Formation of a local moment near a vacancy in a spin liquid

S. A. Krivenko and G. G. Khaliullin
Kazan' Physicotechnical Institute, Russian Academy of Sciences, 420029 Kazan', Russia[1)]

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An isolated vacancy in a spin liquid in the flux phase engenders a localized state with a free spin. This effect can explain the appearance of local moments in high-T_c superconductor systems with nonmagnetic doping. © *1995 American Institute of Physics.*

The study of impurity effects in various strongly correlated electronic systems yields important information about the structure of the ground state of such systems. In the present paper we investigate the effects of nonmagnetic substitution (vacancies) in a two-dimensional spin liquid. The liquid is described by two mean-field models of resonating valence bonds (RVB) — a uniform RVB model (Ref. 1) and a flux-phase model (Refs. 2 and 3). These models are widely employed for describing the spin properties of high-T_c superconducting systems. Assuming that a static vacancy in a RVB lattice can serve as a model of nonmagnetic substitution of copper ions in high-T_c superconducting systems, we shall discuss the particular RVB states, in which such doping results in the formation of a localized state. The appearance of localized moments near nonmagnetic impurities in high-T_c materials was convincingly demonstrated experimentally by the direct observation of magnetic resonance on these moments.[4,5] As discussed in Refs. 4 and 5 , this effect is also closely related to the anomalous effect of nonmagnetic defects on high-T_c superconductivity. The calculations presented in the present paper show that a vacancy in a RVB lattice does indeed engender a localized state, if the spin liquid is in the flux phase. The free spin-1/2 that appears produces a Curie-like contribution to the susceptibility. The bound-state density is distributed over the lattice sites near the vacancy and decreases as $\sim R^{-2}$ away from it.

1. MODEL

The RVB states with Fermi spin excitations (spinons) correspond, in particular, to the mean-field solutions of the Heisenberg antiferromagnetic model. Representing the spin operators in terms of pseudofermions, $s_i = c^+_{i\alpha}\sigma_{\alpha\beta}c_{i\beta}/2$, and factorizing the exchange interaction in the particle–hole channel, we obtain

$$H_{\rm RVB} = -\sum_{\langle ij\rangle} (\Delta_{ij} c^+_{i\sigma} c_{j\sigma} + {\rm H.c.}), \tag{1}$$

where the summation extends over the nearest bonds. The fermion spectrum is determined by the choice of the phase of the coupling parameters, $\Delta_{ii+\delta} = \langle c^+_{i+\delta} c_i \rangle_\sigma$. Here

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δ indicates the direction of the nearest site; on a square lattice we have $\delta=(x,-x,y,-y)$. Since $\Delta_{ij}=\text{const}$ in a uniform RVB phase, the spinon spectrum $\xi_{\mathbf{k}}=(D/2)(\cos k_x+\cos k_y)$ is gapless.

The flux phase at a square lattice[2] corresponds to the parameterization $\Delta_\delta=\Delta_{-\delta}$ and $\Delta_x=i\Delta_y$. In this case the Hamiltonian (1) can be diagonalized by means of the transformation

$$c_{\mathbf{R}\in A}=\left(\frac{1}{N}\right)^{1/2}\sum_{\mathbf{k}}\exp(-i\mathbf{kR})(c_{1\mathbf{k}}+c_{2\mathbf{k}}),$$

$$c_{\mathbf{R}\in B}=\left(\frac{1}{N}\right)^{1/2}\sum_{\mathbf{k}}\exp(-i\mathbf{kR}+i\varphi_{\mathbf{k}})(c_{1\mathbf{k}}-c_{2\mathbf{k}}), \tag{2}$$

where the $A(B)$ sublattice consists of sites with even (odd) values of R_x+R_y, N is the number of sites, and the summation over the momentum $\mathbf{k}$ extends over the magnetic Brillouin zone. The phase factor $\exp(i\varphi_{\mathbf{k}})=\Delta^*_{\mathbf{k}}/|\Delta_{\mathbf{k}}|$, where $\Delta_{\mathbf{k}}=2\Delta(\cos k_x+i\cos k_y)$. The flux-phase spectrum consists of two branches:

$$H_{\mathrm{RVB}}=\sum_{\mathbf{k}\sigma}\xi_{\mathbf{k}}(-c^+_{1\mathbf{k}}c_{1\mathbf{k}}+c^+_{2\mathbf{k}}c_{2\mathbf{k}})_\sigma,\quad \xi_{\mathbf{k}}=2\Delta(\cos^2 k_x+\cos^2 k_y)^{1/2}. \tag{3}$$

