Mott Transition and Strange Metal in Two Dimensions: A View from Cellular Dynamical Cluster Approximation

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We introduce a Cellular Dynamical Cluster Approximation (CDCA) to study the nature of the Mott insulator-metal transition in the extended Hubbard model on a square lattice. At strong coupling, a $d$-wave Mott insulator is obtained. Hole doping drives a first order Mott transition to a non-Fermi (nFL) liquid metal. Remarkably, this nFL is caused by an Anderson orthogonality catastrophe at low energies due to the non-trivial competition between strong, non-local interactions and hopping. This constitutes the first explicit realisation of Anderson’s Luttinger liquid idea in two dimensions. Many experimental responses in the “strange metal” phase found around optimal doping in cuprates are understood naturally within our approach.

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The problem of high-$T_c$ superconductivity (HTSC) in quasi-two-dimensional cuprates remains an outstanding problem of modern condensed matter physics. HTSC arises from a new, non-Fermi liquid (nFL) state, characterised by highly anomalous normal state response of the underdoped cuprates, continuing up to optimal doping, $x_{opt}$ (where the SC $T_c$ is maximum). Beyond $x_{opt}$, a low-$T$ Fermi liquid state seems to be recovered. (i) Superconductivity itself is unconventional, and of $d$-wave symmetry. Subsequently, it was also found that the normal state pseudogap (in the one-particle spectral function) possesses $d$-wave symmetry. Given the problems encountered in relating the PG phase to precursor pairing fluctuations above $T_c$, a new broken symmetry state, with $d$-density wave ($d$-DW) order, was proposed: the $d$-DW state was hypothesised to compete with $d$-SC, being favoured in the underdoped region above $T_c$. (ii) On the other hand, careful measurements reveal that the cuprates remain insulating (at very low $T$ if one suppresses $d$-SC by high magnetic fields) almost up to optimal doping. Given the amount of disorder involved, this insulator would be a Mott-Hubbard-Anderson insulator. If the Mott transition occurs around $x_{opt}$, a natural question would be to inquire about its relation to the undoped ($x=0$) state? (AF/SC long range order is precluded in 2D by the Mermin-Wagner theorem, but $d$-wave order is not). How does this evolve to a nFL metallic state upon hole doping?

An attempt to reconcile both (i) and (ii) above would require that the Mott transition is an insulator-metal (IM) transition from a $d$-wave insulator to a $d$-wave metal. This gives rise to the question: Is the quantum critical point (QCP) invoked to understand cuprates the one associated with such a $T=0$ Mott transition? (Recall that the $T-x$ phase diagram shows that AF-Neel order is destroyed well before $T_c(x)$ achieves its maximum around $x_{opt}$). If so, one would expect strongly divergent, $d$-wave charge/spin fluctuations around this transition (around $x_{opt}$) to naturally mediate high-$T_c$ SC of $d$-wave type. This would constitute a very new picture of the physical response of cuprates.

Additionally, strong dynamical spectral weight transfer (SWT), a ubiquitous feature of correlated systems, is exhibited clearly as the Mott insulator is doped (this occurs over a region of $O(4.0 \text{ eV})$, and can only be caused by electronic correlations). Theoretically, non-local effects giving rise to $d$-wave correlations can be accessed only by cluster-DMFT (see review in [3]). Such studies indeed find good qualitative agreement with the $T-x$ phase diagram for the cuprates. However, to our best knowledge, the compelling link between the unusual nFL responses, the $T=0$ Mott transition around $x_{opt}$, and the high-$T_c$ SC of $d$-wave type still remains to be described consistently.

Here, with this motivation, we study the Mott transition in a two-dimensional model (without chemical disorder) for cuprates. We construct a new cellular-dynamical mean field approximation (C-DMFA) and use it to study the doping-driven Mott transition from a $d$-wave Mott insulator to a $d$-wave non-FL metal. We consider the extended Hubbard model (EHM) in the strong coupling limit as an effective model for Cu-O layers in cuprates. The Hamiltonian is

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c}) + U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle i,j \rangle} n_i n_j - E_F \sum_{i\sigma} n_{i\sigma} ,$$  

(1)
where \( n_i = \sum_{\sigma} n_{i\sigma} \), and \( U >> V, t \), and \( E_F \) is the chemical potential.

