Superconductivity in High Tc Cuprates: The Cause is No Longer A Mystery

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ABSTRACT

I discuss various direct calculations of the properties of the one-band Hubbard model on a square lattice and conclude that these properties sufficiently resemble those of the cuprate superconductors that no more complicated interactions are necessary to cause high Tc superconductivity.. In particular, I discuss phonon effects and conclude that these may be effective in reducing Tc and the gap in electron-doped materials.

The standard preamble for all kinds of papers on theory (or experiment, for that matter) in the field of high Tc usually contains the phrase "since there is no consensus on the cause of high Tc superconductivity" or words to that effect, and often proceeds to justify thereby yet another implausible conjecture as to some aspect of the phenomenon. Of course one man's consensus is another man's wild disagreement, and you can easily find those who do not agree that there is a consensus on relativity, the quantum theory, or the Standard Model, by doing a simple web search. Not, of course , to mention theories of evolution or of the big bang, which are unpopular in whole states and most legislatures. As a solid stater I thank my stars that the band theory of solids and the BCS model are such obscure targets that they do not garner this kind of disapprobation, although each had its powerful though somewhat irrational opponents in the past–names like Slater and Wigner, even, for the latter.

I would agree that there is or should be no real agreement as to the cause of much of the peculiar phenomenology of the cuprates. Each of us would-be experts has his favorite list of really puzzling questions about them. My own favorites are the peculiar insensitivity of Tc to disorder, and the strange transport properties

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in the normal state. Another mystery is the role of interlayer interaction effects in all kinds of ways, although we can now be reasonably certain that they do not cause superconductivity. Yet it is time , I feel, that it should no longer be legitimate to doubt the "first cause", namely the minimal underlying model which produces, among a bewildering welter of other effects, superconductivity at still unprecedentedly high temperatures. I can speak with a certain lack of bias on this matter because the interlayer tunneling theory which I advocated for five years, and wrote a book about, turns out to be one of those which must be consigned to the dustbin. (Although before I was wrong, I was right, at least partially, as to the correct "first cause".[1])

My confidence is based on two things. First is the rough agreement between a number of different simulations, extrapolations, and variational calculations, and the great similarity between these calculations and the actual experimental data, using a "bare-bones" model for the electrons and their interactions, a model for which there is much independent verification. The second is the experimental data themselves, which in many particulars seem to be trying to tell us the nature of the phenomena.

All of these successful calculations are based on the same simple model for the underlying physics. This model is the one-band Hubbard model, or, as can be shown to be essentially equivalent in the appropriate strong-coupling limit, the $t-J$ model. It is interesting that there seems to be no need to include electron-phonon coupling; I will discuss the reason and possible effects of the phonons later in this article. The appropriate Hamiltonian, then is

$$H = \sum (i|t|j)c*(i)c(j) + U\sum n(i,+)n(i,-) \tag{1}$$

$$H(t-J) = P\sum (i|t|j)c*(i)c(j)P + \sum J(ij)S(i)*S(j) \tag{2}$$

Here P is the projection operator which removes double occupancy of any site. (2) is meaningless without the projection. $+$ and $-$ of course are the spin indices.[2]

The most direct calculations with (2) are the quantum Monte-Carlo simulations of Scalapino and his group[3], and using a somewhat different method, those of Sorella and collaborators[4]. There is considerable controversy between these two groups as to the details of the results; however, what strikes the disinterested observer such as myself is not these differences but the essential similarity of the two. The low-temperature phase for low doping is of course antiferromagnetic ((2) reduces to the Heisenberg model in that case) but with increasing doping one encounters first an inhomogeneous (probably striped) phase and then, at approximately the right temperature and hole density, d-wave superconductivity. The parameters of (1) or (2) are not arbitrary–experiments of many types give us J, and ARPES measurements give us a good estimate of the band structure at high doping, which is t–so that there is only a little freedom to manipulate the various components of t. There are some confirmatory simulations, particularly on ladder systems, which again give us a great deal of understanding of why d-wave superconductivity arises; there are also strong indications of a pseudogap phenomenon in the appropriate place. I am no real expert on this extremely tricky field, and in fact have been a pessimist about its ability to arrive at any decisive results, but at this point I have to confess myself impressed. Of course, the trouble with direct calculations is both that they do not really lead to deep understanding, nor can they say much about such things as excitation spectra and transport properties, but what they can say is: when you start out with this physics, you end up with the observed results. I am not at all an expert in the rather involved and subtle reasoning that goes into these calculations, so will not present them in detail, but there is no question that these are the most extensive direct calculations in existence.

