PHYSICS OF $\pi$-MESON CONDENSATION AND HIGH TEMPERATURE CUPRATE SUPERCONDUCTORS.

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(Dated: May 17, 2009)

The idea of condensation of the Goldstone $\pi$-meson field in nuclear matter had been put forward a long time ago. However, it was established that the normal nuclear density is too low, it is not sufficient to condensate $\pi$-mesons. This is why the $\pi$-condensation has never been observed. Recent experimental and theoretical studies of high temperature cuprate superconductors have revealed condensation of Goldstone magnons, the effect fully analogous to the $\pi$-condensation. The magnon condensation has been observed. It is clear now that quantum fluctuations play a crucial role in the condensation, in particular they drive a quantum phase transition that destroys the condensate at some density of fermions.

PACS numbers: 11.30.Rd; 12.38.-t; 75.25.+z; 78.70.Nx

I. $\pi$-MESON CONDENSATION.

It is well established that the physical vacuum spontaneously violates the chiral symmetry of the Lagrangian of Quantum Chromodynamics (QCD). Existence of $\pi$-mesons ($\pi^+$, $\pi^0$, and $\pi^-$), very light strongly interacting particles, is a manifestation of the spontaneous violation. The $\pi$-mesons are the Goldstone excitations associated with the spontaneous violation. In the case of an ideal chiral symmetry the Goldstone particles must be massless. In reality the chiral symmetry of the QCD Lagrangian is explicitly violated by small quark masses. This generates a nonzero mass of the $\pi$ meson. However, this mass is small, $m_\pi \approx 140$ MeV (Mega electron Volts), compared to the typical mass of a nongoldstone strongly interacting particle $M \sim 1000$ MeV. It was pointed out a long time ago by S. Weinberg that the effective low energy action for $\pi$-mesons is given by the nonlinear $\sigma$-model, see also. A $\pi$-meson propagating in nuclear matter is modified due to the interaction with protons and neutrons. The meson Green’s function is

$$G(\omega, q) = \frac{1}{\omega^2 - c^2 q^2 - m_\sigma^2 c^4 - \Pi(\omega, q)}, \quad (1)$$

where $c$ is speed of light and $\Pi(\omega, q)$ is the polarization operator. It is worth noting that due to Adler’s relation the polarization operator must vanish at $m_\pi, \omega, q \to 0$, $\Pi(0, q) \propto q^2 + m_\sigma^2 c^2$. The idea of $\pi$-condensation in nuclear matter was put forward by A. B. Migdal, see also. For a review see Ref. The idea is pretty straightforward. The Green’s function (1) corresponds to the ground state with zero expectation of the $\pi$-meson field, $\langle \bar{\pi} \pi \rangle = 0$. The polarization operator $\Pi(\omega, q)$ is negative and hence, if the operator is sufficiently large, $-\Pi(\omega, q) > c^2 q^2 + m_\sigma^2 c^4$, the Green’s function (1) attains poles at imaginary frequencies. This indicates instability of the ground state. Using language of condensed matter physics one can say that this is a Stoner instability. Note, that the instability is related to the Goldstone nature of $\pi$-mesons or in other words it is related to the smallness of $m_\pi$. The polarization operator can be more significant than $c^2 q^2 + m_\sigma^2 c^4$ only for small $m_\pi$.

The instability leads to the development of a nonzero expectation values of the $\pi$-meson field $\langle \bar{\pi} \rangle \neq 0$. The expectation value is modulated with some wave vector $Q$ that depends on nuclear density, see Ref. This is the $\pi$-meson condensate.

The polarization operator $\Pi(\omega, q)$ has a contact part and a quasiparticle part. The contact part scales linearly with nuclear density $x$, and the quasiparticle part for sufficiently small $\omega$ and $q$ scales as $\sqrt{x}$. Both contributions vanish at $x = 0$. Therefore, to get to the $\pi$-condensation regime one needs a sufficiently high nuclear density. Unfortunately the normal nuclear density is not sufficient to generate the condensation, this is why the effect has never been observed. To induce the condensation one needs a very strong compression which can be realized only in exotic states of nuclear matter.

