Frustration mechanism for high-temperature superconductivity

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(Submitted 12 May 1988)
Pis'ma Zh. Eksp. Teor. Fiz. **47**, No. 12, 650–653 (25 June 1988)

The suggestion that the carriers of the superconducting current frustrate the magnetic system of a high-temperature superconductor not only disrupts the antiferromagnetic order but also converts magnetic excitations of the emerging quantum (Mott) paramagnet into neutral fermions.

The development of high-temperature superconductivity has attracted increased interest in quantum paramagnetic (Mott) insulators in the past year.[1] From the very beginning of the high-temperature boom, it has been more or less clear that the same charges which carry the superconducting current disrupt the antiferromagnetic order, frustrating the antiferromagnetic interaction. Two possibilities have been considered. In Anderson's RVB model and related models,[1] the superconducting charges are at the copper. In Emery's model,[2] in contrast, the holes are localized at the oxygen.

There are now many pieces of experimental evidence in support of Emery's model (see Refs. 3 and 4, for example). The d^9 hold band of copper is apparently split completely into two "Mott-Hubbard subbands," and the oxygen p band happens to lie precisely between them. It is thus reasonable to adopt Emery's model, to use a spin-1/2 quantum Heisenberg magnetic material to describe the filled lower Mott-Hubbard subband, and to assume that the deviation from stoichiometry generates a number of holes in the oxygen p band.

The frustrating effect of the p holes can be understood quite easily in the metallic limit, in which these holes induce an ordinary RKKY interaction between copper spins. The frustration generated by a few holes has been discussed in detail by Aharoni *et al.*[5]

Wiegmann, Polyakov, and the present author[6,7] recently constructed a topological theory of a 2D quantum Heisenberg magnetic material at zero temperature. In its excitation spectrum we found neutral fermions, as had been introduced by Pomeranchuk[8] in 1941, in order to describe the properties of quantum paramagnets, and as have recently been rediscovered by Anderson[2] in the context of high-temperature superconductivity. Below I will discuss the role played by frustration within the framework of the topological theory.[6] In particular, I point out that it is caused by p holes.

In Ref. 6 we worked in the continuum limit, describing a two-dimensional quantum antiferromagnet by means of a three-component vector field $\mathbf{n}$ of unit length ($n_\alpha^2 = 1; \alpha = 123$) in a $2+1$ Euclidean space $xy\tau$ of quantum statistics. The classical part of the action is written in the form

$$\alpha S^2 \int d\tau d^2x\, (\dot{\mathbf{n}}^2 + (\nabla \mathbf{n})^2). \qquad (1)$$

The spin S in front of the integral imposes the correct expansion as $S \to \infty$. The coefficient α determines the measure of frustration of the original lattice: The value $\alpha = 0$ corresponds to complete frustration. We now know that in La, Sr|Cu|O and Y|Ba|-Cu|O the frustration intensity $1/\alpha$ increases with the concentration of p holes.

The quantity αS^2 may be understood as the reciprocal of an effective temperature

$$T_{eff} = 1/\alpha S^2 \tag{2}$$

of a classical three-dimensional magnetic material with energy (1). A theory of a two-dimensional quantum magnetic material has recently been discussed on the basis of this well-known analogy by Wiegmann[9] and, in particular detail, by Chakravarty *et al.*[10] At a sufficient density of holes, a 2D quantum magnetic material is in a disordered quantum paramagnetic state, which corresponds to a "hot" classical 3D magnetic material. The spin correlation function of a quantum paramagnet is given by the standard 3D expression

$$\langle \mathbf{n}(\mathbf{r}, \tau)\, \mathbf{n}(0, 0) \rangle \sim \exp \left\{ - \frac{(x^2 + y^2 + \tau^2)^{1/2}}{R_c} \right\} . \tag{3}$$