A second approach has been taken by Randeria and Trivedi[5], by Masao Ogata[6], and to some extent by Sorella's group. This is to take seriously the original ansatz of the RVB theory that the ground state wave function could be approximated by Gutzwiller projection of an appropriate product wave function of BCS type, and to determine variationally the energy gap and the chemical poten-

tial of the wave function to be projected (which, they point out, need not be the physical chemical potential) by calculating the energy and varying it. The Randeria group also improves the wave function somewhat by Monte Carlo methods. Again, as before the results resemble very strongly the experimental data insofar as these can be determined from the calculation; in particular, the prediction of d-wave superconductivity for an adequately doped sample is very robust. Ogata finds that for underdoped concentrations he can find mixtures of antiferromagnetism and superconductivity, as is observed in some cases.

There is still a third method of direct calculation which has been applied, starting with early work by Georges and Yedidia[7], and carried to an amazing degree of refinement by Bill Putikka[8] in recent years. This is direct expansion of the power series in 1/T for the partition function, and extrapolation of the results with Pade approximants. This method has played a great role in the past in estimating critical behavior near phase transitions, but hasn't previously been much used in quantum many-body systems. It has been very useful in disposing of red herrings which have appeared in various mean field approximations--showing that the $t-J$ Hamiltonian does not lead to phase separation until J is unphysically large, for instance; and also identifying the very large U, low doping "Nagaoka" ferromagnetic region. But recently Puttika has carried his series out to ten to twelve orders and has been able to calculate n(k) with sufficient accuracy to spot the disappearance of the Fermi surface near the (π, 0) point which is characteristic of the pseudogap regime. The agreement of his results with those of ARPES at the same energy resolution is remarkable.

The model is of course not the real substance. Why does it (the model) work so well? In the first place, the question of layer interactions: these are remarkably weak, which we can take as an empirical fact on the basis that the Tl one-layer cuprate is experimentally seen to exhibit all the phenomena that the others do, though proven conclusively by Moler et. al[9] to have very weak interlayer interaction. The same may be said about the gate-doped $CaCuO2$ sample of Kloc, Schon et. al,[10] where there is only one doped layer, but perhaps total acceptance

of these results should await confirmation on more samples and in other laboratories. The simplification to the simple one-band Hubbard model is often justified by the discussion of Zhang and Rice, which is more or less correct, but I prefer the use of projective canonical transformations a la O K Anderson[11]; and actually the strongest argument was the very early exact calculations on small clusters by Michael Schluter et al[12] who showed that an effective one-band Hubbard model worked very well indeed.

There are two physical aspects which are not in the model and could be important. One is long-range Coulomb forces–one assumes effective screening as in a normal metal, and the only real justification is that it works. Some experimental data bear on this: we have good data on interlayer plasmons which show that the c-axis is a fairly insulating direction, actually, (except for supercurrents) but as far as we can see the intralayer plasmons are indeed high-frequency and may screen reasonably well.

The question which keeps coming up is phonons: why are there almost no relevant phonon phenomena? The answer to this, I would speculate, is two-fold. I believe that it is almost on the level of the calculational results above that the nature of the pseudogap is that it is a pairing phenomenon in the spin sector–i e, that the pseudogap region can be seen as an RVB with d-wave pairing. But the spin sector is not coupled to phonons in lowest order, because a displacement of the local potential does not break the spin degeneracy. In the second term of (2) the electron-phonon interaction couples only to J. It is worth confirming this experimentally, but it is known that in heavy-electron materials the Kondo spins do not couple to phonons. Therefore, the pseudogap is not affected one way or another by phonons (or ordinary impurities) In the point of view that I have called "RVB redux"[13] the superconducting gap is caused by the kinetic energy cost of the opening of the pseudogap, which can only be restored by pair hopping via the anomalous "josephson" terms in the kinetic energy; thus at least for the higher doping regime the SC gap follows the pseudogap.