II. MOTT INSULATOR AND $\sigma$-MODEL

La$_{2-x}$Sr$_x$CuO$_4$ is a prototypical high temperature superconductor. Here $x$ is the doping level, the degree of La substitution by Sr. The parent compound La$_2$CuO$_4$ contains odd number of electrons per unit cell. Oxygen is in a O$^{2-}$ state that completes the 2p-shell. Lanthanum loses three electrons and becomes La$^{3+}$, which is in a stable closed-shell configuration. To conserve charge the copper ions must be in a Cu$^{2+}$ state. This corresponds to the electronic configuration 3d$^9$. Thus, from the point
of view of band theory the compound must be a metal. However, the parent compound is a good insulator. The point is that for a free metallic propagation the electron wave function must include configurations $d^0$, $d^{10}$, and $d^6$. Due to the strong Coulomb repulsion between electrons localized at the same Cu ion ($\sim 10$ eV) the configuration $d^{10}$ has too high energy and this blocks the propagation. Thus electrons remain localized at each Cu ion in the configuration $d^9$. Every Cu ion has spin 1/2 and spins of nearest ions $\vec{S}_i$ and $\vec{S}_j$ interact antiferromagnetically, see e.g. Ref.\textsuperscript{11},

$$H = J \sum_{<ij>} \vec{S}_i \cdot \vec{S}_j .$$

The value of the exchange integral is $J \approx 130$ meV (milli electron Volts), so the energy scale is 10 orders of magnitude smaller than that in nuclear matter. An important point is that La$_2$CuO$_4$ is a layered system. Coupling between layers is weak, $\sim 10^{-5}J$, therefore in a very good approximation the system is two dimensional (2D). Another important point is that Cu ions in layers are arranged in a square lattice, so Eq. (2) describes the Heisenberg model on a square lattice.

It is well known that the ground state of the 2D Heisenberg model has a long range antiferromagnetic order. Picture of the ground state is shown schematically in Fig. 1 Left. The ground state spontaneously violates the SU(2) symmetry of the Hamiltonian Ref.\textsuperscript{2}. This is analogous to the spontaneous violation of the chiral symmetry in the QCD ground state. Elastic scattering of neutrons from the state shown in Fig. 1 Left gives Bragg peaks at the neutron momentum transfer $k = (\pm \pi/a, \pm \pi/a)$. Here $a$ is the lattice spacing. Below I set $a = 1$. In the long wave-length limit the Heisenberg Hamiltonian Ref.\textsuperscript{2} can be mapped to the nonlinear $\sigma$-model with Lagrangian

$$\mathcal{L} = \frac{1}{2\chi_\perp} \vec{n}^2 - \frac{\rho_s}{2} (\nabla \vec{n})^2 ,$$

where the staggered field $\vec{n} (r, t)$ obeys the constraint $\vec{n}^2 = 1$, and the parameters are $\chi_\perp \approx 0.53/(8J)$ and

$$\rho_s \approx 0.18J .$$

For a discussion of the mapping see e.g. the review paper\textsuperscript{13}. In the ground state $\vec{n} = (0, 0, 1)$, where the $z$-axis in the spin space is directed along the spontaneous alignment. This corresponds to Fig. 1 Left. To find excitations one has to represent the staggered field as $\vec{n} = (\vec{\pi}, \sqrt{1 - \vec{\pi}^2})$, where $\vec{\pi} = (\pi_x, \pi_y, 0)$, and substitute this in (3). This gives the Goldstone spin waves with linear dispersion $\omega_q = cq$, where the spin-wave velocity is

