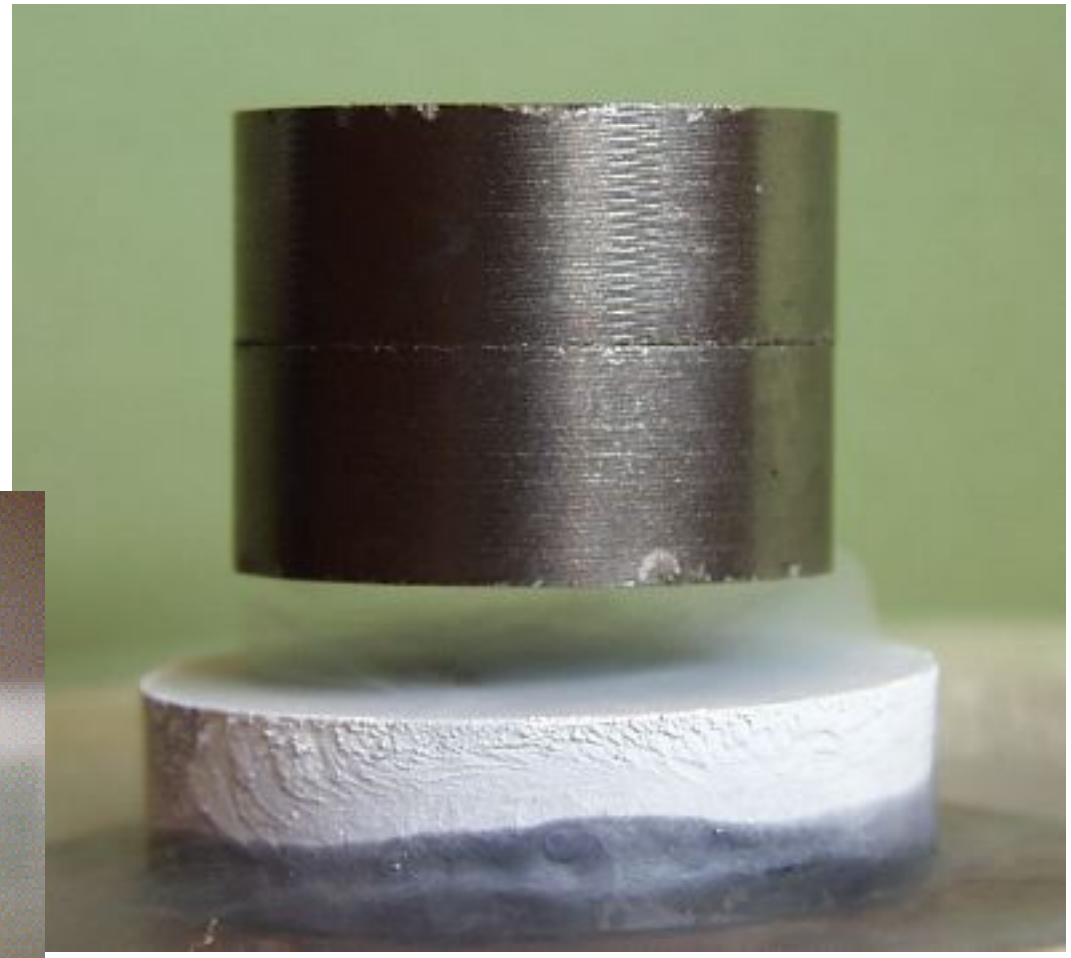
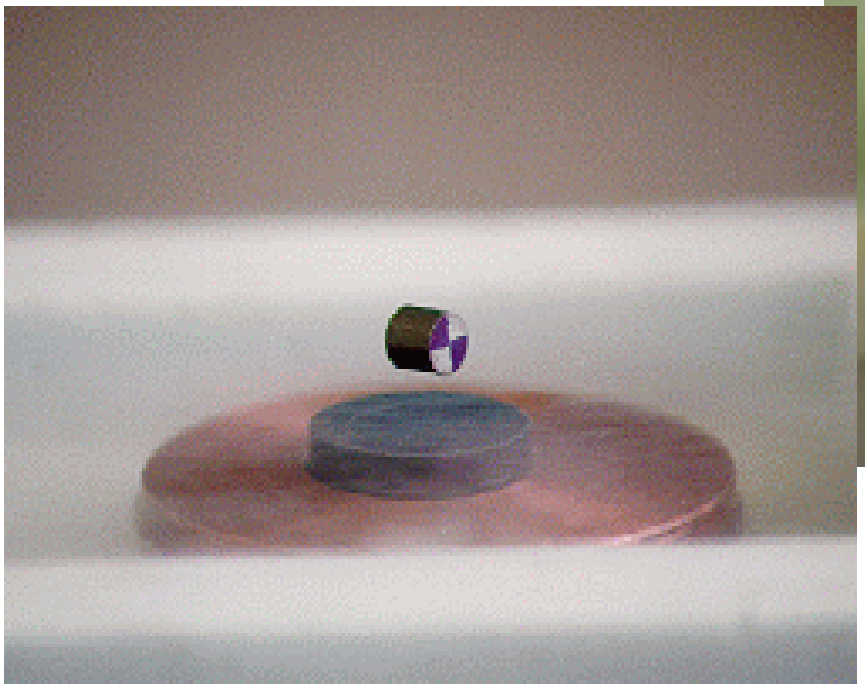
U1.00003 : Anomalous superconductivity near the Mott transition

Perfect diamagnetism (Shielding of magnetic field)

(Meissner effect)





André-Marie Tremblay

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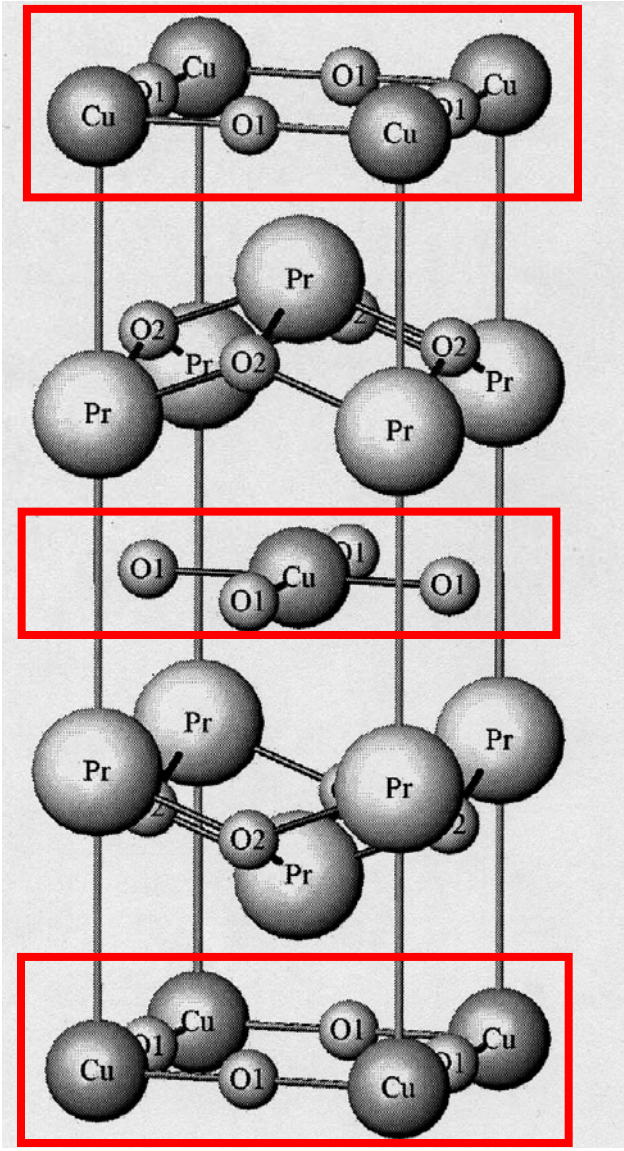
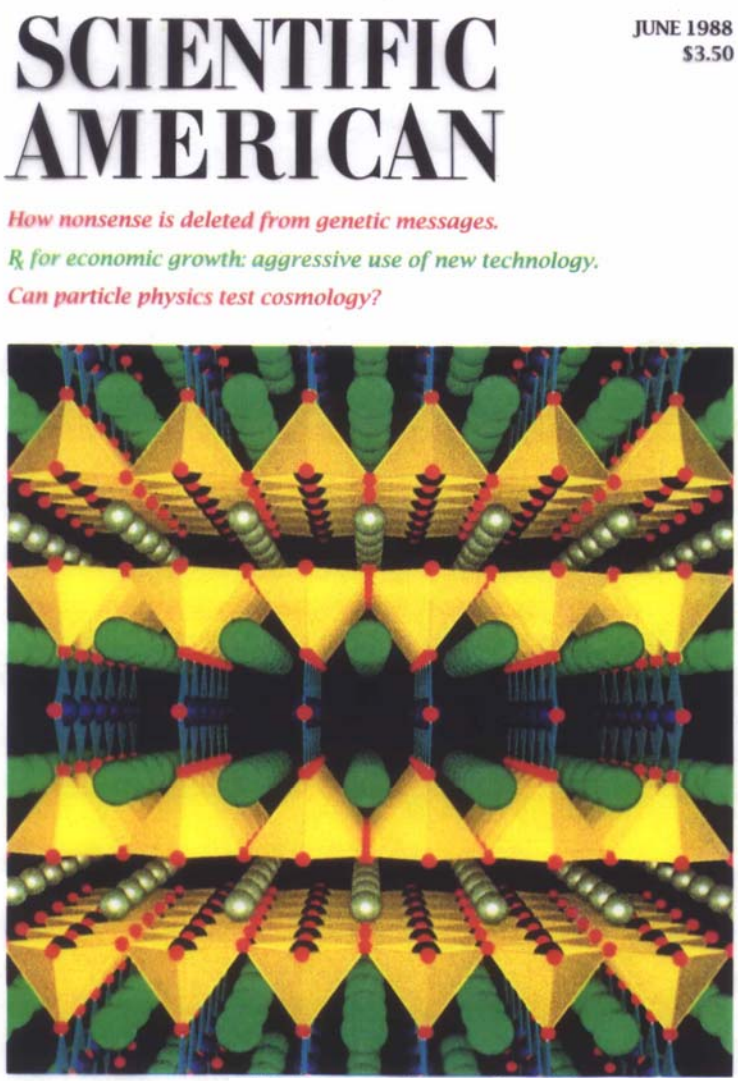
CuO_2 planes





