Why $T_c$ is too high when antiferromagnetism is underestimated? — An understanding based on the phase-string effect

Z. Y. Weng

Texas Center for Superconductivity, University of Houston
Houston, TX 77204-5932
E-mail: zyweng@uh.edu

Abstract. It is natural for a Mott antiferromagnetism in RVB description to become a superconductor in doped metallic regime. But the issue of superconducting transition temperature is highly nontrivial, as the AF fluctuations in the form of RVB pair-breaking are crucial in determining the phase coherence of the superconductivity. Underestimated AF fluctuations in a fermionic RVB state are the essential reason causing an overestimate of $T_c$ in the same system. We point out that by starting with a bosonic RVB description where both the long-range and short-range AF correlations can be accurately described, the AF fluctuations can effectively reduce $T_c$ to a reasonable value through the phase string effect, by controlling the phase coherence of the superconducting order parameter.

It was first conjectured by Anderson [1] that the ground state of the two-dimensional (2D) $t-J$ model may be described by some kind of resonating-valence-bond (RVB) state. Perhaps the most natural consequence of a RVB description is the superconductivity once holes are introduced into the system, which otherwise is a Mott insulator, as preformed spin pairs become mobile, i.e., carrying charge like Cooper pairs.

Even though the RVB state was proposed [1] to explain the then-newly-discovered high-$T_c$ superconductor in cuprates, the mean-field estimate of $T_c$ turned out to be way too high ($\sim 1000$K at doping concentration $\delta \sim 0.1$ [2]) as compared to the experimental ones ($\sim 100$K). Another drawback for the earlier fermionic RVB theory (where spins are in fermionic representation) is that the antiferromagnetic (AF) correlations are always underestimated, which becomes obvious in low-doping limit where long-range AF ordering (LRAFO) cannot be naturally recovered. Even at finite-temperature where the LRAFO is absent, the spin-lattice relaxation rate calculated based on those RVB theories shows a wrong temperature-dependence as compared to that well-known for the Heisenberg model, indicating an absence of
AF fluctuations.

Intuitively, a fermionic RVB state should become superconducting of BCS type at finite doping where the RVB pairs are able to move around carrying charge. But since the RVB pair-breaking process corresponds to AF fluctuations at insulating phase while it also represents Cooper pair-breaking in superconducting state, it is not difficult to see why the underestimate of AF fluctuations in the fermionic RVB theory would be generally related to an overestimated $T_c$.

Of course, the above-mentioned drawback in describing antiferromagnetism does not include all RVB theories. There actually exists a RVB state which can describe the AF correlations extremely well. As shown by Liang, Douct, and Anderson [3], the trial wavefunction of RVB spins in bosonic representation can reproduce almost exact ground-state energy at half-filling (which implies a very accurate description of short range spin-spin correlations). A simple mean-field theory of bosonic RVB studied by Arovas and Auerbach [4] (usually known as the Schwinger-boson theory) can easily recover the LRAFO at zero-temperature and reasonable behavior of magnetic properties at finite temperature.

Thus, one may classify two kinds of RVB states based on whether the spins are described in fermionic or bosonic representation. In principle, both representations should be equivalent mathematically due to the constraint that at each site there can be only one spin. But once one tries to do a mean-field calculation by relaxing such a constraint, two representations will result in qualitatively different consequences: in fermionic representation, even an exchange of two spins with the same quantum number will lead to a sign change of the wavefunction as required by the fermionic statistics. At half-filling, this is apparently redundant as the true ground-state wavefunction only changes sign when two opposite spins at different sublattice sites exchange with each other, known as the Marshall sign [5] which can be easily incorporated into the bosonic RVB description. That explains the great success of the bosonic RVB mean-field theory over the fermionic ones at half-filling.