At low energies the spinon density of states is determined by the neighborhood of the zeroes of $\xi_{\mathbf{k}}$ at the points $(\pm\pi/2,\pm\pi/2)$ and it has a pseudogap character: $\rho_0(\omega)=2|\omega|/\pi D^2$, where $D=4\Delta/\sqrt{2}$ is the half-width of the band.

We are interested in a modification of the ground state of the RVB lattice, in which a single defect — a spin vacancy — appears in the lattice at the site $\mathbf{R}=0$. The absence of pseudofermions at a vacant site, and hence the absence of the spin in it, can be achieved by adding to expressions (1) and (3) a local chemical potential λ_0:

$$H=H_{\mathrm{RVB}}+\lambda_0(n_{0\uparrow}+n_{0\downarrow}),\quad n_\sigma=c^+_\sigma c_\sigma=(c_1+c_2)^+_\sigma(c_1+c_2)_\sigma/2. \tag{4}$$

The Hamiltonian (4) does not contain an interaction and can be easily analyzed. Nonmagnetic substitution is simulated by passing to the limit $\lambda_0\to\infty$ in the calculations.

2. SPINON LOCALIZTION

We shall calculate the density of states in the flux phase with a vacancy. We determine the spinon temperature Green's functions $g_{nm}(\epsilon;\mathbf{k},\mathbf{k}')=\langle -T_r\ c_{n\mathbf{k}}(\tau)c^+_{m\mathbf{k}}(0)\rangle_\epsilon$; the indices n and m denote the number of the subband; here and below the spin index is dropped. Averaging over the states of the Hamiltonian (4), we obtain the expression for the Green's functions

$$g_{nm}(\epsilon;\mathbf{k},\mathbf{k}')=g^0_{nn}(\epsilon;\mathbf{k})\,\delta_{\mathbf{kk}'}\delta_{nm}+g^0_{nm}(\epsilon;\mathbf{k})T(\epsilon)g^0_{mm}(\epsilon;\mathbf{k}'), \tag{5}$$

where $g^0_{nm}(\epsilon;\mathbf{k})=\{i\epsilon-(-1)^n\xi_{\mathbf{k}}\}^{-1}\delta_{nm}$ is the propagator in the absence of a vacancy. In the limit $\lambda_0\to\infty$, the expression for the T matrix, which describes the scattering of spinons by a vacancy, has the form

$$T(\epsilon)=-\frac{1}{NG_0(\epsilon)}, \tag{6}$$

where

$$G^0(\epsilon)=\frac{1}{N}\sum_{kn} g^0_{nn}(\epsilon;\mathbf{k}) \tag{7}$$

is a one-site Green's function in the zeroth approximation of the initial c-fermions. As a result of the pseudogap in the flux-phase spectrum, the function (7) for small ϵ approaches zero as

$$G^0(\epsilon)=-i(4\epsilon/\pi D^2)\ln(\pi D/4|\epsilon|). \tag{8}$$

Correspondingly, the T matrix (6) has a pole at $\omega=0$, which suggests the appearance of a bound state which is pinned at the Fermi level. The presence of a localized spinon state is manifested as a singular correction to the density of states $\rho(\omega)$. It is determined by the function

$$G(\epsilon)=\sum_{kn} g_{nn}(\epsilon;\mathbf{k},\mathbf{k})=NG^0(\epsilon)+\delta G(\epsilon), \tag{9}$$

where the correction associated with the presence of a vacancy is

$$\delta G(\epsilon)=-i\frac{\partial}{\partial\epsilon}\ln G^0(\epsilon)=\frac{1}{i\epsilon}\left(1-\frac{1}{\ln(D/|\epsilon|)}\right). \tag{10}$$

The result (10), from which $\delta\rho(\omega)=\delta(\omega)$ follows, attests to the fact that a vacancy induces a local moment. This results in the appearance of a Curie-like contribution to the uniform spin susceptibility, as can be verified by a direct calculation.

