Investigations of the three band Hubbard model for the cuprates

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We study some aspects of the three-band Hubbard model for the cuprates. Our particular emphasis is on understanding the mapping from *ab-initio* to three band Hubbard model and the step after that i.e. the one band Hubbard model. We utilize ideas from a previous downfolding approach introduced by us. We also clarify some notations about hole vs electron creation operators.

I. MODEL HAMILTONIANS FOR THE CUPRATES

In HJC's notes from 2009, he gives a broad overview of the cuprates. One of the ideas discussed is the determination of the minimal model that describes the low energy theory of the cuprates. In order to do so, some simple (and probably intuitive) assumptions made by others, were also discussed.

Here is the summary of some points. To begin with, consider the case where the copper oxide plane is undoped. To write down a model effective Hamiltonian, we do not necessarily have to consider all the d electrons of Cu and all the p electrons of O. We can figure out which orbitals are important by analyzing the effect of the Cu-O interaction on their orbital energies. In $La_{2-x}Sr_xCuO_4$, each copper atom is surrounded by four in-plane and two apical oxygens. In YBCO, each copper is surrounded by five oxygens. The arrangement of the oxygens in the lattice is responsible for breaking the d orbital degeneracy of the isolated copper ion. It turns out that the highest filled orbital has $d_{x^2-y^2}$ character. (The choice of spatial coordinates used in the remainder of the paper is such that the copper oxide plane is taken to be the X-Y plane). It is sufficient to work with a reduced basis set - the d orbital of Cu and the p orbitals of O.

What happens to the additional hole when the compound is doped? It is clear from ab-initio calculations and physical considerations that the hole is lost from the oxygens rather than the coppers. This makes the downfolding to the t-J model tricky, but Zhang and Rice argued that it was possible. The justification is somewhat detailed and a brief overview of it has been presented in HJC's 2009 notes.

But let us begin with the three band model as mentioned by Zhang and Rice and also considered by Dopf, Muramatsu and Hanke in their QMC study. Though there are places where the jargon and notation is unclear, I believe most people do work in the hole representation directly. For mathematical convenience, the hole representation is apt and take the vacuum to be the state which comprises of Cu $3d^{10}$ and O $2p^6$ states. The orbitals and the unit cell is shown in Fig. I.

$$H = \sum_{ij,\sigma} t_{ij} d^\dagger_{i,\sigma} p_{j,\sigma} + \sum_{j,j'} \bar{t_{j,j'}} p^\dagger_{j,\sigma} p_{j',\sigma} + E_d \sum_i n_i + E_p \sum_j n_j + U_d \sum_i n_{i,\uparrow} n_{i,\downarrow} + U_p \sum_j n_{j,\uparrow} n_{j,\downarrow} + U_{pp} \sum_{\langle i,j \rangle} n^p_i n^p_j + U_{pd} \sum_{\langle i,j \rangle} n^p_i n^d_j \quad (1)$$

where

$$t_{ij} = -t_{Cu-O}(-1)^{\alpha_{ij}} \quad (2)$$

where $\alpha_{ij} = 1$ if $j = i + \frac{1}{2}\hat{x}$ or $j = i - \frac{1}{2}\hat{y}$ and $\alpha_{ij} = 2$ if $j = i - \frac{1}{2}\hat{x}$ or $j = i + \frac{1}{2}\hat{y}$.

The O-O hopping element is given by,

$$\bar{t_{jj'}} = -t_{O-O}(-1)^{\beta_{jj'}} \quad (3)$$

where $\beta_{jj'} = 1$ if $j' = j - \frac{1}{2}\hat{x} - \frac{1}{2}\hat{y}$ or $j' = j + \frac{1}{2}\hat{x} + \frac{1}{2}\hat{y}$ and $\beta_{jj'} = 2$ if $j' = j - \frac{1}{2}\hat{x} + \frac{1}{2}\hat{y}$ or $j' = j + \frac{1}{2}\hat{x} - \frac{1}{2}\hat{y}$.