Since the bosonic RVB description of antiferromagnetism is proven strikingly accurate at half-filling, one may wonder why we cannot extend such a formalism to the doped case by literally doping the Mott-insulating antiferromagnetism into a metal (superconductor). In fact, people have tried this kind of approach based on the so-called slave-fermion representation but the mean-field theories always lead to the so-called spiral phase [6] which is inherently unstable against the charge fluctuations [7]. In other words, an instability boundary seems to prevent a continuous evolution of the mean-field bosonic RVB description into a short-ranged spin liquid state at finite doping.

It implies that some singular effect must have been introduced by doping which was overlooked in those theories. Indeed, it was recently revealed [8] that a hole hopping on the antiferromagnetic background always leaves a string of phase mismatch (disordered Marshall signs) on the path which is non-repairable at low-energy (because the spin-flip term respects the Marshall sign rule). The implication of the existence of phase string is straightforward: a hole going through a closed loop will acquire a nontrivial Berry phase and a quasiparticle picture no longer holds here.
This explains why the mean-field theory in the slave-fermion representation, where the topological effect of the phase string is smeared out by mean-field approximation, always results in an unphysical spiral-phase instability.

This barrier can be immediately removed once the nonlocal phase string effect is explicitly incorporated into the Schwinger-boson, slave-fermion representation through a unitary transformation – resulting in the so-called phase string formulation [9] where the mean-field treatment generalized from the Schwinger-boson mean-field state at half-filling [4] becomes workable at finite doping. A metallic phase [10] with short-range spin correlations can be then obtained in which the ground state is, not surprisingly, always superconducting.

What becomes special here is that the phase string effect introduces a phase-coherence factor to the superconducting order parameter [10]:

\[ \Delta_{ij}^{SC} \propto \rho_s^0 \Delta^s e^{i/2(\Phi_i^s + \Phi_j^s)} \]

where \( \Delta^s \) denotes the mean-field RVB order parameter for bosonic spinons and \( \rho_s^0 \sim \delta \) is the bare superfluid density determined by holons (both spinon and holon are bosonic in this representation), \( i \) and \( j \) refer to two nearest-neighbor sites. The phase-coherence factor \( e^{i/2\Phi_i^s} \) is related to the spin degrees of freedom as follows

\[ \Phi_i^s = \sum_{l \neq i} \text{Im} \ln (z_i - z_l) \sum_\alpha \alpha n_{l\alpha}^b \]

with \( n_{l\alpha}^b \) being defined as the spinon number operator at site \( l \). The physical interpretation of the phase-coherence factor (2) is that each spinon contributes to a phase-vortex (anti-vortex).

At zero temperature, when all spinons are paired, so are those vortices and antivortices, such that superconducting order parameter \( \Delta^{SC} \) achieves phase-coherence [11]. At finite temperature, free excited spinons or dissolved vortices (anti-vortices) tend to induce a Kosterlitz-Thouless type transition once the "rigidity" of the condensed holons breaks down which may be estimated as the excited spinon number becomes comparable to the holon number [10].

The superconducting transition temperature obtained this way is shown in Fig. 1 versus a spinon characteristic energy scale \( E_g \). The definition of \( E_g \) is shown in Fig. 2 where the local (\( \mathbf{q} \)-integrated) dynamic spin susceptibility as a function of energy is given at \( \delta = 0.143 \) (solid curve) at zero temperature. As compared to the undoped case (○ curve), a resonance-like peak emerges at low-energy \( E_g \) due to the phase string effect. The doping-dependence of \( E_g \) is illustrated in the insert of Fig. 2.

Therefore, in the bosonic RVB state where the AF correlations are well described, the superconducting transition temperature is essentially decided by the low-lying spin characteristic energy. According to Fig. 2, \( J \sim 100 \text{ meV} \) gives rise to \( E_g = 41 \text{meV} \) at \( \delta = 0.15 \) which are consistent with the neutron-scattering data for such a compound [12]. Then at the same \( E_g \), one finds \( T_c \sim 100K \) according to Fig.
FIGURE 1. The relation of $T_c$ with the spin characteristic energy $E_g$ defined in Fig. 2.

