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Gauge theory of high-temperature superconductors and strongly correlated Fermi systems

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In this paper we show that the development of resonating-valence-bond correlations and the subsequent superconducting order in the high-T_c oxide superconductors are described by an U(1) lattice-gauge theory. The insulating state has an almost-local gauge symmetry and doping changes this to a global symmetry, which is spontaneously broken at low temperatures, resulting in superconductivity. New topological excitations associated with the singlet field are found.

There has been an explosion of activity in the field of high-temperature superconductivity since the discovery of superconductivity in doped La_2CuO_4.[1] Significant progress has been made in the understanding of the mechanisms of high-T_c superconductivity.[2] The resonating-valence-bond (RVB) theory of superconductivity proposed by Anderson[3] and being developed by the authors[4-7] and others[8,9] is based on a simple Hubbard model and has been quite successful in explaining many of the experimental results.

The pure La_2CuO_4 is an antiferromagnetic (AFM) insulator which loses long-range AFM order at about 1% doping by Sr or Ba.[10] We have argued[6] that 1% doping removes antiferromagnetic order and stabilizes RVB behavior by the quantum fluctuation arising from the holes. At this level of doping, the superconducting T_c is unobservably small or is absent due to localization of holes. However, we have preexisting Cooper pairs in the RVB state up to a temperature $\sim J$, the antiferromagnetic coupling. Superconductivity is absent in this range of temperatures due to the very small electric compressibility of lightly doped systems.

The reduced fluctuation in the number of electrons in any given volume results in large quantum mechanical phase fluctuations suppressing any long-range superconducting order. The present authors and Zou[5] characterized this by a Ginzberg-Landau theory with a very small gradient term arising from the divergent Landau Fermi-liquid parameter F_0^s. Though qualitatively correct, this does not bring out the RVB or superconducting correlation completely. In the present paper we show that the nature of RVB and superconducting correlation is described by a lattice gauge theory. The new local symmetry close to the insulating state arises from the (almost) conservation of particle number on each site. The behavior of the Wegner-Wilson loop correlation function quantifies the RVB correlation. We find new topological excitations associated with the singlet field. These are analogs of magnetic charges in a 2-plus-1 dimensional U(1) lattice-gauge theory of electrodynamics. We believe that the present theory also points towards the solution of two outstanding problems, namely, the characterization of the RVB state in Mott insulators as well as the so-called Kondo coherence in mixed-valence and heavy-fermion systems both having enhanced singlet correlation or quantum coherence but not true spontaneous symmetry breaking under normal conditions. We find features which are similar to that in the problem of confinement in quantum chromodynamics. The present theory is a microscopic theory of superconductivity which avoids the complications of Gutzwiller projections (as encountered by the BZA theory,[4] for example) in a physical way by identification of proper symmetries and fields. It also provides simple and powerful calculational methods for physical quantities. Our theory is also a natural description of Fermi systems with very short (singlet) coherence length of the order of lattice parameters.

For convenience we start with the exactly half-filled band Mott insulator in a simple square lattice which is described by the Heisenberg antiferromagnetic Hamiltonian

$$\mathcal{H} = J\sum(\mathbf{S}_i\cdot\mathbf{S}_j - \tfrac{1}{4}) \ , \tag{1}$$

where $J = 4t^2/U$ and t is the hopping integral and U is the "Hubbard U." Pairs of indices like ij will always stand for nearest-neighbor bonds in what follows, unless otherwise mentioned. As is well known, this Hamiltonian is derived from the Hubbard Hamiltonian as an effective Hamiltonian of the insulator for large U/t. The physics of the RVB comes out clearly when we write the Pauli spin operators in terms of the electron operators c to get[4]

$$\mathcal{H} = -J\sum b_{ij}^\dagger b_{ij} \tag{2}$$

with the local constraints $n_{i\uparrow}+n_{i\downarrow}=1$, where $b_{ij}^\dagger=(1/\sqrt{2})(c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger - c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger)$ is the single creation operator. This Hamiltonian has the important *local gauge symmetry* $c_{i\sigma}^\dagger \rightarrow e^{i\theta_i}c_{i\sigma}^\dagger$. It is physically obvious and can be shown mathematically by an extension of Elitzur's theorem[11] that this local symmetry cannot be spontaneously broken and the thermal average $\langle b_{ij}\rangle=0$ at all temperatures (even in the presence of a global symmetry-breaking field which tends to zero).