A quantity whose value we are interested in is the "charge transfer energy" $\Delta = E_p - E_d$ which Weber, Giamarchi and Varma compared to $\Delta^0 = E^0_p - E^0_d$. They say

$$\Delta = \Delta^0 - E_{DC} \quad (4)$$

where $E_{DC} = U_d(n_d - 0.5)$ is a double counting correction and U_d is the Coulomb repulsion and n_d is the hole density on the Cu atom. They worked in the hole notation and estimated Δ^0 to be around 3-4 eV which they claim corresponds to $\Delta = 0 - 1$ eV in their calculations. Note that in the hole notation $E_p > E_d$

We will choose a set of parameters which may not be the correct ones. However, we will develop some downfolding ideas based on the experiments with this model. The reduction to one band (i.e. involving only the "effective" copper orbitals) was/is controversial and is the subject of some speculations presented next.

II. THREE TO ONE BAND - OPTIMIZING THE UNITARY

I used the above notations in my code and ask the question - what if we did not have the intuition of Zhang and Rice i.e. what if we did not know a "reasonable map" from the d-p orbitals to the "effective dressed" d-like orbitals that enter the

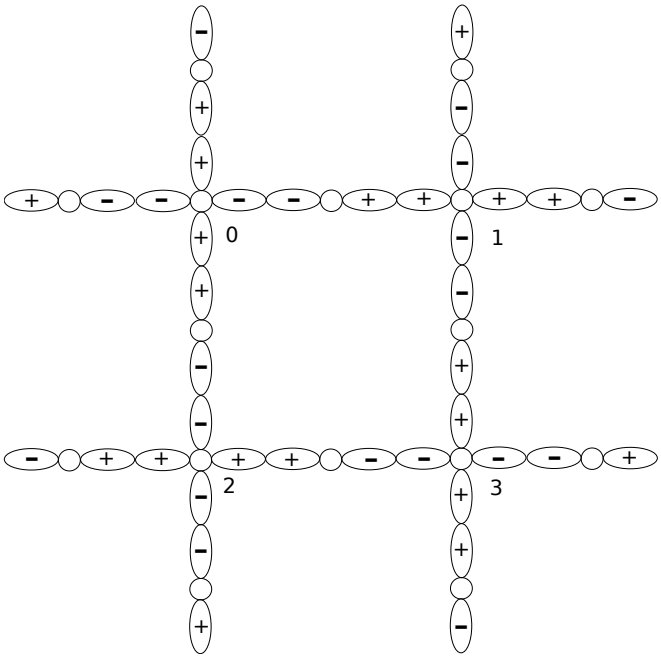

Figure 1. Orbitals involved in the three band model for the cooper-oxygen compounds.

one band model.

To do so, I encode this transformation as,

$$\tilde{c}_i^\dagger = \sum_{ij} U_{ij} c_j^\dagger \tag{5}$$

where $\tilde{c}_i$ is a transformed hole operator and c_j is the bare hole operator. Both c and its tilded version could refer to either d or p orbitals. So for a 2×2 unit cell, I have a 12×12 unitary matrix that I am trying to optimize. Of course, I am interested in only a subset of the rotated orbitals for the low energy physics. To be more explicit, I ask if it is possible to obtain a "effective" $\tilde{d}$ orbital that is a mixture of the bare d and bare p orbitals. The hope is that these set of rotated orbitals will give me a effective 1-band Hubbard-like model in terms of the $\tilde{d}$ alone.

I take the 3-band model provided by L. Wagner based on downfolding of QMC calculations. I begin with putting 1 hole per Cu i.e. I put in 4 holes for the 2x2 periodic cluster. This is the "undoped" case. As expected, my 1-body density matrix (a 12×12) matrix, calculated separately for the up and down electrons. Not being very intelligent about optimizing this unitary, I directly use the Nelder Mead method. In my cost function, working in the hole notation. I demand several things,

1. At half filling, the rotated d orbitals are exactly half filled i.e. their up occupation is 0.5

2. At half filling, the rotated p orbitals are completely unoccupied; their occupation is 0.

3. The reduced 4×4 matrix must respect symmetries of the underlying square lattice of coppers (only).

Actually, I am just demanding a block (or partial) diagonalization of the one-body matrix, so there should be an efficient way for doing this. However, let me cut to the chase and discuss what I do get from my method.

