The 2D Hubbard Model: what do we know, what do we think we know, and what would we like to know

Coda: questions on criticality from STS experiments on pnictides

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Support: NSF-DMR-1308236
Something I learned from Gil:

Interesting Superconductivity

$\iff$

Quantum Criticality
This talk

Two examples providing perspective on this important idea

1. The two dimensional Hubbard Model

2. Stripe Ordering in the Pnictides
References and Collaborators

Emanuel Gull
U. Michigan


Rafael Fernandes
U. Minn.

Abhay Pasupathy
Columbia

- J. Leblanc..A. J. Millis..E. Gull, arxiv: 1505.02290
The Hubbard Model

\[ H = - \sum_{ij} t_{i-j} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

Parameters:
- Bandwidth 8t
- Interaction U
- carrier concentration n (x=1-n)
1988: P.W. Anderson said

The 2d square-lattice Hubbard model captures the essential features of the physics of the cuprates

2015: We have good reason to believe Anderson was correct.
We have reasonable confidence that

The 2d square-lattice Hubbard model has

- momentum space differentiation (anisotropic scattering)
- $d_{x^2-y^2}$ superconductivity in a superconducting dome with $T_c$ of the correct order of magnitude
- a pseudogap producing many of the features observed in the cuprates

In the Hubbard model the pseudogap and superconductivity are competing phenomena
?Why do we believe this?
Moderate interaction
(U=4\(t\); all dopings)

Theoretical control:
• methods agree for ground state
• \(T>0\)—lattice diagr. MC and extrapolated DMFT agree
Strong interaction (U=8t; n=1; T=0.5t)

Theoretical control:
• methods agree for k-dependence of self energy at lowest Matsubara freq.
Interesting case: moderate-strong interaction; general doping, low $T$

Getting to the point of demonstrated convergence, but not there yet. For dynamics, $T>0$: only DMFT
Dynamical Mean Field Theory (DMFT)

DMFT: approximation to electron self energy

\[ \Sigma(k, \omega) = \sum_{a=1 \ldots N} f_a(k) \Sigma^a(\omega) \]

The \( f_a(k) \) determine the ‘flavor’ of DMFT

The \( \Sigma^a(\omega) \) come from solution of auxiliary problem plus self-consistency condition

\( N \to \infty \) recovers exact solution
Momentum space version of DMFT

M. H. Hettler, M. Mukherjee, M. Jarrell, and H. R. Krishnamurthy PRB 61, 12739 (2000)

tile Brillouin zone: choose N momenta \( K_a \), draw an equal area patch around each one.
N->infinity: recover exact result

\[
\Sigma_p(\omega) \rightarrow \Sigma_p^{\text{approx}}(\omega) = \sum_a \phi_a(p) \Sigma_a(\omega)
\]

\( \phi_a(p) = 1 \) if p is in the patch containing \( K_a \) and is 0 otherwise

Find \( \Sigma_a \) from N-site quantum impurity model + self consistency condition
For interesting U, doping and T: not (yet) numerically exact

Variation among accessible clusters (4, 8, 16) =>
qualitative (~25%) accuracy

<table>
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<tr>
<th>Cluster size</th>
<th>$n^h_{\text{diff}}$</th>
<th>$n^e_{\text{diff}}$</th>
<th>$\Delta_g$</th>
<th>$n^h_{\text{SST}}$</th>
<th>$\Delta_{\text{SST}}$</th>
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<td>0.66</td>
<td>1.27</td>
<td>1.4</td>
<td></td>
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</tr>
<tr>
<td>4</td>
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<td>1.38</td>
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<tr>
<td>4*</td>
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<td>1.39</td>
<td>1.8</td>
<td>0.96</td>
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<td>1.23</td>
<td>1.1</td>
<td>0.93</td>
<td>1.9</td>
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<td>16</td>
<td>0.65</td>
<td>1.35</td>
<td>1.4</td>
<td>0.91</td>
<td>2.1</td>
</tr>
</tbody>
</table>

PRB82 155101

8 site: ```sweet spot```--momentum resolution to distinguish zone diagonal from corner but can get to low T for U not too small
Phase diagram: Mott insulator separated from fermi liquid by pseudogap for hole but not electron doping

$\Delta/\tau \sim 0.15 - 0.3$

$\beta t \sim 20$

$\Delta = -0.15t$


Phase diagram: Mott insulator separated from fermi liquid by pseudogap for hole but not electron doping

$t' = -0.15t$

Fermi-Liquid-like regime

Mott insulator

PG / Momentum Selective

Cuprates along this line

Fermi-Liquid-like regime

Line of Quantum phase transitions

Momentum selective phase: partially gapped fermi surface

gap opens around zone face

t' = -0.15t
Momentum selective phase: partially gapped fermi surface

$\mathbf{t}' = -0.15t$

but not along zone diagonal
Pseudogap: marked by appearance of pole in self energy ($N>4$)