$$c = \sqrt{\frac{p_s}{\chi_\perp}} .$$

Thus, the spin waves (magrons) are completely analogous to $\pi$-mesons. Moreover, there is a weak spin-orbit interaction in La$_2$CuO$_4$ that gives a small spin-wave gap $\Delta_{s\omega}$. $\omega_q = \sqrt{c^2 q^2 + \Delta_{s\omega}^2}$. The gap is about $2 - 4$ meV, see e.g. the review paper Ref.\textsuperscript{14}. The relative value is $\Delta_{s\omega}/J \sim 1/40$. Thus the explicit violation of the SU(2) symmetry in cuprates is even smaller than the explicit violation of the chiral symmetry in QCD where $m_\pi/(1000$ MeV) $\sim 1/7$. Therefore, hereafter I disregard the spin-wave gap. The Green’s function of the magnon in the parent compound is

$$G_0 = \frac{1}{\omega^2 - c^2 q^2 + i0} .$$

Thus, the spin waves are propagating in the $xy$-plane.

III. DOPING BY STRONTIUM, MOBILE HOLES

Lanthanum loses three electrons and Sr can lose only two, therefore the substitution La by Sr effectively remove electrons from CuO layers, or in other words injects holes in the system, see Fig. 1 Right. For simplicity the spin pattern in Fig. 1 Right is taken the same as in Fig. 1 Left. In reality the pattern is changed and the entire story is about the change. The injected holes can propagate through the system. In the momentum space minima of the hole dispersion are in the points $k_0 = (\pm \pi/2, \pm \pi/2)$ as it is shown in Fig. 2 see e.g. the review paper Ref.\textsuperscript{15}. Because of the existence of two distinct sublattices with opposite spins the correct Brillouin zone

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure1.png}
\caption{Left: Schematic picture of the antiferromagnetic ground state. Right: Doping removes some electrons.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure2.png}
\caption{Dispersion of a single hole injected in a Mott insulator is similar to that in a two valley semiconductor.}
\end{figure}
of the problem is the Magnetic Brillouin Zone (MBZ) shown in Fig. 2. Hole states inside the MBZ form a complete set, so there are four independent half pockets of the dispersion. It is convenient to replace this description by two full pockets as it is shown in Fig. 2 Right. Thus from the point of view of the single hole dispersion the system is similar to the two valley (two pocket) semiconductor. The dispersion in a pocket is somewhat anisotropic, but for simplicity let us use here the isotropic approximation,

$$\epsilon (p) \approx \frac{1}{2} \beta p^2 ,$$

(6)

where $p = k - k_0$. I remind that the lattice spacing is set to be equal to unity, therefore the momentum is dimensionless and the inverse effective mass $\beta$ has dimension of energy. Numerical lattice simulations give the following value of the inverse mass, $\beta \approx 2.2J$. In usual units this corresponds to the effective mass

$$m^* \approx 2m_e .$$

(7)

This value agrees reasonably well with experimental data.

IV. MAGNON CONDENSATION INSTABILITY

The magnon Green’s function in the doped system reads

$$G(\omega, q) = \frac{1}{\omega^2 - c^2 q^2 - \Pi(\omega, q)} .$$

(8)

The polarization operator is due to magnon scattering from holes. This is similar to the case of $\pi$-mesons in nuclear matter, see Eq. [1]. Another similarity is that due to the Adler’s relation the polarization operator at small $q$ is proportional to $q^2$. Similarly to the case of $\pi$-mesons the polarization operator has a contact part and a quasiparticle part. The contact part is always proportional to doping $x$ and hence in the dilute limit, $x \ll 1$, can be neglected. A qualitative difference from $\pi$-mesons comes from the quasiparticle part of the polarization operator. The point is that in two dimensions the quisiparticle part of the polarization operator is doping independent if $q \ll p_F \sim \sqrt{x}$. Here $p_F$ is the Fermi momentum of holes. Independence of concentration of fermions is a well known property of the two-dimensional fermionic polarization operator. To recall the property we remember that at small $q$ and $\omega$ the polarization operator is proportional to the density of states at Fermi surface. In the 3D case the density of states is

$$\int \delta(\epsilon_F - \epsilon_p) \frac{d^3p}{(2\pi)^3} \propto \sqrt{x} .$$