At half filling (i.e. 4 up holes and 4 down holes), I start off with the input (hole) 1-RDM as,

$$\rho_{in} = \begin{pmatrix}
+0.352 & -0.088 & -0.088 & -0.053 & +0.126 & +0.126 & -0.126 & -0.126 & -0.028 & +0.028 & -0.028 & +0.028 \\
-0.088 & +0.352 & -0.053 & -0.088 & -0.028 & -0.126 & +0.126 & +0.028 & +0.028 & -0.028 & +0.126 & -0.126 \\
-0.088 & -0.053 & +0.352 & -0.088 & -0.126 & -0.028 & +0.028 & +0.126 & +0.126 & -0.126 & +0.028 & -0.028 \\
-0.053 & -0.088 & -0.088 & +0.352 & +0.028 & +0.028 & -0.028 & -0.028 & -0.126 & +0.126 & -0.126 & +0.126 \\
+0.126 & -0.028 & -0.126 & +0.028 & +0.074 & +0.050 & -0.050 & -0.074 & -0.050 & +0.050 & -0.026 & +0.026 \\
+0.126 & -0.126 & -0.028 & +0.028 & +0.050 & +0.074 & -0.074 & -0.050 & -0.026 & +0.026 & -0.050 & +0.050 \\
-0.126 & +0.126 & +0.028 & -0.028 & -0.050 & -0.074 & +0.074 & +0.050 & +0.026 & -0.026 & +0.050 & -0.050 \\
-0.126 & +0.028 & +0.126 & -0.028 & -0.074 & -0.050 & +0.050 & +0.074 & +0.050 & -0.050 & +0.026 & -0.026 \\
-0.028 & +0.028 & +0.126 & -0.126 & -0.050 & -0.026 & +0.026 & +0.050 & +0.074 & -0.074 & +0.050 & -0.050 \\
+0.028 & -0.028 & -0.126 & +0.126 & +0.050 & +0.026 & -0.026 & -0.050 & -0.074 & +0.074 & -0.050 & +0.050 \\
-0.028 & +0.126 & +0.028 & -0.126 & -0.026 & -0.050 & +0.050 & +0.026 & +0.050 & -0.050 & +0.074 & -0.074 \\
+0.028 & -0.126 & -0.028 & +0.126 & +0.026 & +0.050 & -0.050 & -0.026 & -0.050 & +0.050 & -0.074 & +0.074
\end{pmatrix} \tag{6}$$

and finally get my unitary and output (hole) 1-RDM to be,

Parameter	Hybertsen (cLDA)	Hanke (Ref.)	Weber (Ref.)	L.K.Wagner (unpublished)
hole/electron notation	hole	hole	hole	electron
E_p -E_d	+3.6	+4.5	varied	+8.94
t_{pd}	+1.3	+1.5	+1.4	+1.77
t'_{pp}	+0.00	? (0.0)	-1.0 (opp sign)	+0.00
t_{pp}	+0.65	+0.75	varied	+0.00
U_d	+10.5	+12	+8	+14.40
U_p	+4.0	+5.25	+2	+ 0.00
U_{pd}	+1.2	0.75	+1.0	+ 0.00
U_{pp}	+0.0	0.0	0.0	+ 0.00