In this stage we do not yet have any neutral fermions. They appear as a result of the frustration and the nontrivial topological term in the quantum action. This topological term is specific to a 2D quantum magnetic material and is a so-called Hopf invariant $\hat{H}$: the mapping $S_3 \to S_2$, $(\Pi_3(S_2))$. $\hat{H}$ takes on only integer values, $H = 0, \pm 1, \pm 2, \ldots$, which are the indices of the splitting of the quantum trajectories of the particles described by action (1). To write an expression for the Hopf invariant, we need to introduce a "current" j_μ, a "magnetic field" $f_{\mu\nu}$, and a corresponding "vector potential" α_μ:

$$j_\lambda = \frac{1}{2} \epsilon_{\lambda\mu\nu} f_{\mu\nu} = \frac{1}{8\pi} n^a \frac{\partial n^b}{\partial x_\mu} \frac{\partial n^c}{\partial x_\nu} \epsilon_{\lambda\mu\nu} \epsilon_{abc} ,$$

$$f_{\mu\nu} = \partial a_\nu / \partial x_\mu - \partial a_\mu / \partial x_\nu ; \qquad \lambda\mu\nu = xy\tau,\ abc = 123.$$

We then have

$$\hat{H} = - \frac{1}{2\pi} \int d^2 x d\tau a_\lambda j_\lambda . \tag{4}$$

The nontrivial nature of a Hopf mapping can be seen in the circumstance that (4) is not local as a functional of the field $\mathbf{n}$.

$\hat{H}$ disrupts the temporal parity $\tau \to -\tau$, thereby imposing some stringent requirements on the values of the renormalized charge θ with which $\hat{H}$ enters the theory:

$$\frac{1}{T_{eff}} \int d\tau d^2 x \, (\dot{\mathbf{n}}^2 + (\nabla \mathbf{n})^2) + i\pi\theta \hat{H} . \tag{5}$$

The square root of minus one here is required for unitarity of theory in the real

$t = \_\tau i$. The temporal parity requires that θ be an integer. In this case, the contribution of the topological term to the partition function

$$Z = \sum_H Z_{cl}(|H|)(-1)^{i\pi\theta H} \tag{6}$$

is ± 1, and Z does not change under time conjugation, $H \rightarrow -H$. In earlier papers[6,7] we made the tempting assumption $\theta = 2S$ and showed that at a high effective temperature T_{eff}, i.e., at a high density of holes, the particles described by action (5) are massless fermions if $S = 1/2$.

At this point it is not clear how we are to extract the topological term in (5) from a lattice Heisenberg Hamiltonian. The reason is that on a lattice the Hopf textures are topologically trivial, so there are no mechanisms in the theory itself which could generate nonzero Hopf invariants. A natural way to obtain them would be to introduce a small unrenormalized constant θ_0 in the theory to disrupt the temporal parity and to look at what would happen in the renormalization process. We would hope that the typical phase diagram would be similar to that in Fig. 1. The p holes might generate a Hopf term by themselves. In this case, the disruption of temporal parity would arise from interactions between copper spins, which correspond to closed contours containing an odd number of p-hole lines (Fig. 2). A summation over the hole spins would then give us the i's that we need in the Hopf part of the action. For example,

$$(\vec{\sigma} \cdot (\vec{\sigma} \times \vec{\sigma})) \equiv 6i$$

(etc.). Furthermore, at first glance, we now see no reason why θ would have to be an integer; according to (6), the implication would be the appearance of parafermions.

There is a second way in which a frustration might disrupt a quantum magnetic order: At a high hole temperature, we do not have any *a priori* knowledge of just which type of order will be disrupted as a result of the frustration. It is quite possible that a marginal ordered state might happen to be a multisublattice noncollinear antiferromagnet, for which the order parameter is the SO(3) group, or the projective space RP_3. The latter can be represented conveniently as a sphere S_3 with diametrical-

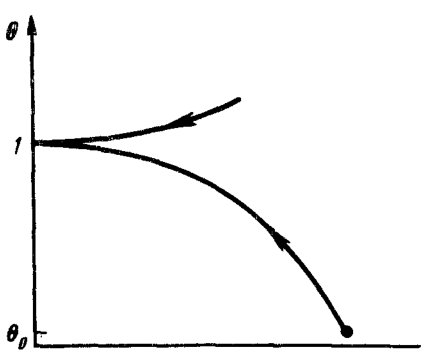

FIG. 1.