(9)

However, in two dimensions

$$\int \delta(\epsilon_F - \epsilon_p) \frac{d^3p}{(2\pi)^3} = \text{const} .$$

(10)

The magnon condensation criterion immediately follows from Eq. [5].

$$- \frac{\Pi(0, q)}{q^2} > c^2 .$$

(11)

Since $\Pi$ is doping independent we must either have the condensation at any doping, or do not have it at all, this depends purely on parameters of the system. Let us now look at experimental data before discussing further theory.

V. NEUTRON SCATTERING EXPERIMENTAL DATA

It has been already pointed out that elastic scattering of neutrons from the parent compound gives Bragg peaks at momentum transfer $k = (\pm \pi/a, \pm \pi/a) = \frac{2\pi}{a}(\pm 1/2, \pm 1/2)$. In notations accepted in neutron scattering literature this is $k = (\pm 1/2, \pm 1/2)$. This scattering measures the “vacuum condensate” corresponding to the parent compound.

A picture from Ref. representing neutron scattering data from the doped compound is reproduced in Fig. [3]. The data clearly indicate a shift of the Bragg peak from the $(1/2, 1/2)$ position. Value of the shift $\delta$ scales linearly with doping $x$. This scaling is shown in the upper part of the picture. Interestingly the shift is directed along the diagonal of the lattice if $x < 0.055$ and the shift is parallel to the lattice if $x > 0.055$. The rotation of the direction is stressed in the lower part of the figure.

Thus, the data clearly indicate a static condensate of magnons with the wave vector

$$Q = 2\pi \delta \approx 2\pi \times 0.95 \times x .$$

(12)

The pion condensate has never been observed, but as we see the magnon condensate that is completely analogous has been already observed. The diagonal direction of the wave vector of the magnon condensate at the very low doping, $x < 0.055$, is related to the quenched disorder in the compound. The corresponding theory has been developed in Ref. It is hardly possible to imagine a quenched disorder in nuclear matter. Therefore, in the present paper I disregard the regime $x < 0.055$. Ideas of the theory describing the magnon condensate at $x > 0.055$ are presented in the next section.
VI. THEORY OF MAGNON CONDENSATION: SPIN SPIRAL

First of all we need to formulate the effective low energy action of the system. The small parameter that justifies the action is the doping level $x$. Since $x \ll 1$ the Fermi momentum of a hole is also small, $p_F \propto \sqrt{x} \ll 1$. Typical energy scales, $\epsilon_F = \beta p_F^2/2 \sim J x$ and $c p_F \sim \sqrt{x} J$ are also low, $\epsilon_F, c p_F \ll J$. This is why the effective long wave-length approach is sufficient. This approach is equivalent to the chiral perturbation theory widely used in $\pi$-meson physics.

The effective low-energy Lagrangian is written in terms of the bosonic $\vec{n}$-field ($n^2 = 1$) that describes the staggered component of copper spins, and in terms of fermionic holons $\psi$. At this instant I am changing terminology, instead of the term “hole” I use the term “holon”. The point is that in normal Fermi liquid a hole carries spin 1/2, this is a straightforward consequence of the ideal gas approximation. In the system under consideration spin is carried by the bosonic field $\vec{n}$. A fermionic hole does not carry any spin, this is the precise meaning of the term “holon”. In spite of the absence of spin the holon field is described by a two component spinor. The corresponding SU(2) operator is called pseudospin. The pseudospin originates from two magnetic sublattices in the system: the holon can reside on either sublattice A or sublattice B. For a collinear antiferromagnetic state sublattice A is the sublattice with spin up, and sublattice B is the sublattice with spin down, see Fig. 1 Right. Most importantly the notion of sublattice remains well defined for twisted spin states for any smooth twist of the spin fabric. For a more detailed discussion of pseudospin and relation between spin and pseudospin see Ref.\textsuperscript{16}. It has been pointed out above that there are two pockets of the holon dispersion. So, there are holons of two types (= two flavors) corresponding to two pockets. All in all, the effective Lagrangian reads\textsuperscript{16}