$$U = \begin{pmatrix} +0.883 & +0.104 & +0.035 & -0.025 & +0.236 & +0.205 & -0.227 & -0.237 & -0.037 & +0.008 & -0.028 & +0.008 \\ +0.034 & +0.883 & -0.013 & +0.093 & -0.020 & -0.251 & +0.242 & +0.005 & -0.008 & -0.019 & +0.195 & -0.224 \\ +0.100 & -0.015 & +0.883 & +0.031 & -0.220 & -0.013 & +0.003 & +0.215 & +0.227 & -0.249 & +0.005 & -0.024 \\ -0.014 & +0.032 & +0.097 & +0.883 & -0.001 & +0.012 & -0.013 & -0.017 & -0.233 & +0.193 & -0.250 & +0.235 \\ -0.238 & +0.016 & +0.242 & -0.008 & +0.936 & -0.016 & +0.002 & +0.065 & +0.030 & +0.019 & +0.041 & -0.020 \\ -0.227 & +0.263 & +0.027 & -0.022 & -0.053 & +0.935 & +0.035 & -0.005 & -0.002 & -0.018 & +0.017 & +0.004 \\ +0.232 & -0.240 & -0.014 & +0.023 & +0.067 & +0.093 & +0.935 & +0.009 & -0.028 & -0.011 & +0.013 & +0.009 \\ +0.211 & +0.025 & -0.222 & +0.018 & +0.048 & +0.061 & -0.070 & +0.944 & -0.055 & +0.015 & -0.008 & +0.017 \\ +0.035 & -0.003 & -0.216 & +0.241 & +0.038 & +0.027 & +0.006 & -0.014 & +0.940 & +0.087 & -0.035 & +0.006 \\ +0.017 & +0.032 & +0.233 & -0.221 & -0.082 & -0.005 & +0.031 & +0.048 & +0.027 & +0.941 & +0.006 & -0.004 \\ +0.030 & -0.191 & +0.002 & +0.243 & -0.027 & +0.052 & -0.079 & -0.009 & -0.034 & +0.059 & +0.943 & +0.026 \\ -0.004 & +0.206 & +0.006 & -0.206 & +0.007 & -0.073 & +0.057 & -0.003 & +0.059 & -0.057 & +0.083 & +0.945 \end{pmatrix} \quad (7)$$

$$\rho_{out} = \begin{pmatrix} +0.499 & -0.189 & -0.189 & -0.000 & -0.001 & +0.002 & +0.005 & -0.003 & +0.006 & -0.001 & +0.006 & -0.004 \\ -0.189 & +0.499 & -0.000 & -0.189 & +0.000 & +0.003 & -0.003 & +0.004 & -0.000 & +0.001 & +0.006 & +0.002 \\ -0.189 & -0.000 & +0.499 & -0.189 & -0.001 & +0.001 & -0.000 & -0.000 & -0.001 & -0.000 & -0.001 & +0.003 \\ -0.000 & -0.189 & -0.189 & +0.499 & +0.002 & -0.001 & -0.002 & +0.003 & +0.002 & +0.008 & -0.001 & -0.001 \\ -0.001 & +0.000 & -0.001 & +0.002 & +0.001 & +0.000 & -0.000 & +0.000 & -0.000 & +0.000 & +0.000 & -0.000 \\ +0.002 & +0.003 & +0.001 & -0.001 & +0.000 & +0.001 & +0.000 & +0.000 & +0.000 & -0.000 & +0.000 & +0.000 \\ +0.005 & -0.003 & -0.000 & -0.002 & -0.000 & +0.000 & +0.001 & -0.000 & -0.000 & +0.000 & +0.000 & -0.000 \\ -0.003 & +0.004 & -0.000 & +0.003 & +0.000 & +0.000 & -0.000 & +0.001 & +0.000 & +0.000 & -0.000 & +0.000 \\ +0.006 & -0.000 & -0.001 & +0.002 & -0.000 & +0.000 & -0.000 & +0.000 & +0.001 & +0.000 & +0.000 & -0.000 \\ -0.001 & +0.001 & -0.000 & +0.008 & +0.000 & -0.000 & +0.000 & +0.000 & +0.000 & +0.001 & +0.000 & +0.000 \\ +0.006 & +0.006 & -0.001 & -0.001 & +0.000 & +0.000 & +0.000 & -0.000 & +0.000 & +0.000 & +0.001 & +0.000 \\ -0.004 & +0.002 & +0.003 & -0.001 & -0.000 & +0.000 & -0.000 & +0.000 & -0.000 & +0.000 & +0.000 & +0.001 \end{pmatrix} \quad (8)$$

We can now ask which one band model best describes this 1-RDM. The only unique element is the nearest neighbor RDM element. We map this renormalized U/t as a function of U_{dd} of the three band model.