$YBa_2Cu_3O_{7-\delta}$

Experimental phase diagram

Electron doping ← → Hole doping

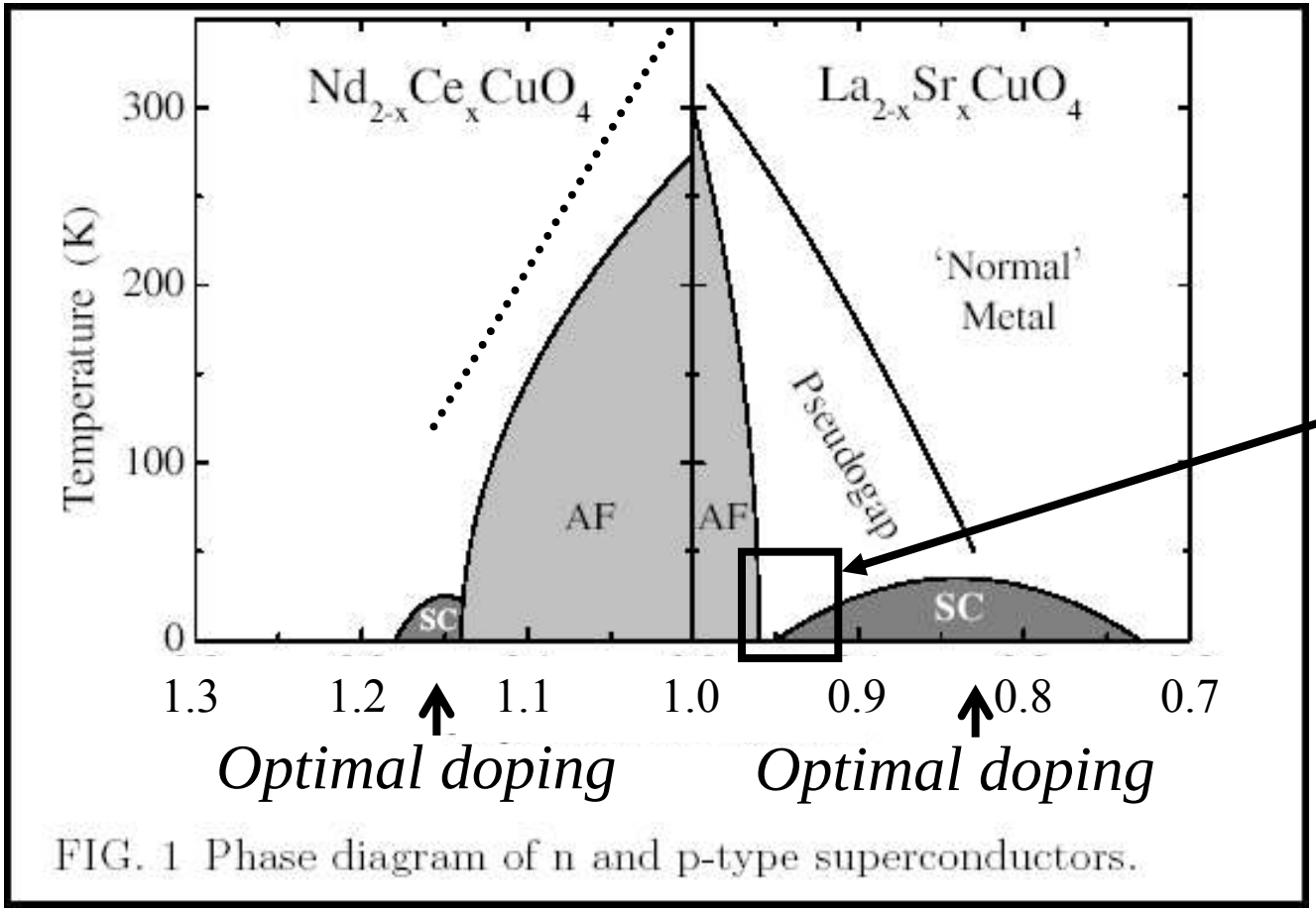


FIG. 1 Phase diagram of n and p-type superconductors.

Stripes

← *n*, electron density

Damascelli, Shen, Hussain, RMP 75, 473 (2003)

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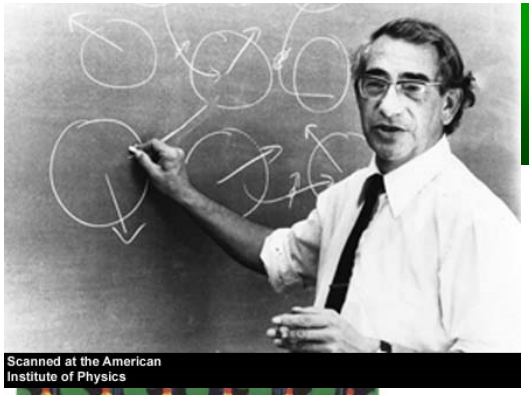
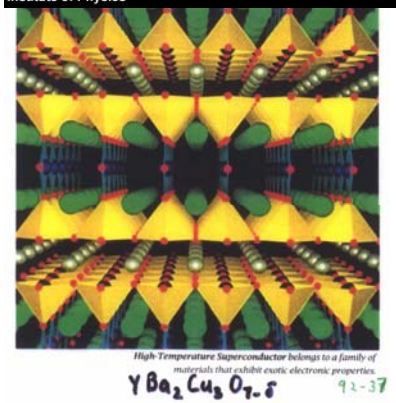
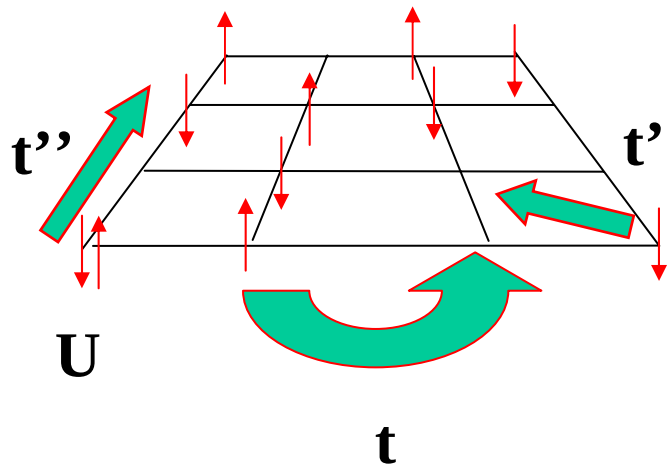
The Hubbard model

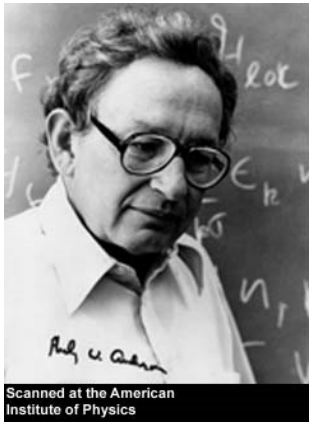


Simplest microscopic model for *Cu* O_2 planes.

