Carrier pairing in spin-liquid state of doped 2D antiferromagnet

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An effective infrared theory which describes the dynamics of charge carriers in a planar CuO_2 antiferromagnet is discussed. This theory reduces to a gauge theory with a topological mass term. The condensation mechanism, the competition between the *s*-wave and *p*-wave pairing, and the effective Ginzburg–Landau Lagrangian are discussed.

The discovery of high-T_c superconductivity in quasi-2D CuO_2 ceramics[1] has stimulated a stream of theoretical papers on alternative superconductivity mechanisms. One direction, originally pointed out by Anderson,[2] starts from the existence of an antiferromagnetism in CuO_2 planes. In the absence of doping, there is a Mott insulator which can be described by a model of highly correlated electrons, in the simplest case by the Hubbard model with a filling of 1/2 and a Néel order. At a low doping level (on the order of 1%) the Néel order is destroyed, and a new phase becomes possible: resonating valence bonds (RVB), which can be described in the infrared region by a gauge theory.[3,4] In the present letter we derive the interaction Lagrangian of free charge carriers (electrons or holes, depending on the deviation of the filling from 1/2) with gauge degrees of freedom, and we analyze the pairing mechanism.

1. We start with the Hamiltonian of the Hubbard model:

$$H = -\sum_{ij} t_{ij}\psi^+_{i\sigma}\psi_{j\sigma} + U\sum_{ij}\psi^+_{i\uparrow}\psi_{i\uparrow}\psi^+_{i\downarrow}\psi_{i\downarrow} - \mu\sum_i \psi^+_{i\sigma}\psi_{i\sigma}\ . \qquad (1)$$

In the limit of pronounced Coulomb repulsion, with $t/U \ll 1$, and in the case of a slight doping, one can derive an effective Hamiltonian which describes the magnetic and charge degrees of freedom:

$$H_{eff} = \sum_{ij} t_{ij}\chi^+_{i\sigma}\chi_{j\sigma} + \sum_{ij} J_{ij}\mathbf{n}_i\mathbf{n}_j(1-\rho_i)(1-\rho_j), \quad J \sim t^2/U\ . \qquad (2)$$

The factors $(1-\rho_i)$, where $\rho_i \chi^+_{i\sigma}\chi_{i\sigma}$, reflect the fact that only sites with a single electron participate in the antiferromagnetic exchange. Free carriers correspond to sites without electrons (holes) or sites having two electrons (free electrons). Following Ref. 4, we find from (2) the Lagrangian

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$$\mathcal{L} = {}^1/_2 \sum_i \int_0^1 du\,(\mathbf{n}_i[\partial_t \mathbf{n}_i \partial_u \mathbf{n}_i\,])(1-\rho_i) - \sum_i \chi^+_{i\sigma}\,\partial_t \chi_{i\sigma}$$

$$- \sum_{ij} \{J_{ij}\,\mathbf{n}_i\mathbf{n}_j\,(1-\rho_i)(1-\rho_j) + t_{ij}\chi^+_{i\sigma}\,\chi_{j\sigma}\,\} + \sum_i \lambda_i\,(1+\mathbf{n}_i\vec{\sigma})\chi_i\ , \tag{3}$$

in which the last term describes the constraint $(1+\mathbf{n}_i\vec{\sigma})\chi_i = 0$, which allows a transfer of only charge, not spin. To solve this constraint, we use a parametrization for $\mathbf{n}_i$ and $\chi_{i\sigma}$:

$$\mathbf{n}_i\sigma = (-)^{P_i} g\sigma^3 g^{-1}, \qquad g = \begin{pmatrix} z_1 & z_2 \\ -\bar{z}_2 & \bar{z}_1 \end{pmatrix} \in SU(2) \tag{4}$$

$$P_i = 0,\, i \in A; \quad P_i = 1,\, i \in B.$$

$$\chi_{i\alpha} = z_\alpha u_i,\quad i \in A\,; \qquad \chi_{j\alpha} = \epsilon_{\alpha\beta}\bar{z}_\beta v_j, \qquad j \in B.$$

