A lattice field theoretical model for high-T_c superconductivity*

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We present a 2+1-dimensional lattice model for the copper oxide superconductors and their parent compounds, in which both the charge and spin degrees of freedom are treated dynamically. The spin-charge coupling parameter is associated to the doping fraction in the cuprates. The model is able to account for the various phases of the cuprates and their properties, not only at low and intermediate doping but also for (highly) over-doped compounds. We acquire a qualitative understanding of high-T_c superconductivity as a Bose-Einstein condensation of bound charge pairs.

1. THE QUESTIONS

The discovery of the new perovskite superconductors [1] opened the path to critical temperatures (T_c) for superconductivity as high as 140 K, surpassing by a factor of seven the highest known T_c for metals or alloys. In fact the physical mechanism for superconductivity seems to be rather different. Traditional superconductors present an *isotope effect*, which calls for a phonon mediated mechanism. They also have a gap (of order of meV) in the excitation spectrum, as shown by the exponential decrease of the specific heat at low temperature. All this can be accounted for by the BCS theory, where electrons of opposite spin and momenta are attractively coupled through a phonon exchange. The basic BCS statement is the existence of a critical temperature at which this attraction *simultaneously* produces the *formation* of bound states of pairs of electrons (with binding energy of the order of the gap) and the *condensation* of those pairs into a *quantum liquid*.

The new superconductors show an intriguing phenomenology:

- Superconductivity appears in doped, ceramic materials, like La_2CuO_4 doped to $La_{2-x}Ba_xCuO_4$, starting at $x \sim 0.05$.
- At x=0 it is an insulating antiferromagnet.
- At large x it may be a normal metal.
- The doping suppresses the antiferromagnetic (AFM) correlation between neighboring CuO_2 planes. However, large ($\xi \sim 10a$) in-plain correlations remain just above T_c. Also, transport phenomena occur mainly in the CuO_2 planes, so everything looks like a d=2 problem, with localized spins on the Cu and mobile holes on the O ions.
- Again the superconductivity is charge-2 in nature (there is a *pairing state*).
- Anomalous *normal* (*i.e.* non superconducting) state: there are experimental indications of a *pseudo-gap phase* (pair formation *before* quantum liquid condensation).

All this poses some essential questions [2]: What is the physical origin of the anomalous *normal* state? How can it be characterized? What is the mechanism for high T_c superconductivity? And what is the *pairing state*?

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2. OUR MODEL

The natural (lattice) field-theoretical approach is effective field theory. For instance, the long wavelength, low temperature (antiferro)magnetic excitations of the the parent compound (undoped La_2CuO_4) are well described by the O(3) Non-Linear σ-model (NLσM) [3]. The basic ingredients of our proposal are:

- Treat localized spins (at Cu), and charge-carriers (at O) independently and, both, dynamically *i.e.* not hole moving on a *fixed* spin background.
- Relativistic lattice field theory, where M.C. and Mean Field calculations are *feasible*.
- Try to catch the essential features of electrons strongly coupled to AFM spin backgrounds (*i.e.* not a microscopic model).

We define a 2+1-dimensional O(3) lattice model, with two flavors of **naive** fermions:

$$S = \frac{1}{2}\sum_{n,\mu,f}\bar\Psi^f_n\sigma^\mu(\Psi^f_{n+\mu}-\Psi^f_{n-\mu}) \qquad (1)$$
$$- \; k\sum_{n,\mu}\vec\phi_n\vec\phi_{n+\mu} + y\sum_n \bar\Psi^{f'}_n(\vec\phi_n\cdot\vec\tau)_{f'f}\Psi^f_n,$$

where $\vec\phi=(\phi_1,\phi_2,\phi_3)$, $\vec\phi^2=1$ and $\bar\Psi,\Psi$ are two-component Dirac spinors in $d=2+1$. The flavors *mimic* the two values of the electron *spin*. The matrices σ^μ,τ_i are Pauli matrices. The spin-fermion coupling y will be related to the doping fraction x. In the large-y region, the change of variable ($\Psi\to\frac{1}{y}\vec\phi\cdot\vec\tau\Psi$,$\bar\Psi\to\bar\Psi$) shows that the fermionic kinetic term is suppressed by a factor $1/y$. Therefore, at both $y=0$ and $y=\infty$ we recover the NLσM. The *insulating* undoped material should be represented by the $y\to\infty$ limit, as suggested by the fermion hopping suppression. Thus small x corresponds to large y (a possible correspondence is $x\sim C^2/(C^2+y^2)$, C being a constant).