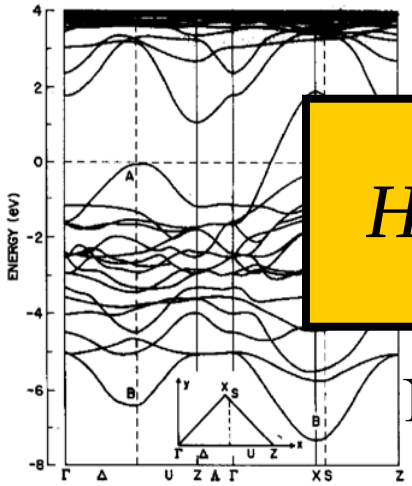




μ



LSCO



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

No mean-field factorization for d-wave superconductivity

Mounting evidence for d-wave in Hubbard

- **Weak coupling (U << W)**
  - AF spin fluctuations mediated pairing with d-wave symmetry
    - (Bickers et al., PRL 1989; Monthoux et al., PRL 1991; Scalapino, JLTP 1999, Kyung et al. (2003))
  - RG → Groundstate d-wave superconducting
    - (Halboth, PRB 2000; Zanchi, PRB 2000, Berker 2005)
- **Strong coupling (U >> W)**
  - Early mean-field
    - (Kotliar, Liu 1988, Inui et al. 1988)
  - Finite size simulations of t-J model
    - Groundstate superconducting
    - (Sorella et al., PRL 2002; Poilblanc, Scalapnio, PRB 2002)

Numerical methods that show Tc at strong coupling

DCA

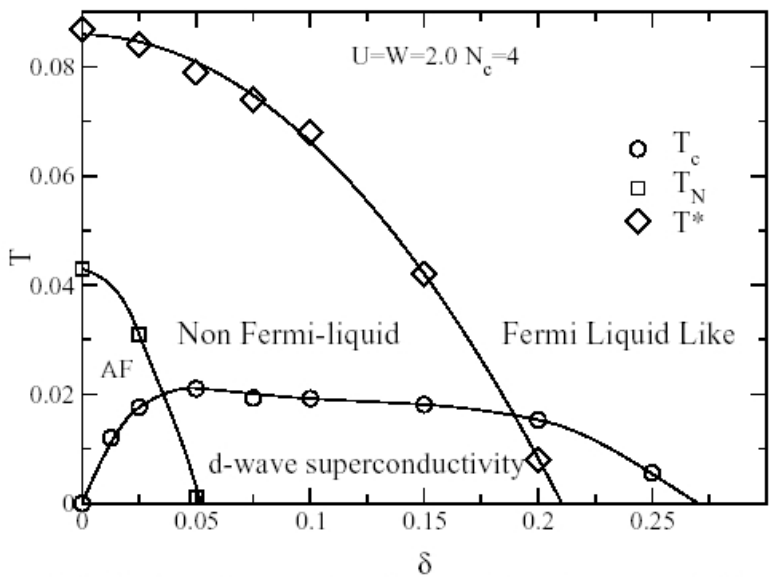


FIG. 5. The temperature-doping phase diagram of the 2D Hubbard model calculated with QMC and DCA for $N_c = 4$, $U = 2$. T_N and T_c were calculated from the divergences of the antiferromagnetic and d-wave susceptibilities, respectively. T^* was calculated from the peak of the bulk magnetic susceptibility.

Th. Maier, M. Jarrell, Th. Pruschke, and J. Keller
Phys. Rev. Lett. 85, 1524 (2000)
T.A. Maier et al. PRL (2005)

Variational

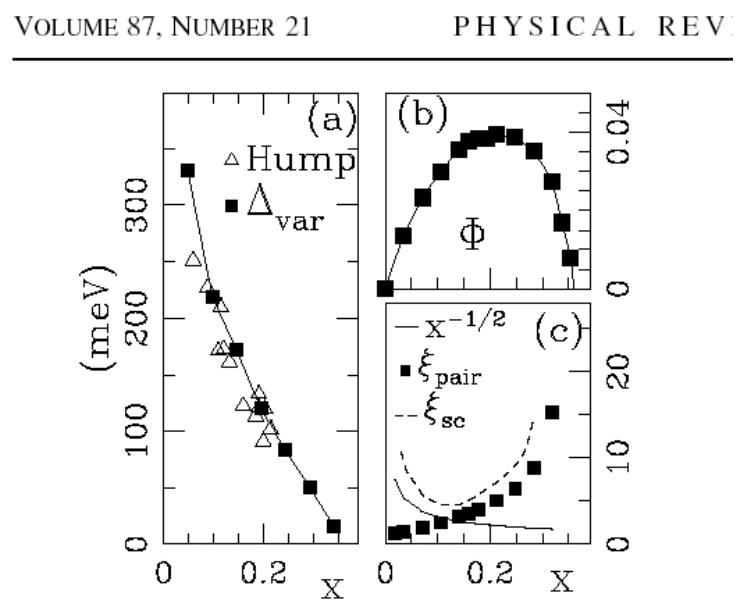


FIG. 1. (a) The variational parameter Δ_{var} (filled squares) and the $(\pi, 0)$ hump scale (open triangles) in ARPES [10] versus doping. (b) Doping dependence of the d-wave SC order parameter Φ. Solid lines in (a) and (b) are guides to the eye. (c) The coherence length $\xi_{sc} \geq \max(\xi_{pair}, 1/\sqrt{x})$.

Paramekanti, M. Randeria, and N. Trivedi
Phys. Rev. Lett. 87, 217002 (2001)

Theoretical difficulties

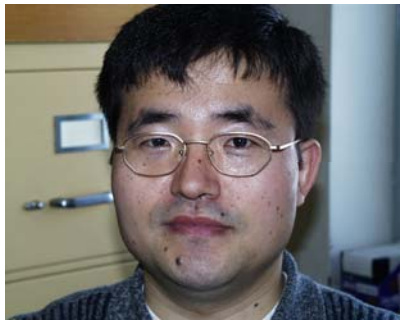
- Low dimension
  - (quantum and thermal fluctuations)

- Large residual interactions (develop methods)
  - (Potential ~ Kinetic)
  - Expansion parameter?
  - Particle-wave?

- By now we should be as quantitative as possible!

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 coupling approaches agree at intermediate coupling.
- Compare with experiment



Bumsoo Kyung

David Sénéchal

Sarma Kancharla

Marc-André Marois

Pierre-Luc Lavertu

UNIVERSITÉ DE SHERBROOKE

Outside collaborators

Gabi Kotliar

Marcello Civelli

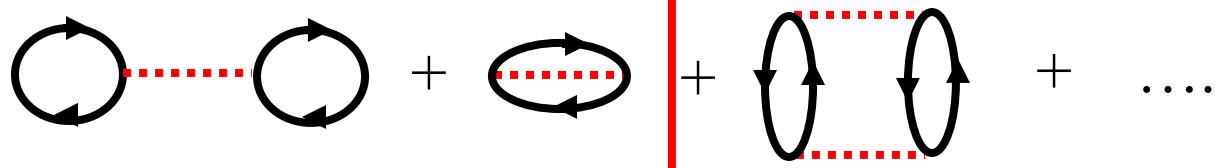
Massimo Capone

Outline

- Methodology
- $T = 0$ phase diagram
  - Variational Cluster Perturbation Theory
  - Cellular Dynamical Mean-Field Theory
  - Anomalous superconductivity : Non-BCS
- Pseudogap

Dynamical "variational" principle

$$\Omega_{\mathbf{t}}[G] = \Phi[G] - Tr[(G_{0\mathbf{t}}^{-1} - G^{-1})G] + Tr\ln(-G)$$

$\Phi[G] =$ 

Universality

$$\frac{\delta\Phi[G]}{\delta G} = \Sigma$$

$$\frac{\delta\Omega_{\mathbf{t}}[G]}{\delta G} = \Sigma - G_{0\mathbf{t}}^{-1} + G^{-1} = 0$$

$$G = \frac{1}{G_{0\mathbf{t}}^{-1} - \Sigma}$$

H.F. if approximate Φ by first order

FLEX higher order

Then Ω is grand potential
Related to dynamics (cf. Ritz)

Luttinger and Ward 1960, Baym and Kadanoff (1961)

Another way to look at this (Potthoff)

$$\Omega_{\mathbf{t}}[G] = \Phi[G] - Tr[(G_{0\mathbf{t}}^{-1} - G^{-1})G] + Tr\ln(-G)$$

$$\Omega_{\mathbf{t}}[\Sigma] = \Phi[G] - Tr[\Sigma G] - Tr\ln(-G_{0\mathbf{t}}^{-1} + \Sigma)$$

$$\frac{\delta\Phi[G]}{\delta G} = \Sigma$$

Still stationary (chain rule)

$$\Omega_{\mathbf{t}}[\Sigma] = F[\Sigma] - Tr\ln(-G_{0\mathbf{t}}^{-1} + \Sigma)$$

M. Potthoff, Eur. Phys. J. B 32, 429 (2003).

SFT : Self-energy Functional Theory

With $F[\Sigma]$ Legendre transform of Luttinger-Ward funct.

$$\Omega_{\mathbf{t}}[\Sigma] = \boxed{F[\Sigma]} + \mathrm{Tr}\ln(-(G_0^{-1} - \Sigma)^{-1})$$

is stationary with respect to Σ and equal to grand potential there.