We should pause here to discuss the nature of this local gauge symmetry. The above local symmetry is not an exact symmetry of all states of the original Hubbard Hamiltonian; it is true only so long as we stay below the Mott-Hubbard energy gap. But it is a symmetry which controls the subspace containing the ground state and low-order excitations, and in this subspace it can be made exact. Here we have an intriguing situation where a rich approximate local symmetry appears depending on the physics of the problem. It is also intriguing that a similar gauge symmetry appears in the Girvin, Macdonald, and Reed theory of the fractional quantum Hall effect.

The RVB state is believed to be the stable ground state of the two-dimensional triangular lattice[12] as well as the lightly doped square lattice Heisenberg spin-$\frac{1}{2}$ antiferromagnets.[5] Hence we will concentrate on the singlet correlation[13] and develop an effective action or free energy corresponding to this. We want to construct a free energy such that

$$\mathrm{Tr}\,e^{-\beta H} \sim \int \prod_{\tau,\langle ij\rangle} d\Delta_{ij}^*(\tau)d\Delta_{ij}(\tau)e^{-\beta F[\Delta(\tau)]} \ , \tag{3}$$

where F is the free energy or effective action expressed in terms of the "order parameter" $\Delta_{ij}(\tau)$ which is attempting to condense. Here τ is the "Euclidean time" variable, and

$$\langle b_{ij}\rangle \equiv \langle \Delta_{ij}\rangle \equiv \frac{\int \pi d\Delta^* d\Delta \Delta e^{-\beta F}}{\int \pi d\Delta^* d\Delta e^{-\beta F}} \ . \tag{4}$$

The free energy $F[\Delta]$ can be evaluated in several ways—one is a formally exact way of converting the quantum average into a functional integral involving Grassman anticommuting variables; or using the Hubbard Stratonovic identity. We will for simplicity adopt an approximate but physically transparent way to calculate $F[\Delta]$ for high temperatures where we neglect the "time" dependence of $\Delta(\tau)$. The procedure is to get the most general Hartree factorization of $\mathcal{H}$ involing Δ to get

$$\mathcal{H}_{\mathrm{HF}} = -J\sum(\Delta_{ij}^* b_{ij}+\mathrm{H.c.}) + J\sum \Delta_{ij}^*\Delta_{ij} \ , \tag{5}$$

with Δ_{ij} being independent complex variables defined on every nearest-neighbor pair. Since the mean-field Hamiltonian is bilinear in fermion variables, the free energy can be evaluated in terms of a determinant involving the matrix Δ_{ij}. *Then we use this free energy in the functional integral [Eq. (4)] to calculate averages. Thus, even though we used a mean-field-type approximate method to calculate the parameters of the effective action, our theory is not a mean-field theory.* Since we are interested in the high-temperature region, close to the mean-field transition temperature, we can expand the free energy in powers of Δ_{ij}.

Since we know that $\langle \Delta_{ij}\rangle=0$ by Elitzur's theorem, the local gauge invariance puts strong restrictions on the form of $F[\Delta]$. The form of F we obtain is

$$F \approx a\sum|\Delta_{ij}|^2 + b\sum|\Delta_{ij}|^4 + c\sum(\Delta_{ij}^*\Delta_{jk}\Delta_{kl}^*\Delta_{li}+\mathrm{H.c.}) + \cdots \ . \tag{6}$$

This form is consistent with local gauge symmetry. The symmetry of this free energy is $\Delta_{ij}\rightarrow e^{i\theta_i}\Delta_{ij}e^{i\theta_j}$. In the third term of Eq. (7) the summation is over elementary plaquettes of the lattice.