FIGURE 2. The local dynamic spin susceptibility function versus energy at $\delta = 0$ (⋄ curve) and $\delta = 0.143$ (solid curve). The insert: $E_g$ versus the doping concentration.
1 which is very close to the experimental number in the optimal-doped $YBCO$ compound.

The overall picture goes as follows. The bosonic RVB order parameter $\Delta^s$ controls the short-range spin correlations which reflects the “rigidity” of the whole phase covering both undoped and doped regimes, superconducting and normal (strange) metallic states. On the other hand, $T_c$ is basically determined by the phase coherence: for those preformed RVB pairs to become true superconducting condensate, the extra phase frustration introduced by doping has to be suppressed. Here we see how the AF fluctuations and superconductivity interplay: the former in a form of RVB pair-breaking fluctuations causes strong frustration on the charge part through the phase string effect and its energy scale thus imposes an upper limit for the transition temperature of the latter. It is interesting to see that AF fluctuations and superconducting condensation do compete with each other, although the driving force of superconductivity already exists in the Mott antiferromagnet in a form of RVB pairing.

To summarize, even though it is very natural for a RVB pairing description of the Mott-insulating antiferromagnetism to develop a superconducting condensation in the neighboring metallic regime, the issue of superconducting transition temperature is highly nontrivial as the AF fluctuations in a form of RVB pair-breaking process are the key effect to scramble the phase coherence of the superconductivity. The underestimated AF fluctuations in a fermionic RVB state are the essential reason causing an overestimate of $T_c$ in the same system. We pointed out that by starting with a bosonic RVB description where both the long-range and short-range AF correlations can be accurately described, the AF fluctuations can effectively reduce $T_c$ to a reasonable value through the phase string effect controlling the phase coherence of the superconducting order parameter.

**ACKNOWLEDGMENTS**

This talk is based on a series of work done in collaboration with D. N. Sheng and C. S. Ting. I would like to acknowledge the support by the Texas ARP program No. 3652707 and the State of Texas through the Texas Center for Superconductivity at University of Houston.

**REFERENCES**

1. P.W. Anderson, Science **235**, 1196 (1987); G. Baskaran et al., Solid State Comm. **63**, 973 (1987); Z. Zou and P. W. Anderson, Phys. Rev. B**37**, 627 (1988).
2. N. Nagaosa and P. A. Lee, Phys. Rev. Lett. **64**, 2450 (1990); P. A. Lee and N. Nagaosa, Phys. Rev. B**46**, 5621 (1992).
3. S. Liang, B. Doucot, and P. W. Anderson, Phys. Rev. Lett. **61**, 365 (1988).
4. D.P. Arovas and A. Auerbach, Phys. Rev. B**38**, 316 (1988).
5. W. Marshall, Proc. Roy. Soc. (London) A**232**, 48 (1955).
6. B. I. Shraiman and E. D. Siggia, Phys. Rev. Lett. 62, 1564 (1989); 61, 467 (1988).
7. Z.Y. Weng, Phys. Rev. Lett. 66, 2156 (1991).
8. D. N. Sheng, et al., Phys. Rev. Lett. 77, 5102 (1996).
9. Z. Y. Weng, et al., Phys. Rev. B55, 3894 (1997).
10. Z. Y. Weng, et al., Phys. Rev. Lett. 80, 5401 (1998); preprint, cond-mat/9809362.
11. V. J. Emery and S. A. Kivelson. Nature, 374, 434 (1995).
12. M. A. Mook, Yethiraj, G. Aeppli, T. E. Mason, and T. Armstrong, Phys. Rev. Lett. 70, 3490 (1993); H. F. Fong, B. Keimer, P. W. Anderson, D. Renzik, F. Doğan, and I. A. Aksay, Phys. Rev. Lett. 75, 316 (1995).