For given interaction, $F[\Sigma]$ is a universal functional of Σ, no explicit dependence on $H_0(\mathbf{t})$. Hence, use solvable cluster $H_0(\mathbf{t'})$ to find $F[\Sigma]$.

$$\Omega_{\mathbf{t}}[\Sigma] = \boxed{\Omega_{\mathbf{t}'}[\Sigma] - \mathrm{Tr}\ln(-(G_0'^{-1} - \Sigma)^{-1})} + \mathrm{Tr}\ln(-(G_0^{-1} - \Sigma)^{-1}).$$

Vary with respect to parameters of the cluster (including Weiss fields)

Variation of the self-energy, through parameters in $H_0(\mathbf{t'})$

M. Potthoff, Eur. Phys. J. B 32, 429 (2003).

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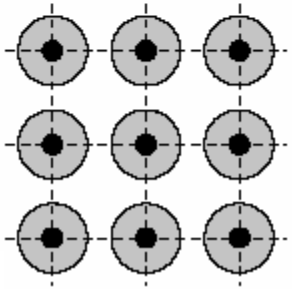
Variational cluster perturbation theory and DMFT as special cases of SFT

M. Potthoff *et al.* PRL **91,** 206402 (2003).

DCA, Jarrell et al.

Savrasov, Kotliar, PRB (2001)

DMFT



Georges Kotliar, PRB (1992).
M. Jarrell, PRL (1992).
A. Georges, *et al.* RMP (1996).

$$T\sum_{\omega_n}\sum_{ij\sigma}\left(\frac{1}{\boldsymbol{G}_{0,\boldsymbol{t}}^{-1}-\boldsymbol{\Sigma}_{\boldsymbol{t}',\boldsymbol{U}}}-\boldsymbol{G}_{\boldsymbol{t}',\boldsymbol{U}}\right)_{ji\sigma}\frac{\partial\Sigma_{ij\sigma}}{\partial\boldsymbol{t}'}=0\,.$$

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Tests VCPT

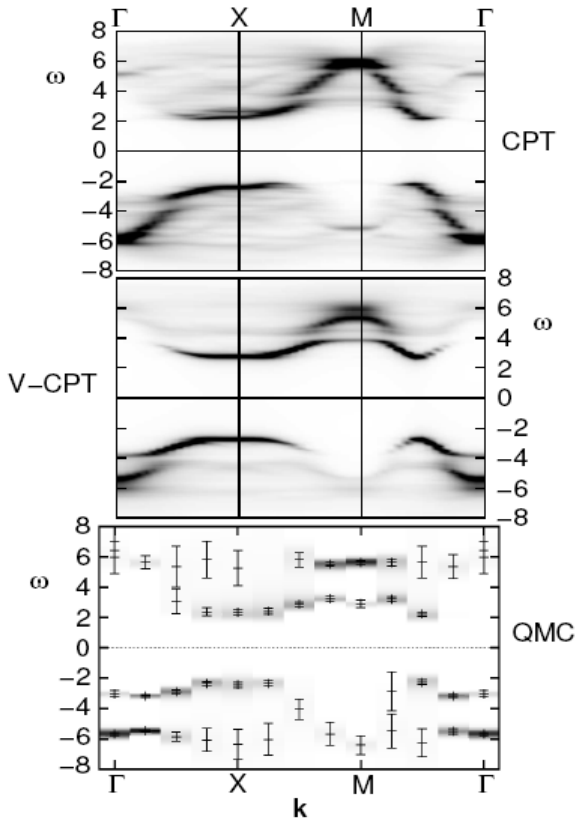
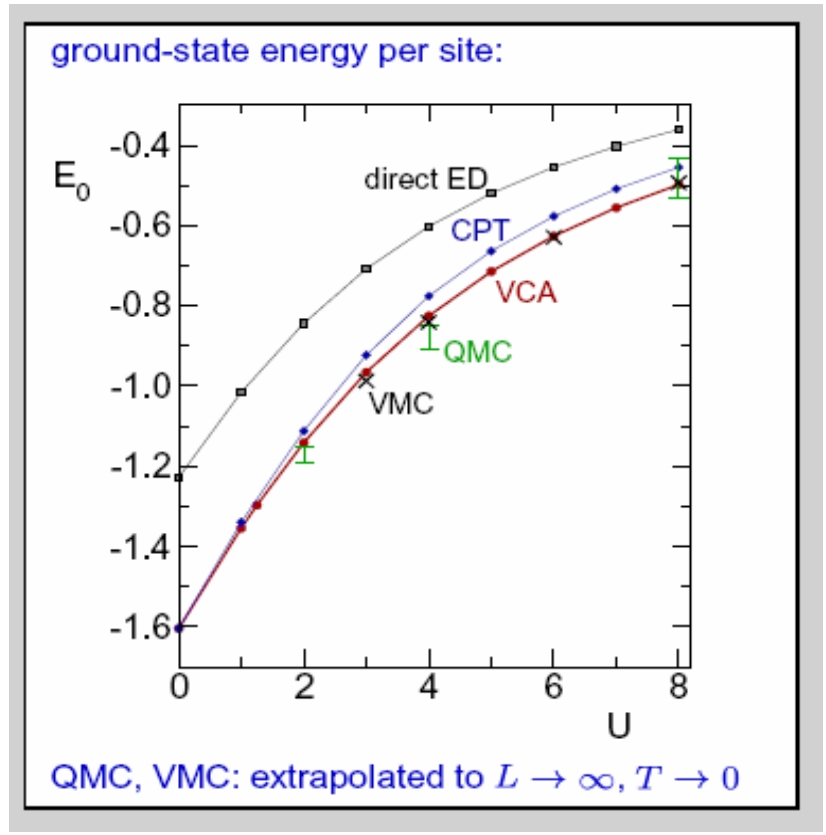


FIG. 11: Density plot of the spectral function for the $D = 2$ Hubbard model at $U = 8$, half-filling and $T = 0$ as obtained by the CPT with $h = 0$ (top) and by the variational CPT with optimal ficticious staggered field $h \neq 0$ (middle). The lattice is covered by $\sqrt{10} \times \sqrt{10}$ clusters. Bottom: QMC (maximum entropy) result, taken from Ref. 37, for the same parameters but for a finite low temperature $T = 0.1$ and an isolated 8×8 cluster. Dark (light) areas correspond to large (small) spectral weight.



Dahnken, Aichhorn, Hanke, Arrigoni and Potthoff, PRB 70, 245110 (2004)

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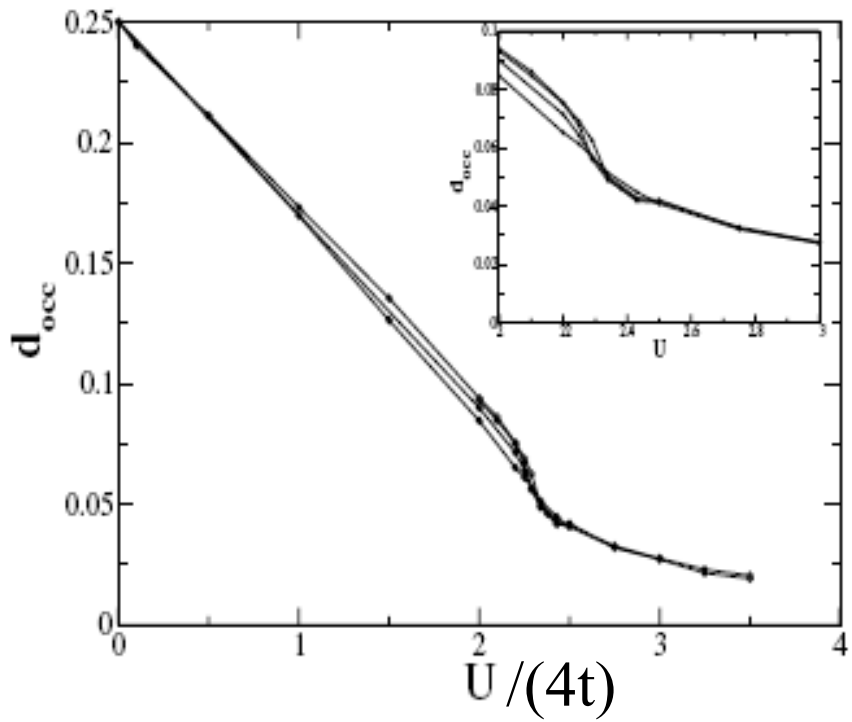
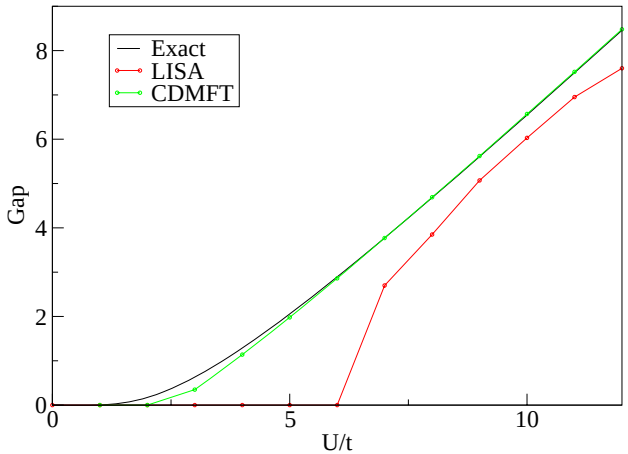
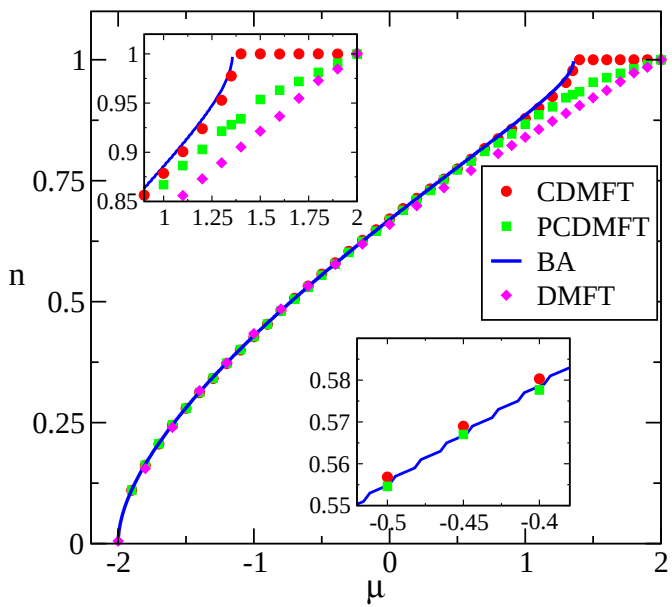
Test: CDMFT
Recover *d* = *infinity* Mott transition