However, there is a possible inadequacy with the entire approach above. We have only considered the half-filled ground state in this entire analysis, whereas all our downfolding ideas are based on the same effective Hamiltonian also describing the low lying excited states.

I can now perform the same procedure when considering $3\uparrow$ and $3\downarrow$ holes and I get the unitary,

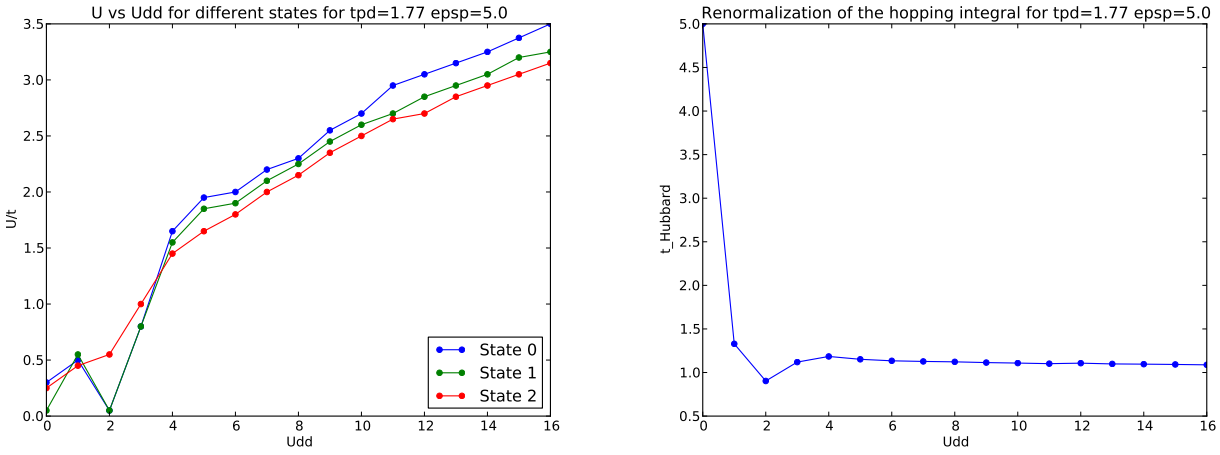

Figure 2. Renormalization of U/t and t as a function of U_{dd} with Lucas' 3-band parameters for the half filled case. These results do not agree with Hanke's study who found t_{pd} renormalized from a value of 1.5 eV to a value of $t = 0.4$ eV. However, to the best of my knowledge they did not renormalize the U/t either, its value was $U_{dd}/t_{pd} = 8$ and $U/t = 8$ in the 3- and 1-band models respectively.

$$U = \begin{pmatrix} +0.796 & +0.025 & +0.112 & +0.068 & +0.280 & +0.310 & -0.319 & -0.271 & +0.074 & -0.055 & +0.030 & -0.034 \\ +0.113 & +0.790 & +0.039 & +0.056 & +0.080 & -0.283 & +0.278 & -0.070 & -0.040 & +0.057 & +0.312 & -0.317 \\ +0.025 & +0.085 & +0.800 & +0.093 & -0.305 & +0.016 & -0.026 & +0.307 & +0.291 & -0.283 & -0.040 & +0.036 \\ +0.059 & +0.082 & +0.052 & +0.807 & -0.037 & -0.053 & +0.053 & +0.045 & -0.296 & +0.306 & -0.277 & +0.283 \\ -0.286 & -0.056 & +0.235 & +0.083 & +0.897 & +0.023 & +0.085 & +0.162 & +0.113 & -0.028 & -0.023 & +0.003 \\ -0.272 & +0.271 & -0.060 & +0.072 & -0.092 & +0.899 & +0.139 & -0.004 & -0.021 & +0.007 & +0.047 & -0.068 \\ +0.336 & -0.288 & +0.016 & -0.049 & -0.004 & +0.064 & +0.887 & -0.008 & +0.046 & -0.052 & -0.044 & +0.058 \\ +0.288 & +0.075 & -0.315 & -0.053 & +0.037 & +0.062 & -0.072 & +0.891 & -0.059 & +0.007 & +0.022 & -0.033 \\ -0.021 & +0.066 & -0.323 & +0.250 & -0.045 & -0.047 & +0.007 & -0.031 & +0.894 & +0.132 & -0.056 & +0.058 \\ +0.048 & -0.029 & +0.291 & -0.327 & -0.027 & +0.062 & -0.006 & +0.065 & +0.074 & +0.889 & -0.010 & -0.018 \\ -0.035 & -0.332 & +0.039 & +0.291 & -0.049 & +0.024 & -0.033 & +0.047 & -0.003 & +0.089 & +0.887 & +0.033 \\ +0.023 & +0.296 & -0.022 & -0.259 & +0.057 & -0.002 & +0.020 & -0.027 & +0.005 & -0.056 & +0.176 & +0.898 \end{pmatrix} \quad (9)$$