$$\mathcal{L} = \frac{\chi_\perp}{2} \vec{n}^2 - \frac{\rho_s}{2} (\nabla \vec{n})^2$$

$$+ \sum_\alpha \left\{ \frac{i}{2} \left[ \psi_\alpha^\dagger D_t \psi_\alpha - (D_t \psi_\alpha)^\dagger \psi_\alpha \right] \right.$$  

$$\left. - \psi_\alpha^\dagger \epsilon(P) \psi_\alpha + \sqrt{2} g (\psi_\alpha^\dagger \vec{\sigma} \psi_\alpha) \cdot [\vec{n} \times (e_\alpha \cdot \nabla) \vec{n}] \right\} .$$

The first two terms in the Lagrangian represent the usual nonlinear $\sigma$ model, see Eq.(14). Note that $\chi_\perp$ and $\rho_s$ are bare parameters, therefore, by definition they are independent of doping. The rest of the Lagrangian in Eq. (13) represents the fermionic holon field and its interaction with the $\vec{n}$-field, $g$ is the coupling constant. The index $\alpha = a, b$ (flavor) indicates the pocket in which the holon resides. The pseudospin operator is $\frac{1}{2} \vec{\sigma}$, and $e_\alpha = (1/\sqrt{2}, \pm 1/\sqrt{2})$ is a unit vector orthogonal to the face of the MBZ where the holon is located.

A very important point is that the argument of the holon kinetic energy $\epsilon$ in Eq. (13) is a “long” (covariant) momentum,

$$\mathcal{P} = -i \nabla + \frac{1}{2} \vec{\sigma} \cdot [\vec{n} \times \nabla \vec{n}] .$$

An even more important point is that the time derivatives of the fermionic field are also “long” (covariant),

$$D_t = \partial_t + \frac{i}{2} \vec{\sigma} \cdot [\vec{n} \times \vec{n}] .$$

It is worth noting that the covariant derivatives in (13) is a reflection of the SU(2) gauge invariance of the system.

An effective Lagrangian similar to (13) was suggested a long time ago by Shraiman and Sigurd.\textsuperscript{17} However, important covariant time-derivatives were missing in their approach. The simplified version\textsuperscript{16} is sufficient for semiclassical analysis of the system. However, the full version (13) is crucial for the excitation spectrum, quantum fluctuations, and especially for stability of the semiclassical solution with respect to quantum fluctuations.
An important note is that the effective Lagrangian (13) is valid regardless of whether the \( \vec{n} \)-field is static or dynamic. In other words, it does not matter if the ground state expectation value of the staggered field is nonzero, \( \langle \vec{n} \rangle \neq 0 \), or zero, \( \langle \vec{n} \rangle = 0 \). The only condition for validity of (13) is that all dynamic fluctuations of the \( \vec{n} \)-field are sufficiently slow. The typical energy of the \( \vec{n} \)-field dynamic fluctuations is \( E_{\text{cross}} \propto x^{3/2} \), see Ref.16, and it must be small compared to the holon Fermi energy \( \epsilon_{F} \propto x \). The inequality \( E_{\text{cross}} \ll \epsilon_{F} \) is valid up to \( x \approx 0.15 \). So, this is the regime where (13) is parametrically justified.

It has been already pointed out that numerical lattice simulations\(^{15}\) give the value of the inverse mass, \( \beta \approx 2.2J \), and the same simulation gives the value of the coupling constant, \( g \approx J \).

