Antiferromagnetic Quantum Critical Behavior and Pseudogap in Electron-Doped Cuprates

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Quantum Criticality in Correlated Materials and Model Systems”, Natal, Brazil, July 21 to August 01, 2014
e-doped cuprates, an example of AFM QCP with superconducting dome
The model
Simplest microscopic model for $CuO$ planes.

$$H = - \sum_{<ij>\sigma} t_{i,j} \left( c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right) + U \sum_i n_i \uparrow n_i \downarrow$$

No mean-field factorization for d-wave superconductivity
Some agreement between experiment and theory
Electron doped: Neutron scattering

Motoyama et al.  

\[ \zeta^* = 2.6(2) \zeta_{th} \]

Vilk, A.-M.S.T *EPL* (1996)  
*J. Physique* (1997)  

Semi-quantitative agreement for both ARPES and neutron
AFM correlation length (neutron)

Hankevych, Kyung, A.-M.S.T., PRL, sept. 2004

t' = 0.175t ; t'' = 0.05t, U=5.75
15% doped case: EDCs in two directions

Exp

TPSC

Armitage et al. PRL 2001

\[ \Delta_{pg} \approx 10k_B T^* \] comparable with optical measurements

$\xi(T)$ at the QCP

$z = 1$
Motoyama, Nature 2007

NCCO
Matsui et al. PRB 2007

$U=6, t'=-0.175, t''=0.05, n=1.2007$

D. Bergeron, D. Chowdhury, M. Punk, S. Sachdev, and A.-M.S. T
Linear resistivity

Fournier et al. PRL 1998
At the QCP for finite $t'$

$U = 6t$, $t' = -0.175t$, $t'' = 0.05t$

D. Bergeron et al.

\[ \rho(T) = AT + BT^2 \]
Linearity for $n > n_c$ and $T_c$

Fitting $\rho(T) = A \ U = 6t, \ t' = -0.175t, \ t'' = 0.05t$

Cooper et al. Science 323 30 (2009)

Outline

• e-doped are in weak to intermediate correlation range
• Methodology and benchmarks
• Pseudogap: Vilk criterion $\xi_{\text{AFM}} > \xi_{\text{th}}$
• Critical point: $z=1$
• Superconductivity
e-doped are in the weak to intermediate range of correlations
e-doped less strongly correlated than h-doped

D. Sénéchal, AMST, PRL 92, 126401 (2004)

- Optical gap 1.3 eV vs 2.0 eV
- Compressibility is larger
e-doped less strongly correlated than h-doped

- Pressure dependence of $T_c$

\[ J = \frac{4t^2}{U} \]
e-doped less strongly correlated than h-doped

Hubbard repulsion $U$ has to…

be not too large

increase for smaller doping

Hankevych, Kyung, A.-M.S.T., PRL, sept. 2004

B. Kyung et al., PRB 68, 174502 (2003)
e-doped less strongly correlated than h-doped

\[ \sigma = \frac{ne^2\tau}{m} \]

\[ n = \frac{k_F^2}{2\pi d} \]

\[ \ell = v_F\tau \]

\[ k_F\ell = 1 \]

\[ \sigma_{MIR} = \frac{1}{d} \frac{e^2}{h} \]
Electron-doped and MIR limit

NCCO

Dominic Bergeron et al. TPSC PRB 84, 085128 (2011)

Onose et al. 2004
Theoretical difficulties

• Low dimension
  – (quantum and thermal fluctuations)

• Large residual interactions
  – (Potential ~ Kinetic)
  – Expansion parameter?
  – Particle-wave?

• By now we should be as quantitative as possible!
Methodology

Weak to intermediate correlations
Theory difficult even for weak to intermediate correlations!