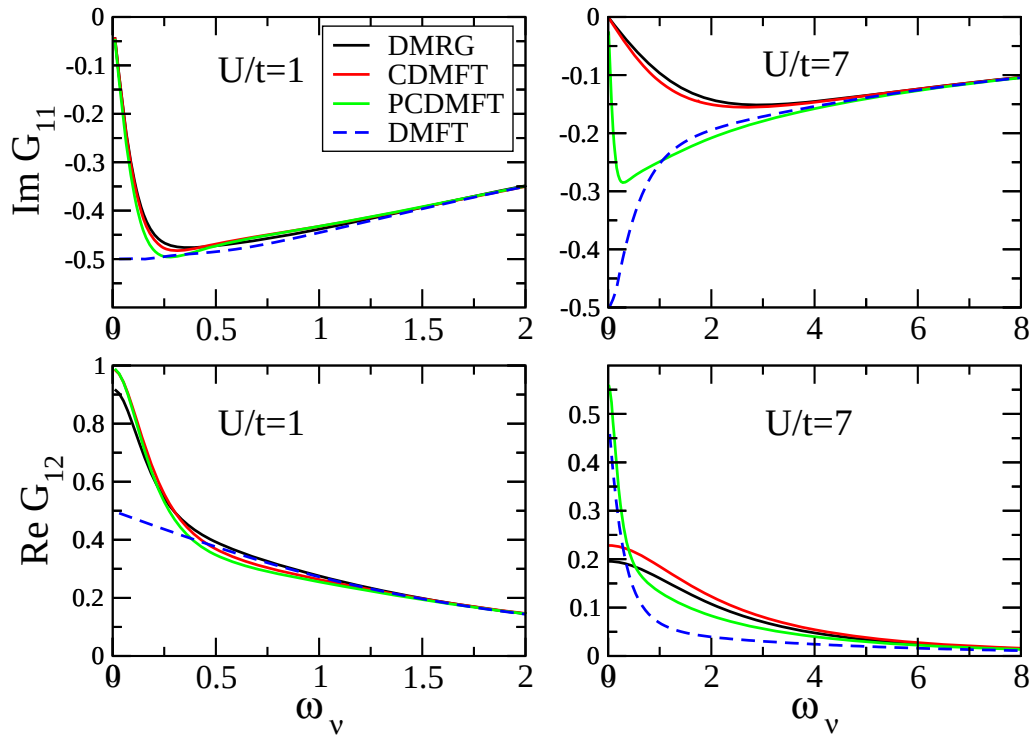
Parcollet, Biroli, Kotliar, PRL (2004)

Tests : CDMFT





1D Hubbard model: Worst case scenario



Excellent agreement with exact results in both metallic and insulating limits

Capone, Civelli, SSK, Kotliar, Castellani PRB (2004)

Bolech, SSK, Kotliar PRB (2003)

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Outline

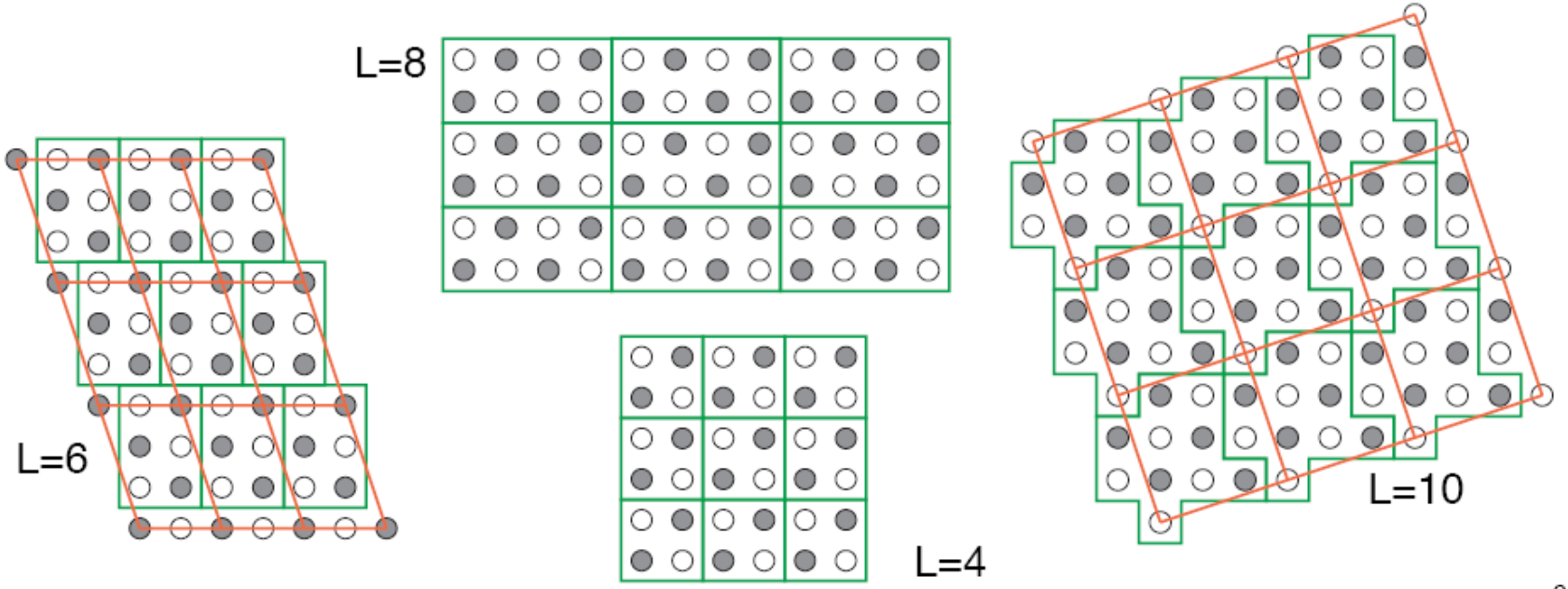
- Methodology
- $T = 0$ phase diagram
  - Variational Cluster Perturbation Theory
  - Cellular Dynamical Mean-Field Theory
  - Anomalous superconductivity : Non-BCS
- Pseudogap

Outline

- $T = 0$ phase diagram
  - Variational Cluster Perturbation Theory

VCPT (VCA)

David Sénéchal



6

The mean-fields decrease with system size

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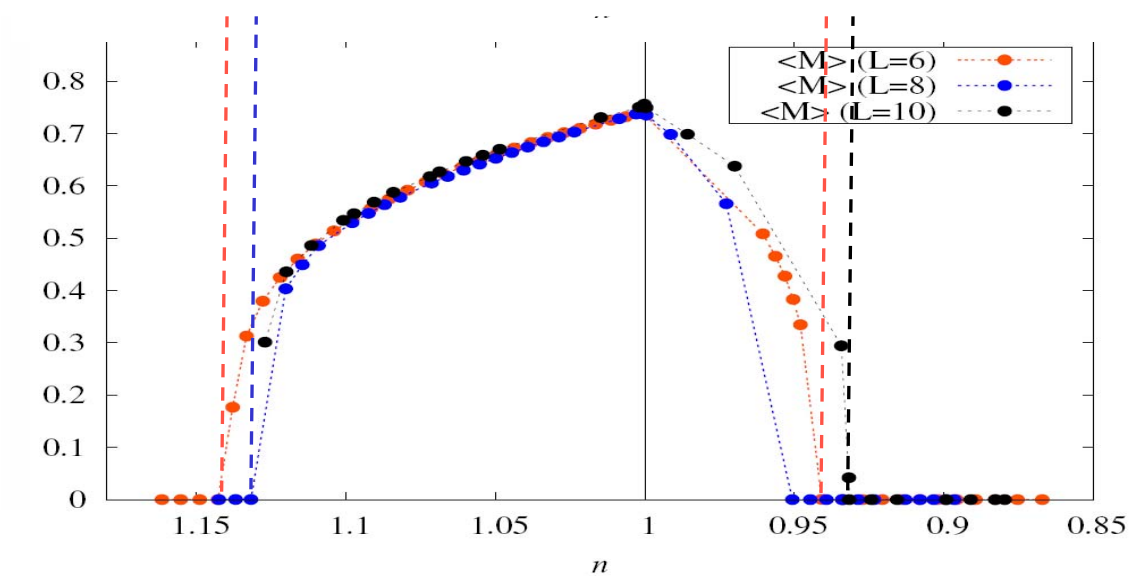
Weiss fields for competing *d-SC* and *AF*