Here A and B are two sublattices. After an integration over the fast variables and renormalizations, we find an effective infrared Lagrangian in which the boson degrees of freedom are described by gauge fields A_μ, which are composite fields at short range, $A_\mu = i\bar{z}\partial_\mu z$. We thus have $\mathscr{L}_{\rm eff} = \mathscr{L}_m + \mathscr{L}_h$, where

$$\mathcal{L}_m = \frac{1}{4\gamma} F^2_{\mu\nu} + \frac{i\theta}{8\pi^2}\,\epsilon_{\mu\nu\lambda} F_{\mu\nu} A_\lambda\ , \tag{5}$$

$$\mathcal{L}_h = \chi^+\Big(-\frac{\partial}{\partial t} + i\tau^3 A_0\Big)\chi + \frac{1}{2m}\,\chi^+(\vec{\nabla} + i\tau^3\mathbf{A}\,)^2\chi\,;\quad \tau^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{6}$$

In the continuum limit, a single isotopic spinor $\chi = (u/v)$ arises from two fermions u and v on sublattices A and B; m is the effective mass of a free carrier (Kane *et al.*,[5] have shown that we have $m \sim \gamma \sim J^{-1}$). The presence of the second term in (5) means that the magnetic system is in a phase of a chiral spin liquid[6] (CSL) with broken P and T parities. Wiegmann[4] has found $\theta = 2\pi$ in this phase.

2. Using the correlation function

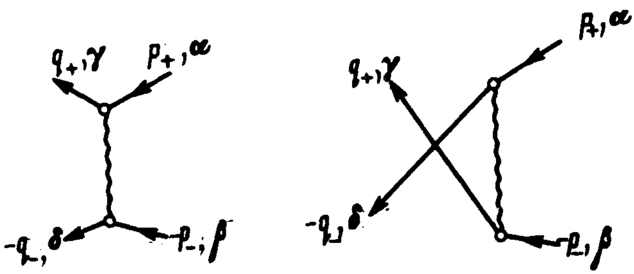

FIG. 1.

$$\langle A_\mu A_\nu \rangle = \gamma \frac{g_{\mu\nu} - k_\mu k_\nu / k^2}{k^2 - \mu^2} + i\gamma\mu \frac{\epsilon_{\mu\nu\lambda} k_\lambda}{k^2 (k^2 - \mu^2)}, \quad \mu = \frac{\gamma\theta}{2\pi^2} = \frac{\gamma}{\pi}. \tag{7}$$

we find the amplitude for the scattering of two particles, ignoring retardation (the static limit) (Fig. 1):

$$\Gamma_{\alpha\beta,\gamma\delta}(q_+, -q_-; p_+, -p_-) = (\tau^3 \otimes \tau^3)_{\alpha\gamma,\beta\delta} \left[V(\mathbf{p}-\mathbf{q}) + U(\mathbf{p}-\mathbf{q}) \frac{\mathbf{p} \wedge \mathbf{q}}{(\mathbf{p}-\mathbf{q})^2} \right]$$

$$+ (1 \otimes 1)_{\alpha\gamma,\beta\delta} W(\mathbf{p}-\mathbf{q}) - \{\mathbf{q} \to -\mathbf{q}, \gamma \leftrightarrow \delta\}, \tag{8}$$

where the potentials V, U, and W are given in the x representation by

$$V(r) = \frac{\gamma}{2\pi} K_0(\mu r), \qquad U(r) = \frac{\gamma}{2m}(1 - \mu r K_1(\mu r)),$$

$$W(r) = \frac{\gamma}{4mr^2}(1 - \mu r K_1(\mu r))^2 .$$

Expression (8) is a particular case of a more general expression which also contains structures of the type $\tau^+ \otimes \tau^-$. These structures arise in models in which jumps of electrons occur not only between copper atoms but also to oxygen atoms (Emery's model[7]). In the process, a charge-carrier interaction χ with an SU(2) triplet of fields $A^a_\mu, \mathscr{L}_{int} = g\chi + \tau^a A^a_0 \chi^+ g'/2m\chi^+ A^a_i \overleftrightarrow{\nabla}_i \tau^a \chi$, $a = 1,2,3$ arises. Again in this case there is a pairing, similar to that which we derive below for example (8).