- **RPA (OK with conservation laws)**
  - Mermin-Wagner
  - Pauli

- **Moryia (Conjugate variables HS)**
  - $\phi^4 = \langle \phi^2 \rangle \phi^2$
  - Adjustable parameters: $c$ and $U_{\text{eff}}$
  - Pauli

- **FLEX**
  - No pseudogap
  - Pauli
Weak correlation methods

- Functional renormalization group
  
  \[
  (a) \frac{\partial}{\partial t} \begin{array}{c}
  \text{Diagram 1}
  
  + \frac{\partial}{\partial t} \begin{array}{c}
  \text{Diagram 2}
  
  + \cdots
  
  \end{array}
  
  \end{array}
  
  
  C. Honerkamp, et al. PRB 63, 035109 (2001)
  
  Rohe and Metzner (2004)
  
  
  
  C. Bourbonnais Sedeki PRB 2012
  
  (b) \frac{\partial}{\partial t} \begin{array}{c}
  \Sigma
  
  = \frac{\partial}{\partial t} \begin{array}{c}
  \text{Diagram 3}
  
  + \cdots
  
  \end{array}
  
  \end{array}
  
  \]

- Other weak coupling methods
  
  
Two-Particle Self-Consistent
TPSC
Theory without small parameter: How should we proceed?

- Identify important physical principles and laws to constrain non-perturbative approximation schemes
  - From weak coupling (kinetic)
  - From strong coupling (potential)
- Benchmark against “exact” (numerical) results.
- Check that weak and strong correlation approaches agree in intermediate range.
- Compare with experiment
TPSC: general ideas

• General philosophy
  – Drop diagrams
  – Impose constraints and sum rules
    • Conservation laws
    • Pauli principle (\( <n_\sigma^2> = <n_\sigma> \))
    • Local moment and local density sum-rules

• Get for free:
  • Mermin-Wagner theorem
  • Kanamori-Brückner screening
  • Consistency between one- and two-particle \( \Sigma G = U<n_\sigma n_{-\sigma}> \)

Vilk, AMT J. Phys. I France, 7, 1309 (1997);
*Theoretical methods for strongly correlated electrons* also (Mahan, 3rd)
Benchmark TPSC with Quantum Monte Carlo
\[ n=1 \]

\[ \xi \sim \exp(C(T)/T) \]

**Calc.:** Vilk et al. P.R. B **49**, 13267 (1994)


QMC + cal.: Vilk et al. P.R. B 49, 13267 (1994)

Notes:
- F.L. parameters
- Self also Fermi-liquid

\[ (0,0) \quad (\pi,0) \quad (\pi,\pi) \]

\[ (0,0) \quad (\pi,\pi) \]

\[ U > 0 \]
\[ \beta = 5 \]
\[ 8 \times 8 \]
TPSC for spin fluctuations

\[ \chi_{sp}^{(1)}(q) = \frac{\chi_0(q)}{1 - \frac{1}{2} U_{sp} \chi_0(q)} \]

\[ \langle (n_\uparrow - n_\downarrow)^2 \rangle = \langle n_\uparrow \rangle + \langle n_\downarrow \rangle - 2 \langle n_\uparrow n_\downarrow \rangle \]

\[ \frac{T}{N} \sum_q \chi_{sp}^{(1)}(q) = n - 2 \langle n_\uparrow n_\downarrow \rangle \]

\[ U_{sp} = U \frac{\langle n_\uparrow n_\downarrow \rangle}{\langle n_\uparrow \rangle \langle n_\downarrow \rangle} \]

Kanamori-Brückner screening
Proofs...