$$H_M = M \sum_a (-1)^a (n_{a\uparrow} - n_{a\downarrow})$$

$$H_D = \sum_{a,b} \Delta_{ab} (c_{a\uparrow} c_{b\downarrow} + \mathrm{H.c.})$$

AF and dSC order parameters, $U = 8t$, for various sizes

$t' = -0.3\ t$
$t'' = 0.2t$
$U = 8t$



Aichhorn, Arrigoni, Potthoff, Hanke, cond-mat/0511460

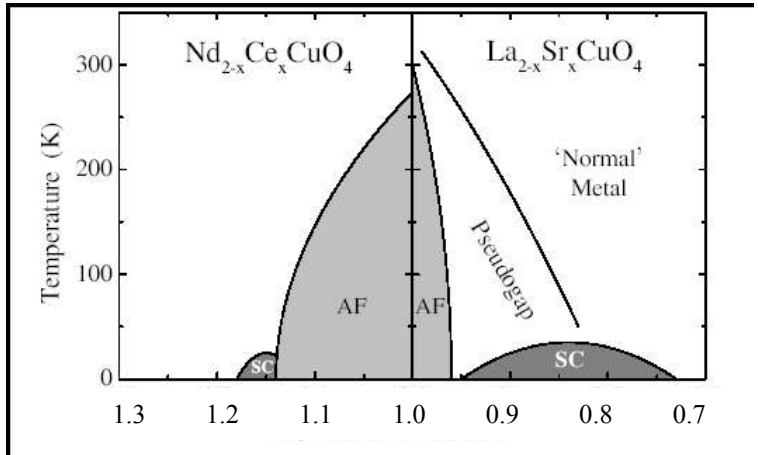


FIG. 1 Phase diagram of n and p-type superconductors.

AF

Sénéchal, Lavertu, Marois, A.-M.S.T., PRL, 2005

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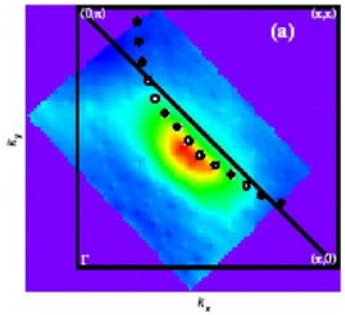
Fermi surface plots, $U = 8t$, $L = 8$

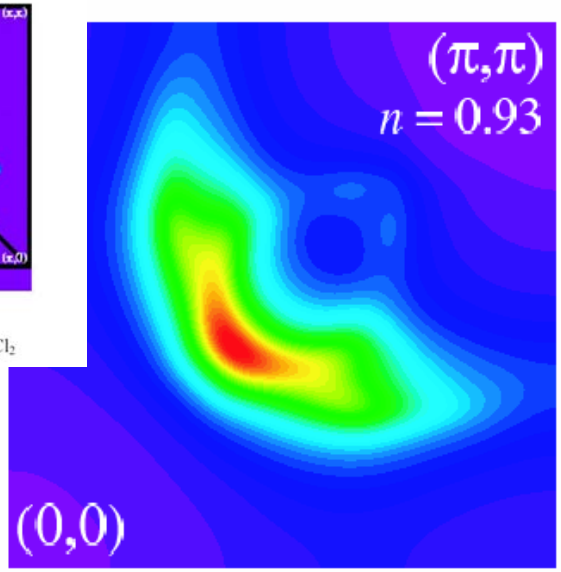
MDC at the Fermi energy

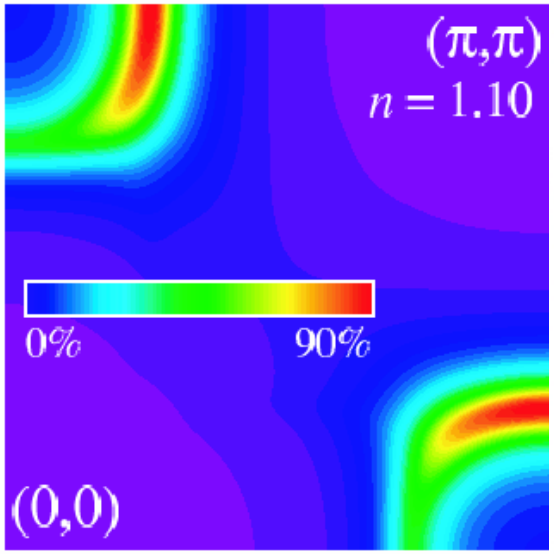
Hole-doped, 10%

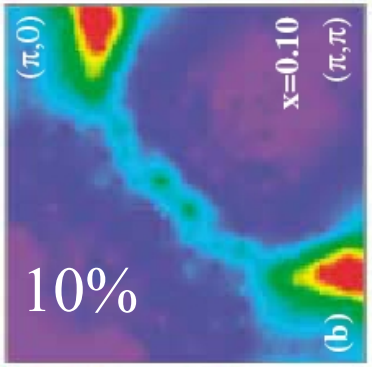


F. Ronning et al. Jan. 2002, $Ca_{2-x}Na_xCuO_2Cl_2$

Ronning *et al.* (PRB 2003)







Armitage *et al.* PRL 2003

FIG. 3: Intensity plot of the spectral function at the Ferr
level, in the first quadrant of the Brillouin zone, for $U = 8t$ c
a $L = 8$ cluster. Left: Hole-doped system ($n = 0.93$). Righ
Electron-doped systems ($n = 1.10$). A Lorentzian broadenir
of $0.2t$ is used.

Outline

- Methodology:
- $T = 0$ phase diagram
  - Variational Cluster Perturbation Theory
  - Cellular Dynamical Mean-Field Theory
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Outline

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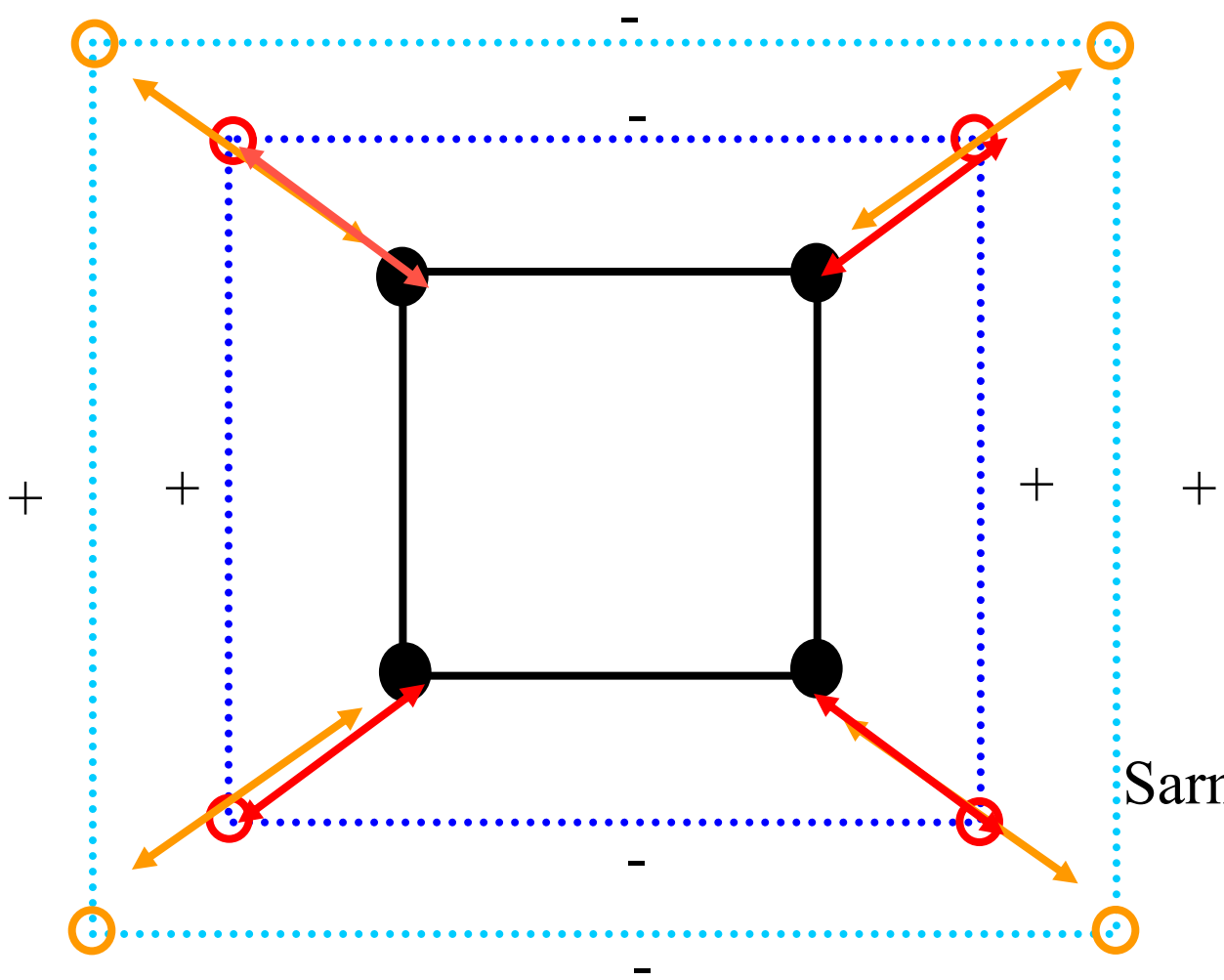
  - Cellular Dynamical Mean-Field Theory
  - Anomalous superconductivity : Non-BCS

CDMFT + ED



Sarma Kancharla

Caffarel and Krauth, PRL (1994)

No Weiss field on the cluster!