The mean-field theory described above gives a value of $a=a_0(k_BT-J/2)$, $b=b_0J(J\beta)^3$, and $c=c_0J(J\beta)^3$, where a_0, b_0, and c_0 are numbers of the order of unity. An exact derivation of the effective action including Gutzwiller projection (that is avoiding double occupancy) is expected to change only the coefficients a, b, c, etc., and not the form of Eq. (7). This is a nontrivial consequence of the local symmetry in the problem. In this sense the parameters a, b, and c may be determined from experiments and can be used as input parameters of our theory. In Eq. (7) only the third term, the "plaquette" term, depends on the phase of the order parameter. It is this term which helps in the development of nontrivial RVB correlation. In the absence of the third term we have essentially fluctuating independent link variables. The plaquette term correlates them, leading to the nontrivial behavior of the gauge invariant Wegner-Wilson loop correlation functions[14,15] defined as

$$W(C) = \langle b_{ij}^\dagger b_{jk} b_{kl}^\dagger \cdots b_{ni}\rangle = \langle \Delta_{ij}^*\Delta_{jk}\Delta_{kl}^* \cdots \Delta_{ni}\rangle \ , \tag{7}$$

where the bonds $ij, jk, \ldots, ni$ form a closed loop C in the lattice. Thus, one of the first consequences of our theory is the realization that the RVB state can be characterized in a most natural way by nonlocal loop correlation functions.

The phase-independent term in the free energy mostly controls the amplitude fluctuation. Thus we can make the approximation $\Delta_{ij} \approx |\Delta_0(\beta)|e^{i\theta_{ij}}$ to get

$$F \approx aN_B\Delta_0^2 + bN_B\Delta_0^4 + c\Delta_0^4\sum\cos(\theta_{ij}-\theta_{jk}+\theta_{kl}-\theta_{li}) \ , \tag{8}$$

where N_B is the number of bonds and

$$\Delta_0^2 = \frac{\int e^{-\beta(a\Delta^2+b\Delta^4)}\Delta^2 d\Delta}{\int e^{-\beta(a\Delta^2+b\Delta^4)}} \ ,$$
$$\therefore W(C) \approx \Delta_0^{2P(C)}\langle\cos(\theta_{ij}-\theta_{jk}+\theta_{kl}-\cdots-\theta_{ni})\rangle \ , \tag{9}$$

where $P(C)$ is the perimeter of the loop C in lattice units.

Equation (8) is precisely the action of a U(1) lattice-gauge theory (with a slightly different convention for the definition and sign of the link variables in the effective action) and we borrow the known results of this well-studied theory. In particular, in two and three dimensions this theory is known to confine for all values of the coupling constant. Hence the Wegner-Wilson loop obeys the "area law" for large loops[13]

$$\langle\cos(\theta_{ij}-\theta_{jk}+\cdots\theta_{ni})\rangle \approx e^{-\sigma A(c)} \ , \tag{10}$$

where σ is the "string tension" and $A(C)$ is the area of the loop. The nonperturbative effects in the three-dimensional U(1) gauge theory keep the system only in the confining phase.[16] This is a remarkable result which shows that in physical dimensions there is likely to be no genuine phase transition at any finite temperature in an RVB spin system. The string tension σ is a function of temperature. We will call $1/\sqrt{\sigma}$ the correlation length (expressed in lattice units) over which the quantum coherence associated with the RVB correlation is the strongest. As T decreases the correlation length increases. It may be possible to measure σ experimentally by some neutron scattering experiments. Another useful quantity is the plaquette-plaquette correlation function which decays exponentially in the confining phase and it also provides a correlation length.

There are interesting topological and nontopological excitations in our theory. Using a Villain type of approximation[17] it is easily shown that there are configurations of this field Δ_{ij} corresponding to magnetic monopoles. They carry integer magnetic charges which are gauge invariant. As mentioned before we call them magnetic charges, because our U(I) theory resembles the electromagnetic lattice gauge theory in 2 plus 1 dimensions which carry magnetic charges. These magnetic monopoles abound at high temperatures and we have a magnetic plasma. These magnetic monopoles are the novel excitations that we have found in the RVB state. It is remarkable that we have topological defects without any spontaneous symmetry breaking.

Since the Δ field is coupled to the underlying electrons any topologically nontrivial configuration is likely to induce a fermionic charge.[18] This point and its consequences are being studied by us. These magnetic monopoles together with their possible induced fermionic charges are entirely new objects that arise in the three-dimensional RVB state.