Analysis of (13) performed in Ref.16 shows that the dimensionless parameter
\[
\lambda = \frac{2g^{2}}{\pi^{3} \rho_{s}} \tag{14}
\]
plays the defining role in the theory. If \( \lambda \leq 1 \), the ground state corresponding to the Lagrangian (13) is the usual antiferromagnetic state and it stays collinear at any small doping. In other words the instability criterion (11) is not fulfilled. If \( 1 \leq \lambda \leq 2 \), the instability criterion (11) is fulfilled and the collinear antiferromagnetic state is unstable at arbitrarily small doping. The ground state is a static or dynamic spin spiral,
\[
\vec{n} = (\cos \mathbf{Q} \cdot \mathbf{r}, \sin \mathbf{Q} \cdot \mathbf{r}, 0) . \tag{15}
\]
The spin spiral state corresponds to condensation of magnons. The pitch of the spiral is
\[
Q = \frac{g}{\rho_{s}} p . \tag{16}
\]
The spiral wave vector is parallel to the lattice,
\[
\mathbf{Q} = Q(1,0) \quad \text{or} \quad Q = Q(0,1) . \tag{17}
\]
If \( \lambda \geq 2 \), the system is unstable with respect to phase separation and/or charge-density-wave formation and hence the effective long-wave-length Lagrangian (13) becomes meaningless.

To find the experimental value of the coupling constant \( g \) it is sufficient to compare (16) with Eq. (12) that summarizes neutron scattering data. This gives \( g \approx J \) in a very good agreement with the prediction of the lattice numerical calculations. Analysis of neutron inelastic scattering data performed in Ref.16 gives the value of inverse mass, \( \beta \approx 2.7 \). This also agrees reasonably well with the lattice simulations, \( \beta \approx 2.2 \). Using values of \( g \) and \( \beta \) found from fit of experimental data, one obtains that
\[
\lambda \approx 1.30 . \tag{18}
\]
Thus, the analysis is consistent, the system is really in the magnon condensation regime.

VII. QUANTUM FLUCTUATIONS AND QUANTUM PHASE TRANSITION TO THE SU(2) SYMMETRIC PHASE

Calculation of quantum fluctuations described by the Lagrangian (13) is a rather technically involved problem. Here I only present results obtained in Ref.16. The length of the vector \( \vec{n} \) stays constant by definition, \( n^{2} = 1 \). However, the static component of \( \vec{n} \) (the ground state expectation value \( \langle \vec{n} \rangle \)) decreases with doping due to quantum fluctuations. Plot of the static component versus doping is shown in Fig. 4. Ultimately, the static part of \( n \)-

**FIG. 4:** The static component of spin versus doping at zero temperature.

field vanishes at \( x = x_{c} \approx 0.11 \). This is a quantum critical point where spontaneous violation of the SU(2) symmetry disappears. At a higher density of fermions, \( x > x_{c} \), the SU(2) symmetry of the ground state is restored. Recently this effect has been clearly observed in neutron scattering from YBa\(_{2}\)Cu\(_{3}\)O\(_{6+y}\) cuprate superconductor\(^{18,19}\).

VIII. CONCLUSIONS

The magnon condensation in high temperature cuprate superconductors is similar to the \( \pi \)-meson condensation in nuclear matter. Neutron scattering from cuprates unambiguously indicates the magnon condensation. So, the effect has been observed. In both cases (magnons and pions) the SU(2) symmetry of the microscopic Hamiltonian is spontaneously broken in the ground state without fermions (physical vacuum in QCD or Mott insulator in cuprates). In presence of fermions (nuclear matter in
QCD or holes in cuprates) the SU(2) condensate evolves, this is the \( \pi \)-meson or magnon condensation (spin spiral).

In the case of cuprates due to the two-dimensional nature of the problem the evolution (condensation) starts at the arbitrary small concentration of fermions. At a sufficiently high concentration of fermions the SU(2) condensate disappears. This is a quantum critical point for restoration of the SU(2) symmetry.

The Lagrangian (13) has an intrinsic instability with respect to superconducting pairing of fermions. How this instability relates to the condensation physics described in the present paper remains an open problem.

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20. More accurately the contact part in the 2D case is proportional to \( x \ln x \). Anyway, it can be neglected.