into tiny vortex tubes. Then this result implies that the spin quasiparticles still turn effectively into bosons but without changing the statistics of the holons into fermions. This is a genuine many-body effect, since one of the bare spinons or holons must be fermionic because of their electronic origin. This unusual result is somewhat paralleled by recent studies on slave-fermion models.[18] There the spinons are naturally represented from the outset as bosons, the holes are fermions and (in the ground state) a phase factor proportional to the doping is associated with the fermions within the mean field approximation. However, that phase does not represent a flux and it leads to the so-called spiral state.

We continue with two remarks on the peculiarities of the model. First, had we considered the continuum model from the outset, there would not have been a unit-flux-quantum-per-plaquette periodicity in the energy as a function of the flux and consequently (with $p_1 = p_2 = 0$ in the above formulas), the competition between the t and J terms would be reestablished and the optimal unit flux per particle could be achieved only for particular values of the doping (the "happy fractions"): $\delta = 1/(\text{odd integer})$. The main reason for this different conclusion lies in the different topology of the lattice and the continuum. Also, the two results correspond to different continuum limits; namely, the particle number per site is kept constant in the first case and the particle number per unit area in the second.

If one moves away from these special values, at least two scenarios are possible: (i) the system will favor the flux corresponding to the nearby happy-fraction value as a background and it absorbs the additional flux by creating quasiparticles with fractional statistics, as happens in the case of the fractional quantum Hall problem and as was suggested recently by Laughlin[8]; (ii) the system phase separates and splits into domains, where the flux takes on the values corresponding to the two neighboring happy-fractional fillings. There is some evidence for phase separation in the t-J model from exact diagonalization on small lattices, especially for large J/t.[19] Of course, the long-range part of the electrostatic energy opposes such a spatial inhomogeneity, but this case should not be excluded *a priori.*[20] The size of these domains is determined by the competition of the magnetic and electrostatic energies and can shrink to the size of the unit cell, in which case the situation is similar to scenario (i). Different, but related mechanisms for phase separation have also been suggested.[21]

Second, we remark on some details of the different techniques applied. Had we not constrained the function space to spatially homogeneous flux states when searching for the minima of the action, we would not have been able to carry through a self-consistent procedure. The reason is that a constant (mean) flux associated with the decoupling of the magnetic exchange term requires a proper nonuniform arrangement of the complex gauge factors along the bonds. When one then introduces the resulting spinon mean field into the holon t term, the resulting effective kinetic energy corresponds not only to a nonuniform magnetic field, but also to a spatially varying hopping amplitude. This would take us out of the Hofstadter problem which requires a uniform hopping. Therefore, our numerical results would not apply. This shows that the energy minimum we obtained by our variational approach is the result of a strongly restricted search and does not necessarily represent a local minimum in an unrestricted space.

We now address the question of the diamagnetic properties of the model. It is clear that for the case of the lattice, in our uniform mean-field treatment, any external flux can be accommodated by changing the internal field such that the total flux remains the optimal value.[6] This means that an external field is not expelled from the material. In this connection, we remark that the absence of flux quantization in a ring geometry for a related model has been demonstrated at the mean-field level.[22] For our model, again in this same uniform mean-field approximation, a gap is present in the spectrum and renders the system insulating. However, investigation of collective modes could reveal the existence of low-energy excitations.[23,24] According to Ref. 23, there is hope for superconductive behavior only in those *extended* mean-field approaches in which the value of the flux is allowed to follow the local changes in the particle density. We note that in the case of the continuum model an external magnetic field leads to an energy increase which is linear in the *magnitude* of the field. Thus a divergent susceptibility is obtained. This is reminiscent of the situation in the anyon gas,[8,24] but it should be emphasized that unlike that situation, we permit the internal fluxes seen by spinons and holons to adjust in such a way as to minimize the energy.

To summarize, we investigated certain flux phases arising in the mean-field approach to the t-J model. First we established for the whole range of parameters that the energy of an electron moving in a uniform magnetic field has a sharp minimum as a function of the flux at exactly one flux quantum per particle. Using this result, we showed that if the hard-core nature of the holons is taken into account, then in a mean-field approximation of the t-J Hamiltonian both the spinons and the holons experience a flux quantum per particle, enabling them to achieve the lowest possible energy within the manifold of spatially uniform flux states. In the case of the continuum model, however, only certain (happy) fractional fillings were possible and we speculated that the system may react to this frustration effect by phase separation, i.e., by developing nonuniform distributions of the electrons. It is worthwhile to mention that some recent experiments on the high temperature superconductors can be naturally explained by assuming phase separation of the electrons.[25]

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