Next, we formulate a new Dynamical Cluster Approximation, which we christen Cellular Dynamical Cluster Approximation (CDCA). Given indications from several experiments \([2, 3]\), our aim is to treat inter-site electronic correlations \( \text{exactly} \) on a single plaquette (2x2) and consider the inter-plaquette correlations (resulting from carrier hopping and n.n interactions) within the CDCA. This is done by mapping the original EHM to an electronic model describing coupled plaquettes, and is a multi-stage procedure as described below: (1) Consider the EHM on a single 2x2 square plaquette, \( C \). In the limit \( U \to \infty \), the EHM reads

\[
\begin{align*}
H &= -t \sum_{\sigma, i,j=1}^{4} (X_{i\sigma} X_{j\sigma} + h.c) + V \sum_{i,j=1}^{4} n_i n_j \\
&- E_F \sum_{\sigma, i=1}^{4} n_{i\sigma} ,
\end{align*}
\]

where the no-double occupancy constraint resulting from the \( U \to \infty \) limit is implied, and appears as a local constraint on \( H \). Using the Gutzwiller approximation \([3]\), this becomes an unconstrained fermion model, but with \( V = V(x), t = t(x) \). (2) Construct the four possible symmetry-adapted linear combinations of the site fermions to “plaquette-centered” fermions: \( a_{\mu\sigma} = U_{i\mu} c_{i\sigma} \) with \( i = [1, 2, 3, 4] \) for a 4-site square. Explicitly, \( a_{1\sigma} = \frac{1}{2}(c_1 + c_2 + c_3 + c_4) \), with \( a_{2\sigma} = \frac{1}{2}(c_1 - c_2 + c_3 - c_4) \), and \( a_{3\sigma} = \frac{1}{2}(c_1 + c_2 - c_3 + c_4) \), and finally, \( a_{4\sigma} = \frac{1}{2}(c_1 - c_2 - c_3 + c_4) \). Notice that \( a_1 \) transforms as an s-wave operator, \( a_2 \) as a d-wave operator, while \( a_3, a_4 \) transform like p-wave operators. The one plaquette Hamiltonian becomes (\( \mu \) centered on \( C \))

\[
H_C = -2t \sum_{\mu, \sigma} (n_{a1\mu\sigma} - n_{a2\mu\sigma}) + V \sum_{\mu, \alpha, \beta} n_{a\mu\alpha} n_{a\mu\beta} \\
- E_F \sum_{\mu, \sigma} n_{a\mu\sigma} ,
\]

where \( \alpha, \beta = [1, 2, 3, 4] \), and \( a_{\mu\alpha} = a_{\mu\alpha}^\dagger a_{\mu\alpha} \). Thus, for half-filling, \( t < 0 \), and \( U \to \infty \), the exact spectrum of the EHM on an isolated square consists of four singly occupied plaquette states, \( E_1 = -2t, E_{2,3} = 0, E_4 = 2t \), which we identify with the “lower Hubbard band” states, and the corresponding states raised upwards by \( V \), which we identify with the “upper Hubbard band” (charge transfer) states. In analogy with the usual Hubbard model, the UHB states correspond to high-energy states describing the dynamics of an electron hopping onto a given local “site” (plaquette) in a specified “orbital” when the other “orbitals” are already occupied. \( H_C \) in the plaquette basis is exactly similar to the local limit of a four-orbital Hubbard model with \( U \to \infty \), and a fictitious “crystal field” term which raises the d-wave state above the doubly degenerate \( p_{x,y} \) and extended-s states. (3) We now connect \( C \) to other plaquettes via the hopping, \( t \), and n.n coupling, \( V \), in the original EHM. To do this, we split the 2D lattice into plaquettes covering the whole lattice. The hopping and n.n coupling between neighboring sites on different neighboring plaquettes (in terms of original site fermions) are then expressed in terms of the plaquette fermions \( (a_{\mu\sigma}) \). In the 2D square geometry, \( V, t \) acting between n.n plaquettes means that sites (2, 3) on plaquette \( \mu \) are connected to sites (1, 4) on \( (\mu + 1) \) along \( x \), while (1, 2) on \( \mu \) are connected to (3, 4) on \( (\mu + 1) \) along \( y \). Namely, the Hamiltonian coupling the given plaquette \( \mu \) to the rest of the lattice is

\[
H'_\mu = -t \sum_{\mu \sigma} \left( c_{1\mu\sigma} c_{2,\mu + e_x,\sigma} + c_{4\mu\sigma} c_{3,\mu + e_x,\sigma} + h.c \right) \\
- t \sum_{\mu \sigma} \left( c_{1\mu\sigma} c_{4,\mu + e_y,\sigma} + c_{2\mu\sigma} c_{3,\mu + e_y,\sigma} + h.c \right) ,
\]

and

\[
H'_V = V \sum_{\mu} (n_{2,\mu} n_{1,\mu + e_x} + n_{3,\mu} n_{4,\mu + e_x}) \\
+ V \sum_{\mu} (n_{4,\mu} n_{1,\mu + e_y} + n_{2,\mu} n_{3,\mu + e_y}) .
\]
square lattice. Thus, we solve \( H = H_C + H' \) using the MO-DMFA.