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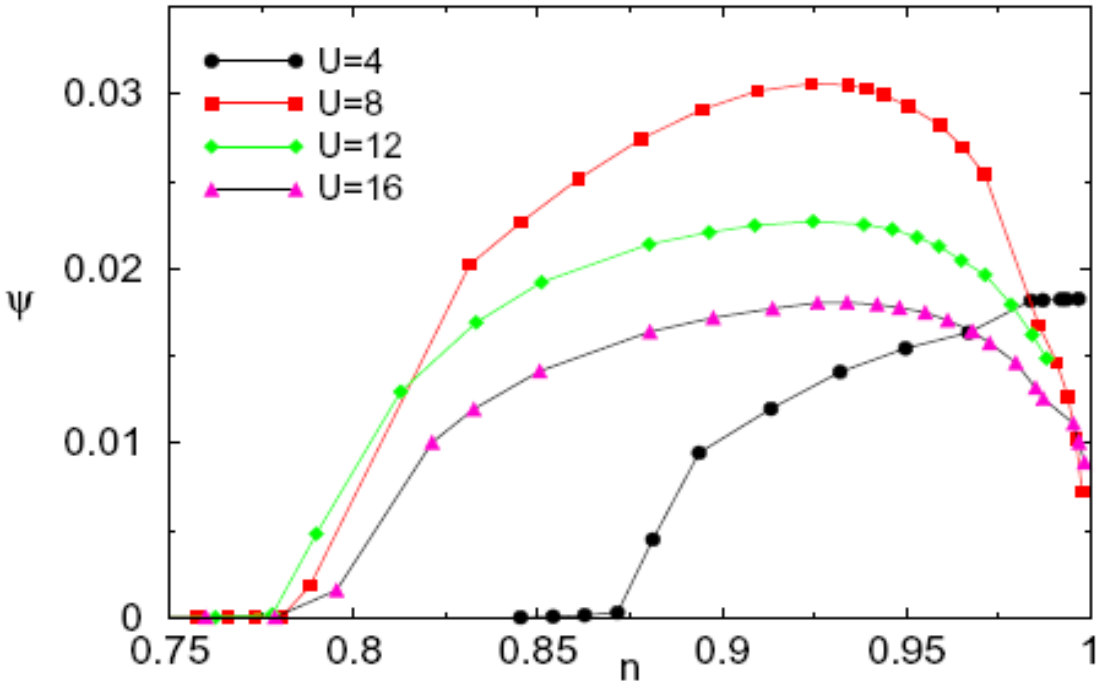
Effect of proximity to Mott (CDMFT)

D-wave OP



t'= t''=0

FIG. 1: SC order parameter ψ as a function of filling n and onsite Coulomb repulsion U, $t' = 0$.

Sarma Kancharla

Kancharla, Civelli, Capone, Kyung, Sénéchal, Kotliar, A-M.S.T. cond-mat/0508205

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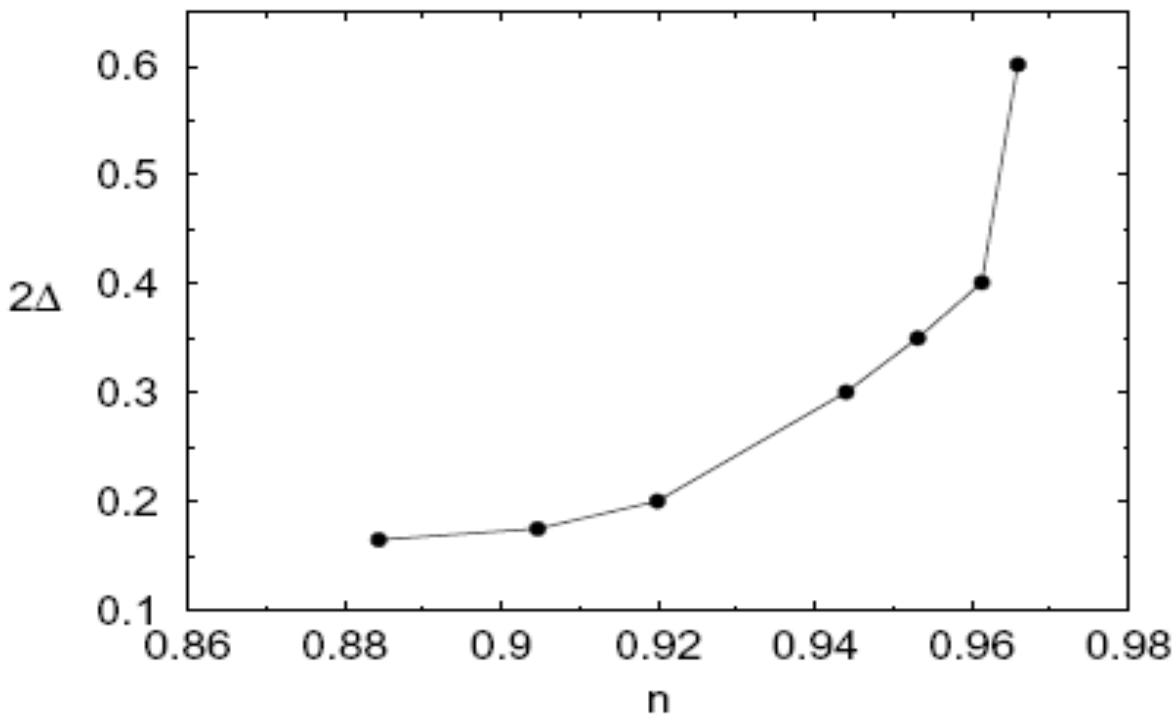
Gap vs order parameter



$t' = t'' = 0$

$\Delta = \psi Z$

FIG. 2: The dSC gap as a function of filling, U=8t, $t' = -0.3t$.

Kancharla, Civelli, Capone, Kyung, Sénéchal, Kotliar,
A-M.S.T. cond-mat/0508205

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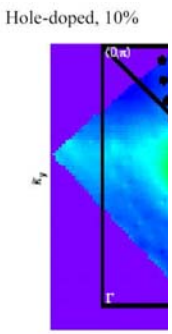
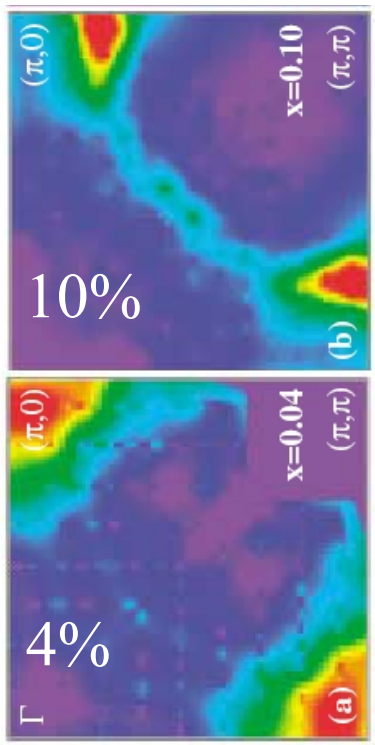
IDC in CDMFT