We believe that the nontopological unstable energetically stable point defects of the Δ field are likely to be the candidates for the spin solitons and charged solitons of KRS.[8] The following limiting case illustrates this. Imagine a dangling (unpaired) spin at the origin in an otherwise RVB vacuum. In this state clearly $\Delta_{0j}=0$, where j are the nearest neighbors of the site at the origin. If we take our mean-field Hamiltonian [Eq. (6)] and put $\Delta_{0j}=0$, the fermion degree of freedom at the origin is decoupled from the rest of the system and its energy is zero. We may identify this with the "midgap state." If this state is occupied we have a neutral soliton and have a charged soliton (hole) if this state is empty. The above situation is to be contrasted with the topological solitons in polyacetylene. The nontopological nature of the spin and charged soliton in our picture may be related to the possible *absence of any discrete symmetry breaking in the RVB state.*

As T decreases, the "time" dependence of the line field $\Delta(\tau)$ becomes important and we have to keep the extra term of the form $\int \Delta_{ij}^*(\tau)\partial/\partial\tau\Delta_{ij}(\tau)d\tau$ in the free energy. All our local symmetries are time independent. So our problem does not reduce to an Euclidean $d+1$ dimensional lattice gauge theory at $T=0$. It is plausible that this theory is in the "Coulomb phase" at $T=0$ where there is no energy gap for spin excitations. In a Coulomb phase there are no energy gaps for excitations.

Now we describe briefly how doping removes the local symmetry allowing only a global symmetry. At sufficiently low temperatures, the global symmetry may be spontaneously broken resulting in superconductivity. The Hamiltonian in the case of non-half-filled bands is

$$\mathcal{H} \approx -t\sum \tilde{c}_{i\sigma}^{\dagger}\tilde{c}_{j\sigma} + \mu\sum_i n_{i\sigma} - J\sum_{\langle ij\rangle}\tilde{b}_{ij}^{\dagger}\tilde{b}_{ij} - J\sum_{\langle ijk\rangle}(\tilde{b}_{ij}^{\dagger}\tilde{b}_{jk} + \text{H.c.}) \; . \quad (11)$$

where $\tilde{c}_{i\sigma}=(1-\tilde{n}_{i-\sigma})\tilde{c}_{i\sigma}$, etc. This Hamiltonian does not have the local symmetry. It has only the global symmetry $c_{i\sigma}\rightarrow e^{i\theta}c_{i\sigma}$. Adapting the same procedure as for the half-filled band, we get an extra "hopping term" $d\sum(\Delta_{ij}^*\Delta_{jk}+\text{H.c.})$ in the free energy [Eq. (6)], where $d\approx\delta Jd_1+\delta\beta^2Jt^2d_2$ (also the parameters a, b, and c and in particular the mean-field transition temperature starts depending on δ). This term breaks the local symmetry and is invariant only under the global symmetry $\Delta_{ij}\rightarrow e^{i\theta}\Delta_{ij}$. This global symmetry can be spontaneously broken and $\langle\Delta_{ij}\rangle$ can be nonzero at low enough temperature. With doping the superconducting coherence length increases and when the coherence length is much greater than the lattice parameter it is appropriate to replace the action [Eq. (6)] including the hopping term by its coarse-grained version which is easily shown to be the Ginzburg-Landau free energy.

In the heavy-fermion and Kondo problems we have a strong tendency to have singlets on impurity sites in dilute systems as well as to have bond singlets in concentrated systems. The development of this singlet tendency as the temperature is lowered has been termed Kondo coherence and it always lacked a clear picture as well as quantification in the case of the Anderson lattice. The link variable Δ_{ij} is definitely the appropriate quantity to be looked at as has been emphasized by Noga.[19] The simplest approximate free energy that we get starting from an Anderson lattice Hamiltonian is exactly Eq. (6) with the additional $d\Delta_{ij}\Delta_{jk}$ term which breaks the local symmetry. The interesting point is that the chemical potential and the parameters like the relative position of the f level, etc., are such that they lead to a very small d term compared to c term in the free energy leading to the impossibility of spontaneous symmetry breaking in spite of the presence of the term which breaks the global symmetry. Most importantly we find that the behavior of the Wegner-Wilson loop and the plaquette-plaquette correlation function characterizes the Kondo coherence. More details of the Kondo-lattice behavior and calculations of the transport and other physical properties of high-temperature superconductors will be discussed in a forthcoming paper.

Note added in proof: Some of the above, particularly mechanisms for superconductivity, has been superseded in the months since submission. Nonetheless the paper represents the first proposal for exploitation of the local gauge version of the RVB theory. For more recent treatments see P. W. Anderson (unpublished) or I. Afflect (unpublished).

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