There is a technical problem for the numerical simulation, as $\vec\phi$ are *constrained* variables not belonging to a *Lie group.* We solve it by introducing *three* conjugate momenta *per spin.* We then

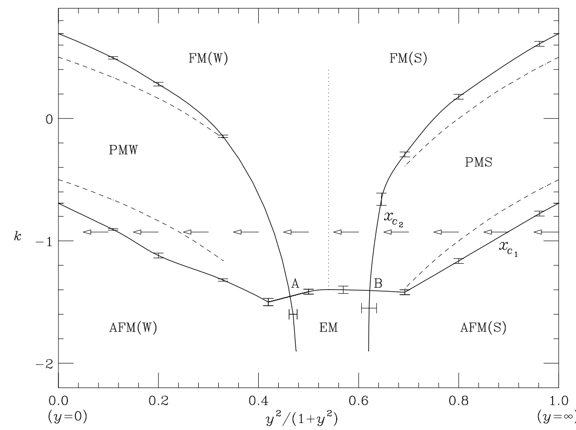

Figure 1. Phase diagram of the action (2), with two fermion families as required by HMC. Dashed lines indicates the MF calculation, while solid are from a MC calculation on a 8^3 lattice.

obtain the Hamiltonian

$$H=\frac{1}{2}\sum_n\vec P^2_n+S(\{\vec\phi_n\}),$$

for which equations of motion preserving the constraint and the energy, can be written:

$$\dot{\vec\phi}_n=\vec P_n\times\vec\phi_n\ ,\ \dot{\vec P}_n=-\vec\phi_n\times\frac{\delta S}{\delta\vec\phi_n}.$$

The standard HMC algorithm is now straightforward. The simulation took 16 days of the 32 Pentium Pro processor parallel computer RTNN based in Zaragoza. In fig. 1, we show the phase diagram of the model at zero temperature. Notice that it is very similar to the familiar diagram of (chiral) Yukawa models [4]. We name their ferrimagnetic phase *exotic magnetic* (EM), to avoid confusion in a condensed matter context. So far, the undoped material could be represented by either of ($\pm\kappa_0$,y=∞) in fig. 1. However, while doping the material, the representative point moves in the plane (κ,y). Doping suppresses the AFM order, so the curve κ=$\kappa(y)$ should start at ($-\kappa_0,y=\infty$). In fig. 1, the arrows sketch the possible *trajectory* of a material with increasing doping.

For the fermionic correlation functions, our results are still at the mean-field level. The small-y region is in a perturbative regime, with *light fermions* of mass $m_f = y\langle\vec{\phi}\rangle$ (a Fermi liquid). In the large-y region, the fermionic kinetic term in the action is $(1/y)\bar{\Psi}\gamma^\mu\partial_\mu\langle\vec{\phi}\cdot\vec{\tau}\rangle\Psi$ at the MF level. Thus, inside the PMS phase ($\langle\vec{\phi}\cdot\vec{\tau}\rangle = 0$), the fermions are essentially non-propagating. However, the operator $\epsilon_{ff'}\Psi^f\Psi^{f'}$ excites a spin singlet of mass $m^2_{pair} = 4(y^2 - 3/2)$, which can get small in the PMS phase, that is a *light charge-2 spin singlet bound state*, as in (chiral) Yukawa models [5]. Inside the FM(S) phase, the kinetic term is not so strongly suppressed ($\langle\vec{\phi}\rangle \neq 0$). Thus, carriers are expected to propagate. In the AFM(S) phase the original fermions (and doublers) do not propagate. But fermions with wavenumbers $\pm\pi/2$ are found to propagate (strongly resembling the *Schrieffer pockets*).

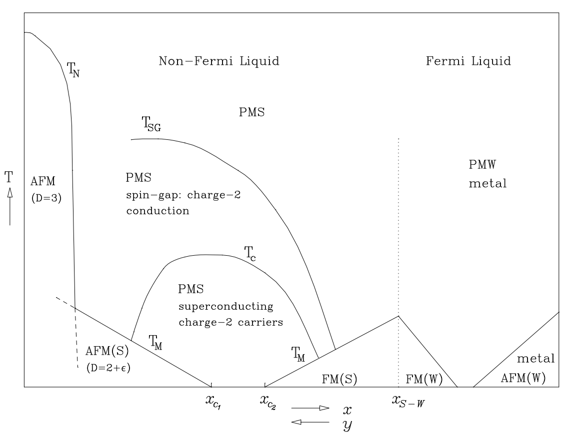

Figure 2. Qualitative temperature (T) and doping (x) phase diagram, from the model (2).

Now, we can qualitatively discuss the behavior with the temperature (see fig. 2, and ref. [6]). The T=0 axis can directly be read off from the arrow line in fig. 1. As we enter the PMS phase, we should expect the light, charge-2 bound states to be Bose-Einstein condensed, yielding superconductivity. As the temperature rises, the BE condensation will disappear, and the system enters a region with heavy single fermions and uncondensed light charge-2 pairs. This we expect to correspond to the *pseudo-gap* phase. At even higher temperatures, the pairs will break up (yielding an insulating phase at the MF level). We also obtain Fermi liquid behavior at large x (small y).

3. OUR ANSWERS

- **Physical origin of anomalous** *normal* **state?** A dynamical, antiferromagnetically interacting spin background, *strongly* coupled to fermions (*heavy* $\phi\Psi$ fermions).
- **Characterization of anomalous** *normal* **state?** heavy single charges ($\phi\Psi$) and *light bosonic* charge-2 bound states.
- **Mechanism of high-T_c?** Bose-Einstein condensation of previously formed *stable* pairs.
- **What is the pairing state?** A bound state of *heavy* fermions, tied by spin-waves in a *disordered* phase: a **PMS-pair**.

Moreover, this pairing mechanism, as well as the non-coincidence of pair formation and *quantum liquid* condensation, are likely to occur in other spin-fermion models.

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