This is rather a speculative argument, and I am going immediately to say that in fact there are phonon effects on Tc. For most phonons these are reasonably small because, as has been exhaustively proven for ordinary superconductors, the electron-electron interaction due to phonons is very local and acts primarily between Wannier functions on the same site. In our Hubbard model, it acts simply as a modulation of U. But of course the reason why we have a d-wave is that it has zero amplitude at the origin and hence avoids the repulsive U, and neither U nor phonons are effective. But I think there is one phonon which can be expected to couple rather strongly to our d-electrons, and much more strongly to electrons than to holes (note that in our projective theory (2) there is no particle-hole symmetry.) This is the phonon which represents the Jahn-Teller displacement which breaks the $d_{x^2-y^2}$ vs d_{z^2} degeneracy (see Fig 1). An electron site has no $(x^2 - y^2)$ hole and thus tends to relax the Jahn-Teller distortion, while a hole site simply adds to the distortion a little. As is easily seen from the figure, the phonon which couples best is at wave vector π, π and hence couples the peaks in the gap function $\pi, 0 - > 0, \pi$ This phonon has been the subject of considerable discussion recently but rather off the point. What it will do is to cause a repulsive interaction for the d-wave gap and hence lower the superconducting Tc for electrons relative to holes., an effect which is observed but has seemed rather puzzling. It is noteworthy that in a couple of recent measurements (see, for instance, [10]) the pseudogap and T* are about the same for electron and hole dopings at the same level, but T_c is much reduced.

In fact, if the effect is rather localized in k-space we might expect the two gaps to behave as in Fig. 2, with the $\pi, 0$ peak depressed for the SC gap relative to the general point along the Fermi surface. This seems to explain the ARPES observations that the peak of the gap function is not at the $0, \pi$ points but rather there is a local minimum there, as we have sketched in Fig. 2 (not, of course, to scale)

One implication of this picture is that we would expect an isotope effect for the electron-doped materials, but a negative one. A crude calculation, assuming

without any justification that the BCS gap equation is valid, would suggest

$$\partial(\ell n\, T_c)/\partial(\ell n\, fopt) \;=\; -\mu/(J-\mu) \tag{3}$$

where $fopt$ is the optical phonon frequency, μ the phonon coupling constant, and J the effective antiferromagnetic exchange . (3) might be valid in the overdoped regime. For reasons mentioned but not emphasized in my book, (which include a great deal of experience) I am not very convinced of the accuracy or relevance of isotope effect measurements, but perhaps the gate-doping possibility, which avoids the necessity of making a new sample for every measurement, is a new opportunity.

In conclusion, my point here is that there is a great deal of consensus on the model which underlies high T_c cuprate superconductivity, and there ought to be more: I think we have proved our point. But there is much more to be done and specifically, for instance, we are so far unable to give a closed-form gap equation.

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FIGURE CAPTIONS

(1) The phonon which is likely to interact strongly with electrons around the 0, points. Its displacements are those of the Jahn-Teller distortion caused by an x^2-y^2 hole, so that it might be expected to be particularly soft for electron doping.

(2) The reduction in the superconducting gap which might result from the repulsive interaction caused by the optical phonon of Fig. 1.