The Bethe–Salpeter equation for bound states near a singularity in the total energy of the pair, E, is (Fig. 2)

$$\psi_{\alpha\beta}(\mathbf{p}, E) = \sum_{\mathbf{q},\omega} \Gamma_{\mu\nu,\alpha\beta}(\mathbf{q}, -\mathbf{q}; \mathbf{p}, -\mathbf{p}) G_{\gamma\mu}(\mathbf{q}) G_{\delta\nu}(-\mathbf{q}) \psi_{\gamma\delta}(\mathbf{q}, E)$$

$$\psi_{\alpha\beta}(\mathbf{p}, E) = \sum_{\mathbf{q},\omega} \Gamma_{\gamma\delta,\alpha\beta}(\mathbf{q}, -\mathbf{q}; \mathbf{p}, -\mathbf{p}) \langle \chi^+_{\mathbf{q},\gamma} \chi^+_{-\mathbf{q},\delta} \rangle . \tag{9}$$

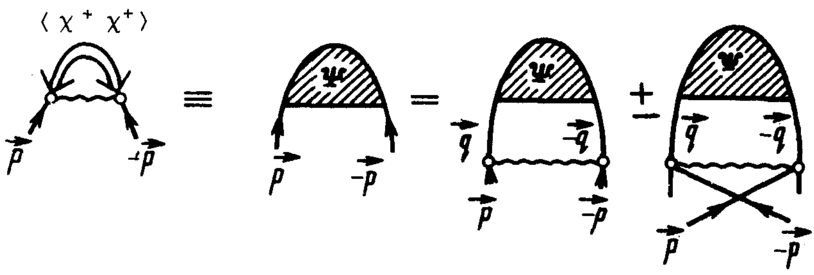

FIG. 2.

Equations (9) split into an isospin-symmetric part ψ_S and an isospin-antisymmetric part ψ_A, and an attraction of particles with opposite isospins arises in each channels: $\tau_1^3 + \tau_2^3 = 0$. If the carriers had a spin, a spin attraction would have arisen in addition to the isospin attraction.[8] From (8) and (9) we find

$$\psi_{A,S}(\mathbf{p}, E) = \sum_{\mathbf{q}} \frac{1 - n_{\mathbf{q}} - n_{-\mathbf{q}}}{\epsilon_{\mathbf{q}} + \epsilon_{-\mathbf{q}} - 2\epsilon_F - E} \{ [V(\mathbf{p}-\mathbf{q}) + U(\mathbf{p}-\mathbf{q}) \frac{\mathbf{p}\Lambda\mathbf{q}}{(\mathbf{p}-\mathbf{q})^2} - W(\mathbf{p}-\mathbf{q})]$$

$$\pm [\mathbf{q} \to -\mathbf{q}] \} \, \psi_{A,S}(\mathbf{q}, E). \tag{10}$$

Because of the long-range potentials W and $U[\mathbf{p}\Lambda\mathbf{q}/(\mathbf{p}-\mathbf{q})^2]$, which fall off as $1/r^2$ the usual solution $\psi = \text{const}$ on the Fermi surface $|\mathbf{q}| = q_F$ is incorrect. These terms essentially lead to a shift of the effective angular momentum in the two-particle problem; this effect must be taken into account before taking the limit of the many-particle problem near the Fermi surface. It is easy to show that at distances greater than μ^{-1} there is a shift of $2s$ in the angular momentum, where $s = \pi/2\vartheta$ is the effective spin ("spin transmutation"[9]), and in the case $\vartheta = 2\pi$ we find[10] $s = 1/4$. After some straightforward manipulations, we find equations for the harmonics $\psi_m(q)$ ($m = 2k$ for ψ_A and $m = 2k + 1$ for ψ_S):