which is about 10-20 percent different from the unitary obtained in the half filled case.

Thus one proposal to optimize the unitary is to simultaneously try to "block diagonalize" several 1-RDM's i.e. RDM's of various excited states. This diagonalization must be preferably done for eigenstate so that we can impose more constraints on our cost conditions. But most importantly, the unitary transformation we have proposed above may not be a simple one-particle rotation.

In fact there are indications from the Zhang-Rice paper that this may NOT be true at all. This is because Zhang and Rice effectively considered a higher body tansformation. Recall that their singlet ψ_i^- involved a two body term. Their modified kinetic energy involved a three body term. Note this three body term comes in the t-J model as there are 2 number operators multiplying $d_i^\dagger d_j$ Thus the t-J model is actually not even a two body Hamiltonian.

Thus the more general idea out of this discussion is to look for a unitary acting on the many-body space of orbitals.

III. WHAT IS THE "LIKELY" PHYSICS FROM QMC PARAMETERS

I now discuss what the likely physics is expected to be if L.K.Wagner's QMC parameters are used for the phase diagram.

IV. ACKNOWLEDGEMENTS

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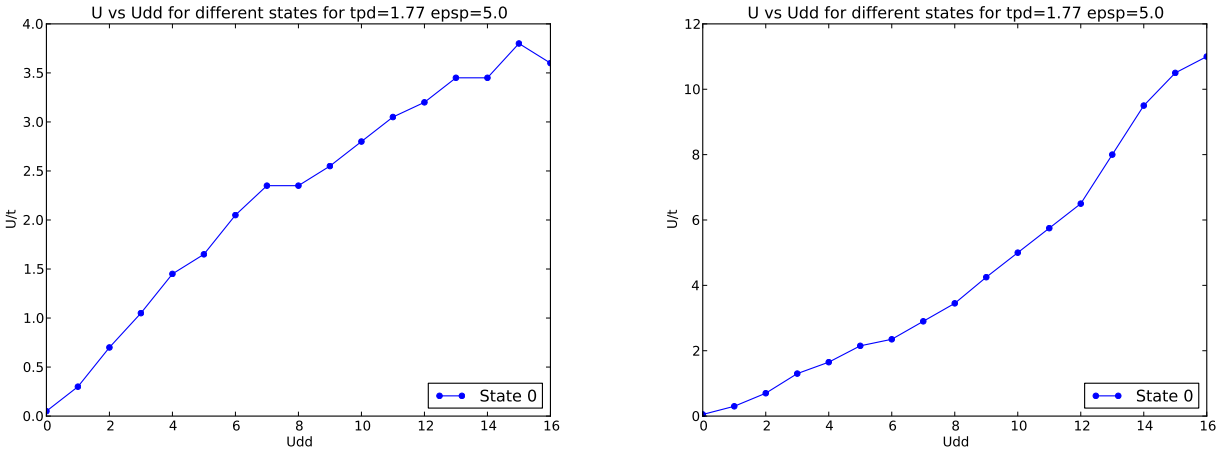

Figure 3. Renormalization of U/t and t as a function of U_{dd} with Lucas' 3-band parameters for (left) 1u,1d hole and (right) 3u, 3d holes. The holes see an effectively increased interaction when there are more of them.