In order to make progress, we use insights gained from detailed analyses of the general multi-orbital problem in usual DMFA \[9, 10\]. Here, multi-orbital models without the inter-orbital, intersite pairing terms were solved using IPT and QMC, both leading to qualitatively similar conclusions. The Mott insulator has ferro-orbital (in our case \( d \)-wave) order: this is a \( d \)-wave Mott insulator. Away from \( n = 1 \), the highest-lying (\( d \)-wave) band becomes metallic, while the lower-lying (here, one or more of \( s, p_x, p_y \)) bands remain Mott insulating. For our model, this would describe a first order Mott transition from a \( d \)-wave insulator to a \( d \)-wave metal for any \( x = (1-n) > 0 \) in absence of chemical (doping-induced) disorder. As we show below, this \( d \)-wave metal is not a Fermi liquid.

We solve our cluster (mapped 4-orbital) problem using multi-orbital iterated perturbation theory (MO-IPT). As discussed in recent \[11\] work, the MO-IPT turns out to be an accurate solver for multi-orbital problems at arbitrary fillings, \( n \leq 1 \). We refer the reader to relevant references \[3, 11\] for methodical details. We focus on the Mott-Hubbard I-M transition as a function of hole doping. The role of the \( d \)-wave p-h (PG) and SC orders are described in an accompanying work \[18\]. Here, we focus on the region of the \( T - x \) phase diagram for cuprates without \( d \)-wave PG/SC order; i.e, on the strange metal phase terminating at \( T = 0 \) at \( x_{opt} \).

We now describe our results. In Fig. 1 we show the “orbital” resolved and total one-particle spectral function for our model with \( V = 4.0 \text{ eV}, \omega W = 8t = 4.0 \text{ eV} \) for half-filling. First, it is clear that the occupied states closest to \( E_F(= 0) \) have \( d \)-wave symmetry (observe that \( d \otimes s' = d, p_x \otimes p_y = d \)). The Mott-Hubbard gap, \( \Delta_{MH} \approx 1.0 \text{ eV} \). Very interestingly, different “orbital” DOS have different Mott gaps: this is a benchmark feature of the (\( d \)-wave) ground state breaking the lattice point-group symmetry. In terms of original \( c \)-fermions, these features result directly from an explicit (and exact to \( O(1/D) \)) consideration of the competition between strong, intersite correlations and one-electron hopping in the strong coupling (\( U >> V, t \)) limit of the EHM. Together with the rich Hubbard band structures in Fig. 1 it describes the internal structure of the Mott-Hubbard gap (inaccessible in \( d = \infty \)). We predict that polarised optics, XAS, Raman measurements would show anisotropic spectral features reflecting those found in the DOS: this may already have been seen.

To extend our calculation to \( n < 1 \), the MO-DMFT equations need to be constrained by the Friedel-Luttinger sum rule, \( 4n = 4(1-x) = \int_{-\infty}^{E_F} \rho_{total}(\omega) d\omega \) for our cluster problem. \( E_F \) is then determined self-consistently within the MO-DMFT loop at each stage using \( \rho_{total}(\omega) \) computed in each iteration, and the process is iterated to convergence. The spectral functions for \( n < 1 \) are shown in Fig. 2. As expected generally, hole doping transfers dynamical spectral weight over large energy scales \( O(4.0 \text{ eV}) \) from the Hubbard bands into the Mott gap. The MIT is discontinuous, with the carrier density, \( (n) \), jumping discontinuously from zero to a finite value off half-filling (not shown), as generically expected within MO-IPT \[9\]. What is more interesting, and crucially important, is that this SWT is also strongly “orbital”

![FIG. 1](image1.png)  
**FIG. 1:** The “orbital resolved” and the total many-particle density of states (DOS) for the 2D EHM at half-filling, \( (n) = 1 \). Notice the appearance of “orbital” dependent Mott-Hubbard gaps, and the \( d \)-wave insulator, as explained in the text.

![FIG. 2](image2.png)  
**FIG. 2:** Same as in Fig.(1), but for hole doping, \( x = 0.1 \) (dashed lines) and \( x = 0.2 \) (solid lines). The “orbital selective” character of the Mott transition is explicitly seen, as is the fact that the ex-\( s \)-wave DOS remains Mott localised in the metallic phase.
dependent: clearly, our results show that the highest-lying \(d\)-wave DOS becomes the most metallic, the \(p_{x,y}\) DOS much less so, while the ex-\(s\)-wave DOS remains Mott insulating. In “orbital” language, this is an “orbital selective” Mott transition, discussed in detail in recent LDA+DMFT work on real oxides \([8, 9]\). In our CDCA applied to the 2D EHM, this feature directly follows from the strong, dynamical scattering between electronic channels with different “orbital” symmetries in a situation where these are split on the single cluster (reminiscent of crystal-field splitting in usual multi-orbital models \([9, 10]\)).