$$\psi_m(p) = \int_0^\infty \frac{q\,dq}{4\pi} \frac{1 - 2n_q}{\xi_q - E} V_{m+2s}(p, q) \psi_m(q), \quad \xi_q = \frac{q^2}{2m} - \epsilon_F, \tag{11}$$

where $V_{m+2s}(p,q) = \int_0^{2\pi} (d\varphi/2\pi) V(\mathbf{p}-\mathbf{q}) \exp(i(m+2s)\varphi)$. Substituting in $V(\mathbf{p}-\mathbf{q})$ from (8), we find

$$V_{m+2s}(p, q) = \frac{\gamma}{\mu^2} \left(\frac{pq}{\mu^2 + p^2 + q^2} \right)^{|m+2s|} \tag{12}$$

Equation (11) has a singularity at $E = -\Delta_m$, where

$$\Delta_m \approx \epsilon_F \exp \{ -4\pi(\mu/m)^2 \left(\frac{\mu^2}{2m\epsilon_F} \right)^{|m+2s|} \} \tag{13}$$

determines the gap for pairing with an angular momentum m at absolute zero.

3. We would like to call attention to a remarkable fact concerning degeneracy: Condensates with angular momenta m and $-(m + 4s)$ $[-(m+1)$ in our case$]$ arise simultaneously as the temperature is lowered. This competition is a direct consequence of the spin transmutation. An important point is that a competition between an s wave and one of the p waves arises in a realistic case; the sign of the projection of the angular momentum is determined by $\text{sgn}\vartheta$. The degeneracy is lifted when the short-range interaction is taken into account, and in the case of a repulsive core (a screened Coulomb interaction) the condensate will form in the p wave. By virtue of $m = \text{sgn}\vartheta$, the P and T parities of the ground state will be broken. In other words, a macroscopic breaking of these symmetries will occur.

Under conditions such that bound states exist even in the two-particle problem (see Ref. 8, where pair formation in the p wave in the weak-coupling case is discussed), the scenario of a Cooper instability is realized only if there is a sufficiently high carrier density, $n = m\epsilon_F/2\pi$. In the case $n^{1/2} < L_b^{-1}$, where L_b is a characteristic size of the pair in the two-particle problem, the system can legitimately be treated as a nonideal Bose gas. The binding energy exceeds the degeneracy temperature, and a $2D$ superfluidity arises in the system of charged bosons at the temperature[11] $T_c = \pi n_B/m\ln\ln\mu^2/n_B$, where the density of bosons is $n_B = n/2$ at small values of n and decreases substantially at $n \sim L_b^{-2}$, leading to a transition to $T_c \sim \Delta_0 = \Delta_{\mathrm{sgn}\,\vartheta}$ [see (13)].

Introducing the resultant momentum of the pair, $\mathbf{Q}$, in Eq. (10), and carrying out a gradient expansion in the external electromagnetic field $\mathbf{A}_{\mathrm{ex}}$, $\mathbf{Q} \to \mathbf{Q} - 2e\mathbf{A}_{\mathrm{ex}}$, we find a Ginzburg–Landau functional. It contains, in addition to the standard terms, a P-odd term which is proportional to sgn $\vartheta\mu_B(J/t)|\psi|^2 \,\mathrm{curl}\,\mathbf{A})_z$. The source of this term is the orbital current of the condensate (the p wave). This term leads to an additional magnetic moment (per site) on the order of $n(J/t)\mu_B \sim 10^{-3}\mu_B$ and also to several experimentally observable effects, such as a Faraday effect (a rotation of the polarization plane of reflected light) and a directional dependence of the lower critical field H_{c1}. One might say that by virtue of this term a situation which would be favored from the energy standpoint in a layered bulk sample would be an alternation of the signs of ϑ in neighboring layers, so that no macroscopic magnetic field would be generated in the sample. A detailed discussion of the scenario outlined here will be published separately.

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