As far as we can tell (have looked down to $T=T/80$ at half filling, $N=8$) transition to PG state is smooth (second order) for 8 and 16 site clusters. First order transition found in 4-site CDMFT is peculiar to that approach.
Order parameter: gap in (0, Pi) sector sharply defined only at T=0

T=0: sharp transition
T>0: crossover

Crossover

Sharp T=0 transition
Pseudogap associated with enhanced antiferromagnetic spin correlations

but no direct sign of magnetic quantum criticality
Pseudogap associated with enhanced antiferromagnetic spin correlations

These are equal-time impurity-model correlations. We are working on getting the real dynamical correlations (vertex corrections needed).
Spin correlations at other wavevectors not enhanced
No charge `nematicity’

NO enhancement of inter-patch density fluctuations is visible
However, sensitivity to breaking C4 symmetry

Transition can happen in one node before the other => large anisotropy

See Okamoto, Senechal, Civelli and Tremblay, arXiv:1008.5118
Pseudogap Summary

• Intrinsic property of 2D Hubbard model
• Not directly connected to Mott gap
• Within ‘DCA’ theory
  – Phase transition at T=0
  – Crossover at T>0
  – Associated with pole in self energy
  – Associated with spin correlation
  – No obvious charge nematic fluctuations; coupling to hopping anisotropy
Now: superconductivity
SC in DMFT

Pioneers: (2x2 cluster)

--Maier, Jarrell, Pruschke, Keller, PRL 85, 1524 (2000).

Lots of subsequent work (mainly 2x2 clusters):

Large clusters: Superconductivity established


High T susceptibility: clusters up to N=26 at x=0.1 U=4t (too small for Mott phase)

MJSKW result confirmed by lattice diagr MC
Our work: construct the sc state and determine some properties

Phase diagram, different clusters

$T=t/40$

$N=4$ a bit of an outlier. 8 and 16 differ at small $U$ but have similar doping dependence at larger $U$
Comparison to very recent result

Semiquantitative agreement

DMET (G. Chan, arxiv:1504.01784)
Transition temperature and gap

t~0.3eV => $T_c^{\text{max}} \approx 170\text{K}$
Transition temperature and gap

![Diagram showing transition temperature and gap](image)
Transition temperature and gap

Superconductivity cut off by pseudogap. Transition is first order
Some other physical properties
Raman scattering

Calculation

Data
Sacuto et al
Temperature dependence of kinetic energy

Pseudogapped regime

Fermi liquid regime

This trend in KE change is observed in optics: Santander-Syro, Lobo, Bontemps arXiv:0404.2901
Temperature dependence of kinetic energy

Pseudogapped regime

Fermi liquid regime

SC and PG are competing "phases". PG reduces kinetic energy: SC weaks PG, allows KE magnitude to rise
Superconductivity and the pseudogap

![Diagram showing the relationship between temperature, hole concentration, and superconducting phases.](image-url)
Evolution of photoemission Spectra

Fermi liquid regime

margins of pg regime

Transition regimes

Pseudogap regime
Two points:

SC gap
SMALLER than pseudogap

In SC+PG regime:
clear `peak-dip-hump’ structure
Standard interpretation of ”hump” shakeoff

Leading edge of ”hump” is interpreted as a threshold for creating an excitation.
Mathematically

\[ A(k, \omega) = \text{Im} \left[ G(k, \omega) \right] = \frac{\Sigma^{(2)}(\omega)}{(\omega - \varepsilon_k - \Sigma^{(1)}(\omega))^2 + (\Sigma^{(2)}(\omega))^2} \]

Two sources of peak in \( A \)

Shakeoff: onset of structure in imaginary part with real part non-zero (off resonance)

**THIS IS NOT WHAT HAPPENS IN THE HUBBARD MODEL**

Alternative: resonance—real part of \( G^{-1} \) vanishes
We find: ‘hump’ is a resonance coming from a zero crossing of the real part of the self

\[
\frac{\Sigma^{(2)}(\omega)}{(\omega - \varepsilon_k - \Sigma^{(1)}(\omega))^2 + (\Sigma^{(2)}(\omega))^2}
\]

‘hump’ when

\[
\omega - \text{Re}\Sigma(\omega) = 0
\]
Pairing mechanism

Distinguish normal (N) and anomalous (A) components of self energy. Split normal part into Matsubara-frequency odd and even parts

\[ \Sigma_{o,e}^{N} = \frac{\Sigma^{N}(k,\omega_{n}) \mp \Sigma^{N}(k,-\omega_{n})}{2} \]

Define gap function

\[ \Delta(i\omega_{n}) = \frac{\Sigma^{A}(i\omega_{n})}{1 - \frac{\Sigma_{o}^{N}(i\omega_{n})}{\omega_{n}}} = \int \frac{dx}{\pi} \frac{\Delta^{(2)}(x)}{i\omega_{n} - x} \]
In conventional superconductors

Lead

Imaginary part of gap function peaked at frequencies of pairing phonons

Scalapino, Schreiffer, Wilkins, PBR 148 263 1966
In the Hubbard model


All the pairing comes from low frequencies; most from very low frequencies
Particle-hole asymmetry: different from experiment

Implication: electron doped cuprates are different materials (more weakly correlated?)
What we would like to know

1. This is all (dynamical) mean field theory: other phases are found only if you look for them…is what we found preempted by another phase?