It is easy to see that such spinon localization does not occur in a uniform RVB phase. In this phase, formally, the bare density of states given by expression (7) does not approach zero at low energies, and the T matrix near the Fermi level is a regular function.

The result (10) can also be obtained by performing a calculation on the basis of the $s+id$ phase[3] with a vacancy. This is obvious, since both formulations of the flux phase are equivalent[6] because of the SU(2) symmetry. In terms of the $s+id$ formulation, spinons from different sites form singlet pairs with a d symmetry. Qualitatively, the removal of a spinon at a vacant site converts its partner from a condensate into a free spin. The situation is essentially similar to the formation of a local moment near a Kondo hole in half-filled Kondo insulators,[7] when the removal of a single f center results in localization of its partner from the conduction band. Purely formally, the flux-phase theory in the $s+id$ formulation[3] is equivalent to the BCS theory with a d symmetry. The fact that in the unitary limit a nonmagnetic impurity induces impurity states in anisotropic superconductors has been known for a long time.[8,9] This circumstance is now often brought into discussions of the effect of impurities on the superconducting properties of high-T_c systems. Our analysis (possibly) shows that the low-energy impurity states in high-T_c systems probably are largely of a purely spin origin. We emphasize that the formation of a local moment near a static vacancy in a quantum antiferromagnet has also been observed in numerical calculations.[10]

3. DISTRIBUTION OF THE LOCAL MOMENT

An idea of the spatial distribution of an impurity state can be obtained by calculating the Green's function $G(\epsilon;\mathbf{R},\mathbf{R})=\langle -T_\tau c_{\mathbf{R}}(\tau)c^+_{\mathbf{R}}(0)\rangle_\epsilon$ of the initial c-pseudofermions. The vacancy correction for it is

$$\delta G=|A(\epsilon,\mathbf{R})|^2/G^0(\epsilon),\quad \mathbf{R}\in A,\quad \delta G=-|B(\epsilon,\mathbf{R})|^2/G^0(\epsilon),\quad \mathbf{R}\in B, \tag{11}$$

where

$$A(\epsilon,R)=\frac{1}{N}\sum_{\mathbf{k}n} g^0_{nn}(\epsilon;\mathbf{k})\exp(i\mathbf{kR}),$$

$$B(\epsilon;R)=\frac{1}{N}\sum_{\mathbf{k}n} g^0_{nn}(\epsilon;\mathbf{k})(-1)^{n+1}\exp(-i\varphi_{\mathbf{k}}+i\mathbf{kR}). \tag{12}$$

Expressions (11) show that the singular part of the density of states is distributed only over the sites of the B sublattice, as expected from physical considerations (we recall that the removed spin belonged to the A sublattice). Near the vacancy the correction for $\rho(\omega)$ at low frequencies ($R\omega/D\ll 1$) behaves as

$$\delta\rho_B(\omega,\mathbf{R})=\Phi(\mathbf{R})\frac{2}{\pi R^2}\frac{\delta(\omega)}{\ln(\pi D/4|\omega|)}. \tag{13}$$

The complicated angular dependence of the quantity (13) is determined by the function $\Phi(\mathbf{R})=1/2-\cos 2\theta(\cos \pi R_x-\cos \pi R_y)/4$ (here θ is the angle between the x axis and the vector $\mathbf{R}$), and it decreases as R^{-2} with increasing distance from the vacancy. We note that summing $\delta\rho(\omega,\mathbf{R})$ over the entire lattice gives the result obtained above: $\delta\rho=\delta(\omega)$.

A nonmagnetic substitution in the flux phase induces a local moment. If this moment is directly related to the formation of local moments near nonmagnetic impurities in high-T_c systems, then this would mean that pairing effects are present in the spin degrees of freedom even in the normal phase of these systems.

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[1)]e-mail: khaliu@ksc.iasnet.com

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