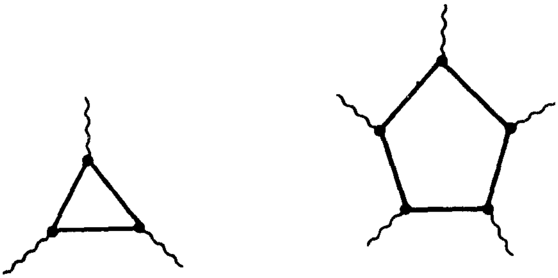

FIG. 2.

ly opposed identified points. The order parameter is thus the four-component unit vector $\vec{\nu}$ ($\nu_a^2 = 1; a = 1234$) with the joining condition $\vec{\nu} \equiv -\vec{\nu}$.

The classical part of the action remains of the same form. The topological term which disrupts the temporal parity, however, is of a completely different nature. It is now a trivial degree D of the mapping $S_3 \to S_2$, ($\Pi_3(S_2)$). The total action takes the form

$$\frac{1}{T_{eff}} \int d\tau d^2x \, (\dot{\vec{\nu}}^2 + (\nabla \vec{\nu})^2) + i\pi\theta \hat{D}, \qquad (9)$$

where $\hat{D}$ is given by the well-known local expression

$$\hat{D} = \frac{1}{4\pi^2} \int d\tau d^2x \, \epsilon_{\lambda\mu\nu} \nu^a \frac{\partial \nu^b}{\partial x_\lambda} \frac{\partial \nu^c}{\partial x_\mu} \frac{\partial \nu^d}{\partial x_\nu} \epsilon_{abcd} \, .$$

It is easy to verify that the term $\hat{D}$ in (9) cannot alter the nature of the excitations. They remain bosons with a correlation function of the type in (3) in the disordered state. Anderson *et al.*[11] recently presented argument supporting the suggestion that in the case of a magnetic order describable by the SO(3) group there would be another factor which would cause excitations to become fermions. They identified the quantum trajectories of these fermions with stable disclinations $\Pi_1(\mathrm{SO}(3)) = Z_2$.

The arguments presented by Anderson *et al.*[11] also apply to a third type of marginal order, which might in principle be generated by a frustration. In addition to a simple **n** or SO(3) we could imagine a so-called spin liquid crystal.[12] In it, the states **n** and $-$**n** would be identical, so in place of S_2 we would have a projective plane RP_2, where again there exists a stable disclination $\Pi_1(RP_2) = Z_2$.

In one way or another, we can distinguish two different classes of quantum disorder which might be produced by holes in a 2D Heisenberg magnetic material. In the first of these classes, in which the nonvanishing order is described by a three-component vector **n**, we would have, presumably depending on the spin S and the density of the p holes, either a quantum paramagnet, (3), or a fermion (or parafermion) liquid. In the second class, of a four-component vector ν, the excitations are always fermions, or—if the arguments of Anderson *et al.* are not completely convincing—we would again have a quantum paramagnet with a correspondingly different structure of antiparamagnons in (3).

The pairing mechanisms might be different in the Fermi liquid or the quantum paramagnet. In the first place, since the charged holes are by assumption at the oxygen, rather than at the copper, the well-known topological restriction[1,9] drops out of the picture, and a neutral fermion and a hole can form a boson of charge e. Clearly, the direct Coulomb repulsion would play no role in this process. In order to explain the half-integer quantization of the flux, however, we would have to assume that in a real Bose condensate there is a significant portion of bosons with a charge of $2e$, whose formation would now depend substantially on the relation between the Coulomb repulsion between singly charged bosons and the forces produced by neutral fermions. A scenario based on the presence of singly and doubly charged ions in a condensate seems particularly likely; as we know quite well from quantum mechanics,[13] a pairing of bosons in the 2D case would be possible if there were any attraction, no matter how slight. We should of course not forget that there is an old and reliable method to call on when we are dealing with two impurities (p holes) in a neutral Fermi liquid.

Without neutral fermions, an attraction between holes in a quantum paramagnet is produced through an exchange of antiparamagnons, (3), or their analog for SO(3). Birgenau *et al.*[14] recently calculated the corresponding transition temperature for La,Sr|Cu|O.

An exchange of antiparamagnons might of course also prove effective in a Fermi liquid, if the distance between holes in the pairs turned out to be smaller than the fermion deconfinement radius.

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Translated by Dave Parsons