Fig. 1

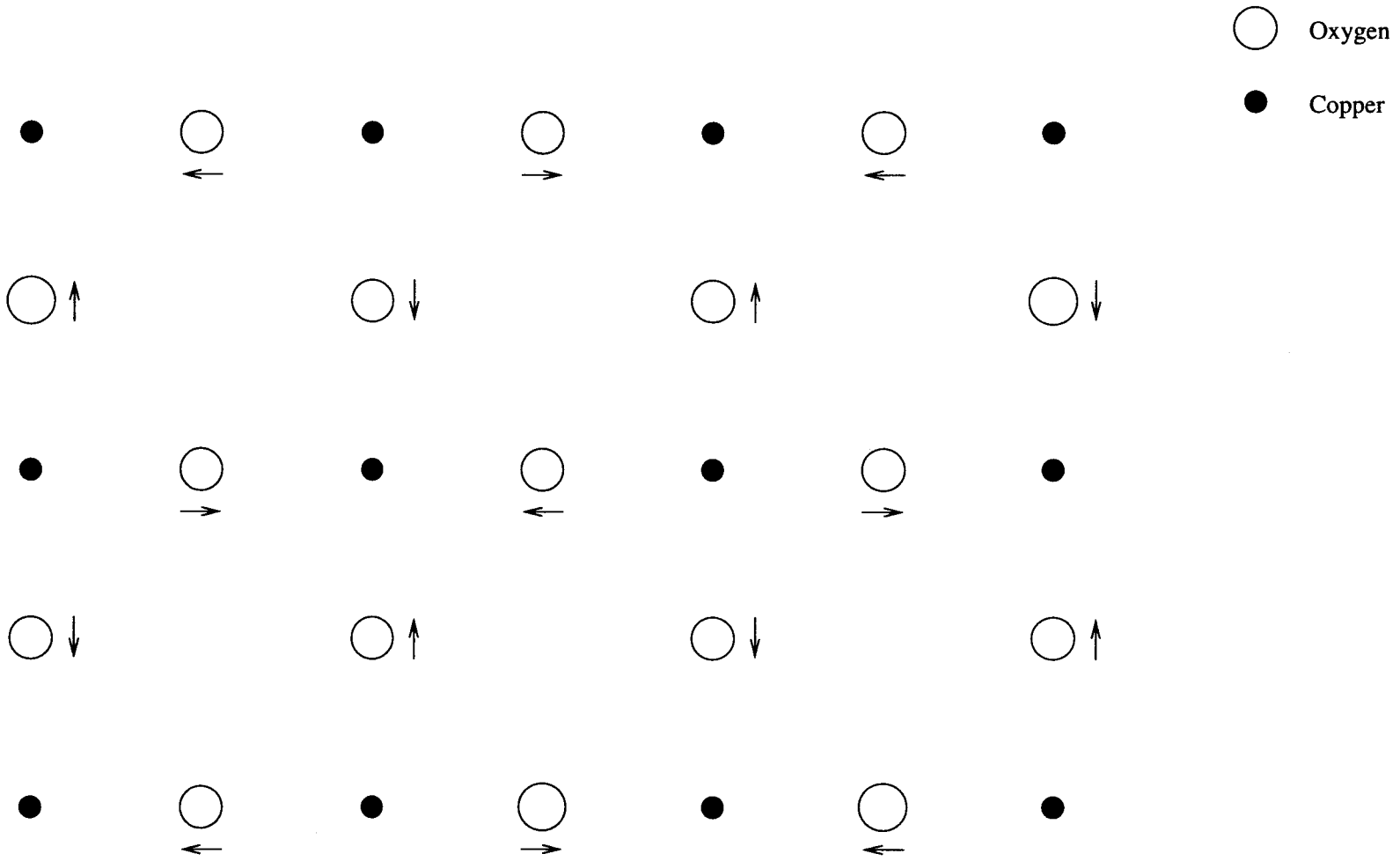
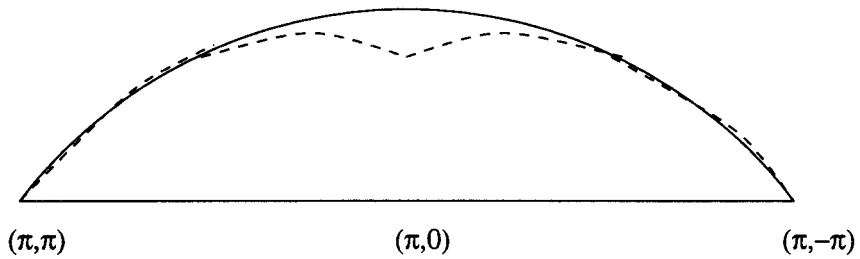


Fig. 2



Pseudogap

Superconducting gap