$U = 4$
$\beta = 5$
$n = 1$
Self-energy in TPSC

\[
\chi_{sp}(q) = \frac{\chi_0(q)}{1 - \frac{1}{2}U_{sp}\chi_0(q)}
\]

\[
\left\langle (n_\uparrow - n_\downarrow)^2 \right\rangle = \left\langle n_\uparrow \right\rangle + \left\langle n_\downarrow \right\rangle - 2\left\langle n_\uparrow n_\downarrow \right\rangle = \frac{T}{N} \sum_q \chi_{sp}^{(1)}(q) = n - 2\left\langle n_\uparrow n_\downarrow \right\rangle
\]

\[
U_{sp} = U \frac{\left\langle n_\uparrow n_\downarrow \right\rangle}{\left\langle n_\uparrow \right\rangle \left\langle n_\downarrow \right\rangle}
\]

Kanamori-Brückner screening

\[
\Sigma^{(2)}(k) = U n_\sigma + \frac{U T}{8N} \sum_q \left[ 3U_{sp}\chi_{sp}^{(1)}(q) + U_{ch}\chi_{ch}^{(1)}(q) \right] G_\sigma^{(1)}(k + q)
\]

Does not assume Migdal. Vertex at same level of approximation as G

Internal accuracy check

\[
\frac{1}{2} \text{Tr} \left( \Sigma^{(2)} G^{(1)} \right) = U \left\langle n_\uparrow n_\downarrow \right\rangle = \frac{1}{2} \text{Tr} \left( \Sigma^{(2)} G^{(2)} \right)
\]
A better approximation for single-particle properties (Ruckenstein)

\[ 1 - \sum \frac{1}{2} = - \frac{1}{3} + \frac{1}{3} \]

Y.M. Vilk and A.-M.S. Tremblay, Europhys. Lett. 33, 159 (1996);

N.B.: No Migdal theorem
Pseudogap: $\xi_{AFM} > \xi_{th}$ (Vilk criterion)
Precursor of SDW state
(dynamic symmetry breaking)

- Hankevych, Kyung, A.-M.S.T., PRL, sept 2004
Vilk criterion:  
effect of critical fluctuations on particles (RC regime) 

\[ \Sigma(k_F, i\xi_n) \propto T \int d^d q \frac{1}{q_{\perp}^2 + q_{\parallel}^2 + \xi^{-2}} \frac{1}{ik_n + \varepsilon_{-k+q}} \]

\[ \text{Im} \Sigma^R(k_F,0) \propto -\frac{T}{\nu_F} \xi^{3-d} \]

in 2D:  \[ \xi > \xi_{th} \quad (\xi_{th} \equiv \hbar \nu_F / \pi \ k_B T) \]

\[ \Delta \varepsilon \approx \nabla \varepsilon_k \cdot \Delta k \approx \nu_F \hbar \Delta k = k_B T \]

in 3D: Marginal

in 4D: quasiparticle survives up to \( T_c \)

Y.M. Vilk and A.-M.S. Tremblay, Europhys. Lett. 33, 159 (1996);
Hot spots from AFM quasi-static scattering
Exponent at the critical point


D. Bergeron, D. Chowdhury, M. Punk, S. Sachdev, and A.-M.S. T
Touching condition

D. Bergeron, D. Chowdhury, M. Punk, S. Sachdev, and A.-M.S. T
Origin of the change of power law
$d$-wave superconductivity
\[ \Delta_p = -\frac{1}{2V} \sum_{p'} U(p - p') \frac{\Delta_{p'}}{E_{p'}} \left( 1 - 2n\left(E_{p'}\right) \right) \]

Exchange of spin waves?
Kohn-Luttinger

\[ T_c \text{ with pressure} \]

Béal–Monod, Bourbonnais, Emery
P.R. B. 34, 7716 (1986).
D. J. Scalapino, E. Loh, Jr., and J. E. Hirsch
P.R. B 34, 8190-8192 (1986).
Kohn, Luttinger, P.R.L. 15, 524 (1965).

Kyung, Landry AMST
PRB 68, 174502 (2003)

QMC: symbols.
Solid lines analytical.