A very remarkable fact now emerges. Since the ex-\(s\)-DOS remains Mott insulating in the metal, strong scattering between the quasi-itinerant \(d\)-DOS and the localised ex-\(s\)-DOS results in an exact mapping of our problem to an effective Falicov-Kimball model \([8, 9]\), with resulting X-ray edge (XRE) behavior. The \(d\)-wave DOS then shows a power-law fall off at low energy in contrast to the smeared lorentzian of a FL metal: 
\[
\rho_d(\omega) \simeq |\omega|^{-(1-\alpha)}, \text{ with } \alpha = \tan^{-1}(V(x)/W(x)) \text{. Hence, so does the total DOS.}
\]

The corresponding self-energy is \(\Sigma(\omega) \simeq |\omega|^{-(1-\alpha)}\), with \(\alpha < 1\) for \(V > 0\) \([12]\). This implies no FL quasiparticle residue: \(Z_{FL} = 0\), and the metallic state is a non-Fermi liquid. Amazingly, this is exactly in agreement with Anderson’s proposal \([13]\) for the breakdown of FL theory in the 2D Hubbard model. It is indeed remarkable that a close numerical estimation of the DOS near \(E_F = 0\) gives \(\alpha \simeq 0.2, 0.1\) for \(x = 0.1, 0.2\). To our best knowledge, this is the first explicit demonstration of Anderson’s conjecture within C-DMFT schemes. Recall that XRE behavior was suggested in the past \([14]\) in multi-channel, single-impurity Anderson (and their \(D = \infty\) lattice counterparts) models.

Armed with this insight, several unusual features of optimally doped cuprates are understood naturally. The photoemission intensity, as measured in PES, measures the one-particle Green’s function in the sudden approximation: hence, \(I_{PES}(\omega) \simeq \omega^{-(1-\alpha)}\) as \(\omega \to E_F\), as observed \([15]\). The in-plane optical conductivity, \(\sigma_{xx}(\omega) \simeq \omega^{-(1-2\alpha)}\) from a direct scaling argument, and drops like \(\omega^{-0.6}(x = 0.1), \omega^{-0.8}(x = 0.2)\) very close to that measured experimentally \([15]\). Using an “extended Drude” fit \([15]\), we also obtain that the scattering rate, \(\gamma^{-1}(\omega) \simeq \omega^{(1-2\alpha)}\), as indeed observed. Further, the optical phase angle, \(\phi = \tan^{-1}(\sigma_2/\sigma_1) = (1 - 2\alpha)\pi/2\), is independent of \(\omega\), and increases with decreasing \(x\), as seen. Finally, the electronic Raman scattering intensity in the \(B_{1g}\) channel follows from the local limit of the Shastry-Shraiman relation (valid in our MO-DMFT) for intraband transitions \([10]\): 
\[
I_R^{B_{1g}}(\omega) = \omega \sigma_1(\omega) \simeq \omega^{2\alpha}, \text{ and is very weakly } \omega\text{-dependent, again as seemingly observed. Very interestingly, this non-FL behavior extends up to rather high energies } O(1.0 \text{ eV}), \text{ fully consistent with that used phenomenologically in optical analysis } [13]. \]

Following Anderson \([17]\), the tunnelling spectrum will also exhibit power-law anomalies, reflecting that of the DOS.

What is the dominant instability of this singular non-FL phase? Using the XRE mapping, it is clear that the “excitonic”correlation function, \(\chi_{12}^x(\omega) = \int_{-\infty}^{\infty} d\tau e^{i\omega \tau} \langle a_{1\sigma}^\dagger(\tau) a_{2\sigma}(0) \rangle \simeq |\omega|^{-(2\alpha - \omega^2)}\) is also singular. This implies soft \(d\)-wave \(p - h\) modes, and so the dominant instability will be to a \(d\)-wave \(ph\) pseudogapped state. Details will be presented elsewhere \([18]\).

In conclusion, we have formulated a new cluster-DMFT to treat the effects of intersite electronic correlations (exactly) on the Mott transition in the 2D EHM. The \(d\)-wave Mott-Hubbard insulator found for \(n = 1\) undergoes a first-order Mott-Hubbard transition to a \(d\)-wave, non-FL metal upon hole doping. Remarkably, in absence of the \(d\)-pseudogap, this nFL metal shows low energy singular behavior of the one-particle DOS/\(d\)-wave “excitonic” correlator, exactly as postulated by Anderson. Our results provide an appealing, microscopic explanation for a host of normal state anomalies characterising the “strange metal” phase of cuprates near optimal doping.

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