2. Stripes and other ordered states are (presently) beyond the reach of this approach. What is their importance?

3. What is the spin fluctuation spectrum?
Conclusions: Hubbard model
Conclusions: Hubbard model

What we know

- pseudogap
- $d_{x^2-y^2}$ SC
- $T_c^{\text{max}} \sim 180K$
- more than sign of charge carriers changes between e- and h-doped
Conclusions: Hubbard model

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What we think

- PG and SC are `intrinsic’
- charge, nematic, stripe fluct s are `along for ride’
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What we want to know

how do the results relate to antiferromagnetism

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Coda: SDW order and fluctuations in Iron Arsenide Superconductors.
With Abhay Pasupathy & Rafael Fernandes

(Caricature of) standard theory of quantum criticality: Generalized linear response

Key quantities:

\[ \chi(q, \omega) \]

Exponents \((\omega \text{ and } q \text{ dep.})\)

Amplitude of \(\chi\) not important
NaFeAs: `stripe' (0,\(\pi\)) order below 43K
`nematic' order below 54K

Park…Inosov PRB 86 024437

Y. Zhang,\(^1\) C. He,\(^1\) Z. R. Ye,\(^1\) J. Jiang,\(^1\) F. Chen,\(^1\) M. Xu,\(^1\) Q. Q. Ge,\(^1\) B. P. Xi,\(^1\) J. Wei,\(^2\) M. Aeschlimann,\(^2\) X. Y. Cui,\(^3\) M. Shi,\(^3\) J. P. Hu,\(^4\) and D. L. Feng\(^1,\) *
SDW rearranges the Fermi surface

Data:

Calculation:

\[ M \text{ Yi}^{1,2}, \ D \text{ H Lu}^3, \ R \ G \text{ Moore}^1, \ K \text{ Kihou}^{4,5}, \ C \text{-H Lee}^{4,5}, \ A \text{ Iyo}^{4,5}, \ H \text{ Eisaki}^{4,5}, \ T \text{ Yoshida}^{5,6}, \ A \text{ Fujimori}^{5,6}, \ Z \text{-X Shen}^{1,2} \]
Quasiparticle Interference Reveals the Reconstruction

E. P. Rosenthal\textsuperscript{1}, E. F. Andrade\textsuperscript{1}, C. J. Arguello\textsuperscript{1}, R. M. Fernandes\textsuperscript{2}, L. Y. Xing\textsuperscript{3}, X. C. Wang\textsuperscript{3}, C. Q. Jin\textsuperscript{3}, A. J. Millis\textsuperscript{1} and A. N. Pasupathy\textsuperscript{1*}

N. Phys. 10 225 (2014)
Structure in QPI reveals fermi surface
As you raise the temperature, expect the SDW-derived features to go away

\[ T < T_N \sim 43K \]  
\[ T_N < T < T_{\text{nematic}} \]  
\[ T_{\text{nematic}} < T \]

Here I show you joint DOS for simplicity. Full QPI calculations give the same physics.
This is not what happens
More easily visualized as a line cut

Key Result: SDW-like features persist to high $T$, in fact up to $T=2T_N$
Model

‘Lee-Rice-Anderson’ ansatz

\[ \Sigma(\omega, k) = \frac{\Delta^2}{\omega - \varepsilon_{k+Q} - \frac{i}{\xi}} \]

This is broadened backscattering (no `coherence factors in normal state)
The short ranged SDW calculations use the standard QPI formula but with the Lee-Rice-Anderson G in a simplified 3-band approximation to the pnictide bands.
Vary correlation length

\[ \Sigma(\omega, k) = \frac{\Delta^2}{\omega - \varepsilon_{k+Q} - \frac{i}{\xi}} \]

To get peaks in line cuts need to keep Delta at approximately the T=0 value., have correlation length not too short.
In other words

Data imply large amplitude, slow fluctuations of density wave order, persisting up to ~2x observed transition temperature

Paramagnetic phase has hidden structure
Poetically
Poetically
We used to think of the fermi sea as a (relatively) placid lake with modest ripples (RPA fluctuations).
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Which picture is correct. If large amplitude density wave fluctuations are present, how do we surf on them
Happy Birthday Gil!!

With happy memories of stimulating scientific discussions and looking forward to many more of the same!