Kyung, Landry, A.-M.S.T.
$T_c$ from TPSC

$t' = 0$


S. Roy, PhD thesis 2007
Vilk et al. J. Physique (1997)
T. Maier, M. Jarrell, T. Schulthess, P. Kent, and J. White, PRL 95, 237001 2005

$T_c = 0.023$
More on superconductivity: $n=1$
Relation between symmetry and wave vector of AFM fluctuations

Hassan et al. PRB 2008
$T_c$ depends on $t'$

FIG. 5. (Color online) The $d_{x^2-y^2}$ superconducting critical temperature $T_c$ as a function of $t'$ at $U=2.5, 3,$ and $4$ for $n=1$. The inset shows the $d_{xy}$ superconducting critical temperature $T_c$ as a function of $t'$ for $U=3.6$ and $4$.

Hassan et al. PRB 2008
$T_c$ in RC regime or not

$\xi_{AFM} \sim 10$ at optimal $T_c$

$\xi_{th} > \xi_{AFM}$

Hassan et al. PRB 2008
Conditions for $d$-wave superconductivity

Hassan, Davoudi, AMST PRB 77, 094501 2008

- Symmetry related to that of commensurate spin fluctuations
- $T_c$ increases with $U$
- DOS does not play dominant role
- Optimal frustration
  - In underfrustrated $T_c < T_X$
  - In overfrustrated $T_c > T_X$
  - In all cases $\xi > a$
Stifening AFM and new mode

Figure 2

arXiv:1308.4740 [pdf]
Charge ordering in the electron-doped superconductor $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$

Eduardo H. da Silva Neto, 1,2,3,4,* Riccardo Comin, 1,* Feizhou He, 5 Ronny Sutarto, 5 Yeping Jiang, 6 Richard L. Greene, 6,4 George A. Sawatzky, 1,2,4 and Andrea Damascelli 1,2,4,†

Motoyama et al.
Increased nesting away from $n = 1$

TPSC: First step

- Consistency between one- and two-particle quantities:
  \[
  \Sigma_\sigma(1, \bar{1}) G_\sigma(\bar{1}, 2) = -U \langle T_\tau n_{-\sigma}(1)c_\sigma(1)c_\sigma^+(2) \rangle,
  \]
  \(l = (r_1, \tau_1)\).

- TPSC ansatz:
  \[
  \Sigma_\sigma(1, \bar{1}) G_\sigma(\bar{1}, 2) \approx U_{sp} G_{-\sigma}(1, 1^+) G_\sigma(1, 2), \quad \text{with} \quad U_{sp} = U \frac{\langle n_\uparrow(1)n_\downarrow(1) \rangle}{\langle n_\uparrow(1) \rangle \langle n_\downarrow(1) \rangle}.
  \]

- \(\Rightarrow\) Spin irreducible vertex:
  \[
  \Gamma_{sp}(1, 2; 3, 4) = \left. \frac{\delta \Sigma_\uparrow(1, 2)}{\delta G_\uparrow(3, 4)} - \frac{\delta \Sigma_\uparrow(1, 2)}{\delta G_\downarrow(3, 4)} \right| = U_{sp} \delta(1 - 3) \delta(1^+ - 4) \delta(1^- - 2)
  \]

- We also use a local charge irreducible vertex:
  \[
  \Gamma_{ch}(1, 2; 3, 4) = \left. \frac{\delta \Sigma_\uparrow(1, 2)}{\delta G_\uparrow(3, 4)} + \frac{\delta \Sigma_\uparrow(1, 2)}{\delta G_\downarrow(3, 4)} \right| \approx U_{ch} \delta(1 - 3) \delta(1^+ - 4) \delta(1^- - 2)
  \]
Hole-doped: Link to Mott transition up to optimal doping

Doping dependence of critical point as a function of $U$

Sordi et al. PRL 2010, PRB 2011
Conclusion

• e-doped better understood with one-band Hubbard than h-doped (less strongly correlated)

• Mechanism for pseudogap is different on h-doped side (Related to Mott physics) (Vilk criterion not satisfied)

• Certain anomalies explainable by charge order? Or interference between channels?
Collaborators

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