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 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, ceramice materials, like La$_2$CuO$_4$ doped to La$_{2-x}$Ba$_x$CuO$_4$, 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-plane 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: 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?
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 parent compound (undoped La$_2$CuO$_4$) are well described by the O(3) Non-Linear $\sigma$-model (NL$\sigma$M) [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:

\[
S = \frac{1}{2} \sum_{n,\mu,\nu} \bar{\Psi}_n^f \sigma^\mu (\Psi_{n+\mu}^f - \Psi_{n-\mu}^f) + \frac{\kappa}{2} \sum_{n,\mu} \bar{\phi}_n \phi_{n+\mu} + \frac{y}{2} \sum_n \bar{\Phi}_n^f (\phi_n \cdot \bar{\tau}) f'_f \Phi_n^f,
\]

where $\phi = (\phi_1, \phi_2, \phi_3)$, $\phi^\dagger = 1$ and $\Phi, \bar{\Phi}$ are two-component Dirac spinors in $d = 2 + 1$. The flavors mimic the two values of the electron spin. The matrices $\sigma^\mu, \tau_i$ 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 ($\Psi \rightarrow \frac{1}{y^\dagger} \bar{\phi} \cdot \bar{\tau} \Phi, \bar{\Phi} \rightarrow \bar{\Psi}$) shows that the fermionic kinetic term is suppressed by a factor $1/y$. Therefore, at both $y = 0$ and $y = \infty$ we recover the NL$\sigma$M. The insulating undoped material should be represented by the $y \rightarrow \infty$ 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 $\bar{\phi}$ are constrained variables not belonging to a Lie group. We solve it by introducing three conjugate momenta per spin. We then obtain the Hamiltonian

\[
H = \frac{1}{2} \sum_n \bar{P}_n^2 + S(\{\bar{\phi}_n\}),
\]

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

\[
\ddot{\bar{\phi}}_n = \bar{P}_n \times \bar{\phi}_n, \quad \ddot{\bar{P}}_n = -\bar{\phi}_n \times \frac{\delta S}{\delta \bar{\phi}_n}.
\]

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. [8] 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 $(\pm \kappa_0, y = \infty)$ in fig. [8]. However, while doping the material, the representative point moves in the plane $(\kappa, y)$. Doping suppresses the AFM order, so the curve $\kappa = \kappa(y)$ should start at $(-\kappa_0, y = \infty)$. In fig. [8], 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 $(1/y) \bar{\Psi} \gamma^\mu \partial_\mu (\vec{\phi} \cdot \vec{\tau}) \Psi$ 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 $m_{\text{pair}}^2 = 4(y^2 - 3/2)$, 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. \[3\], 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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