$t' = -0.3\,t,\ t'' = 0\,t$
$U = 8t$

Armitage *et al.*
PRL 2003

ning *et al.* PRB 2003





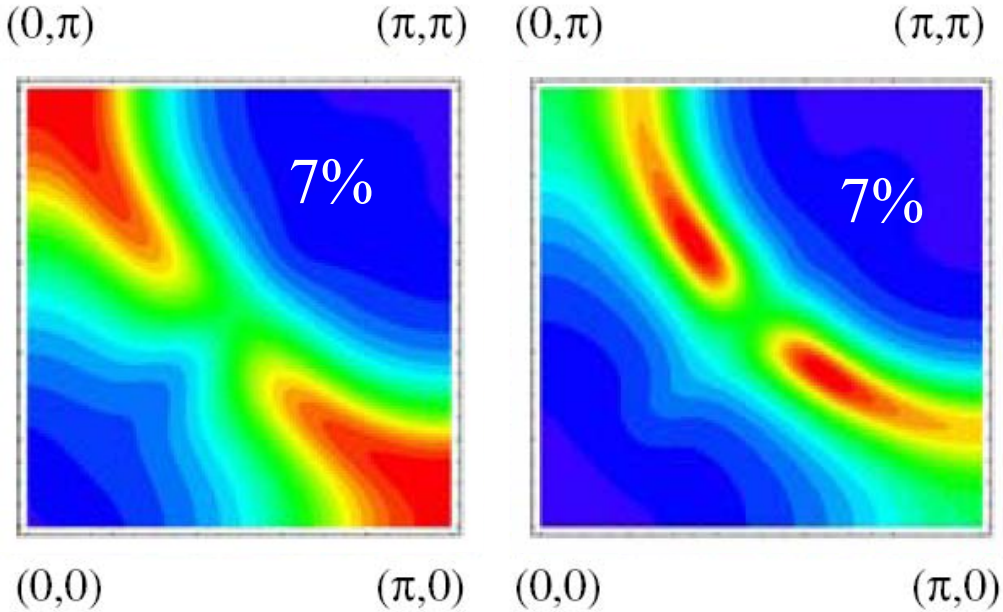


FIG. 5) in first quadrant of the Brillouin zone, U=8t. Energy resolution, $\eta = 0.1t$ (left and middle). Left: Hole-doped dSC (t'=-0.3t, n=0.96), Middle: Electron-doped dSC (t'=0.3t, n=0.93), Right: Same as middle with $\eta = 0.02t$.

Kancharla, Civelli, Capone, Kyung, Sénéchal, Kotliar,
A-M.S.T. cond-mat/0508205

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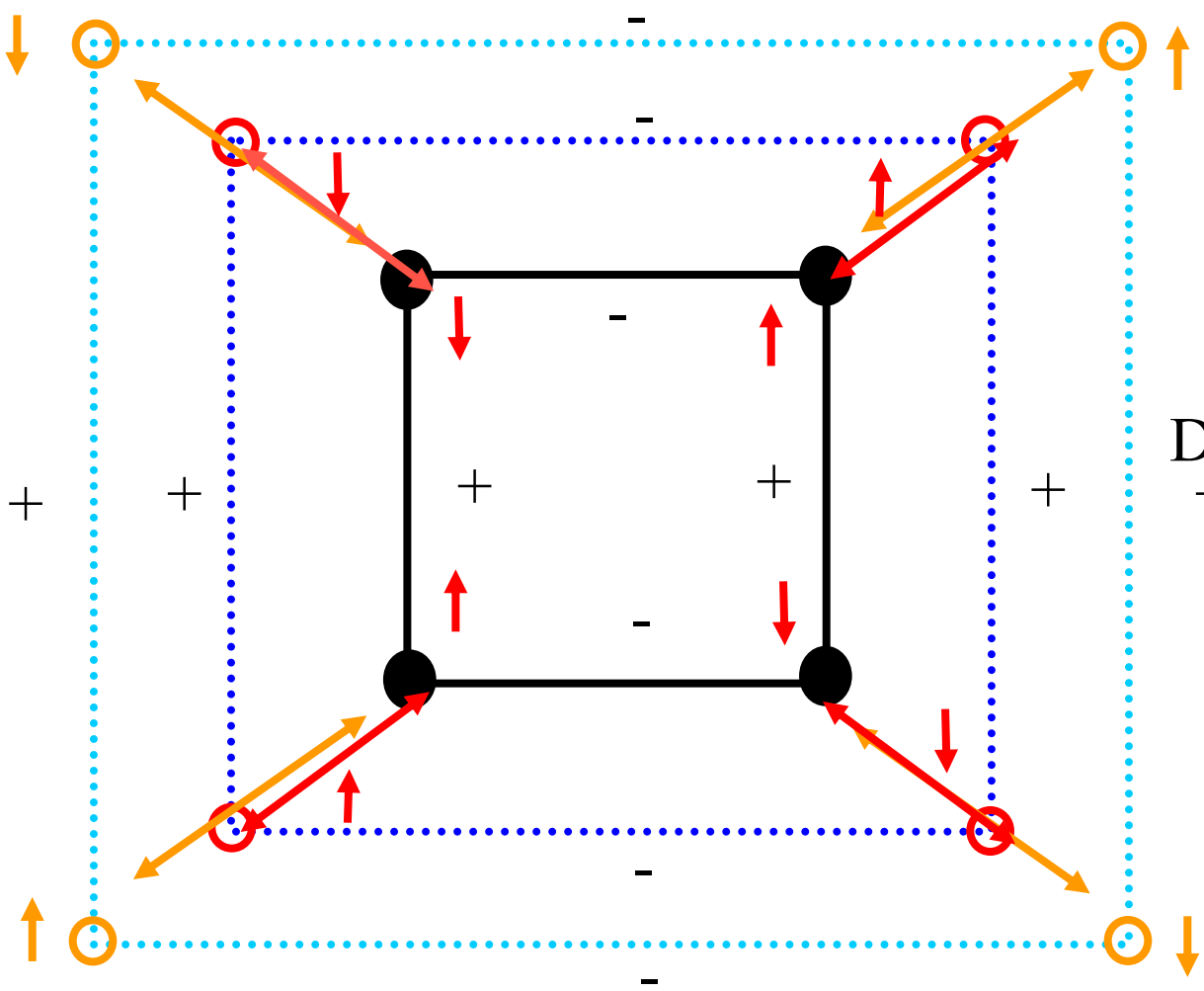
Competition AFM-dSC – using SFT



David Sénéchal

See also, Capone and Kotliar, cond-mat/0603227,
Macridin et al. DCA cond-mat/0411092

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Preliminary

$t' = -0.3\,t,\ \ t'' = 0.2\,t$
$U = 8t$

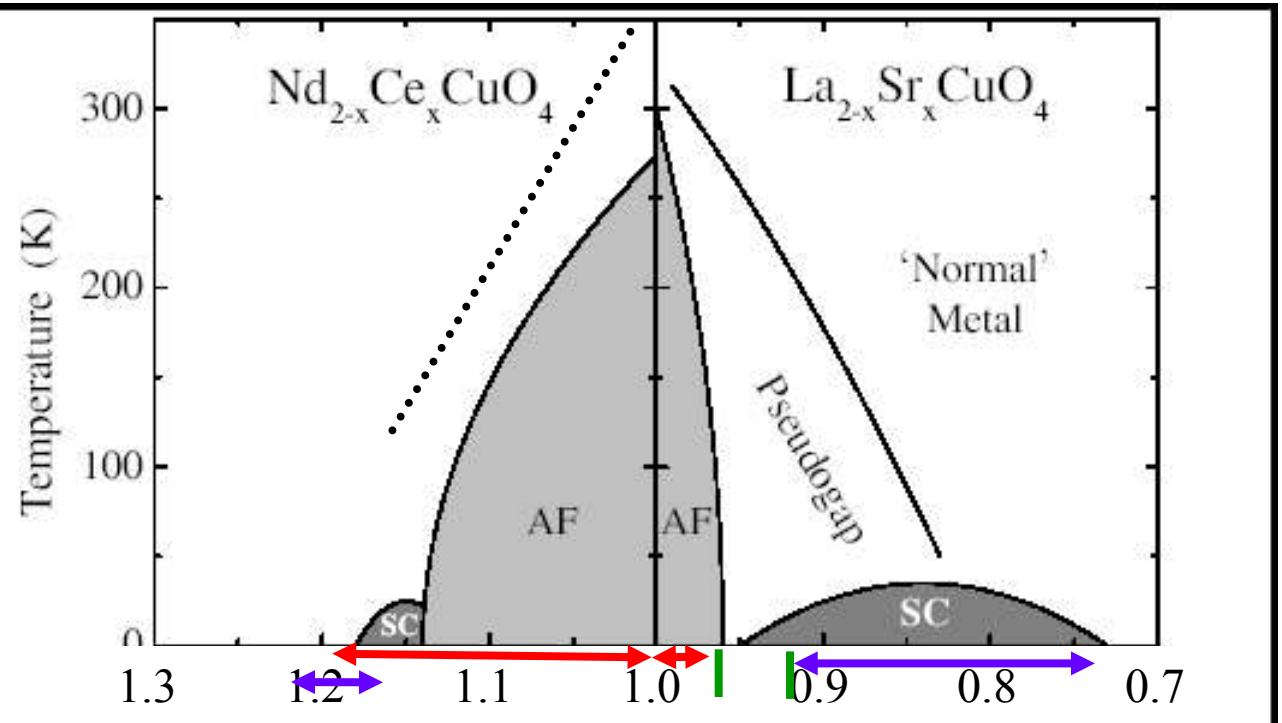

FIG. 1 Phase diagram of n and p-type superconductors.

n, electron density Damascelli, Shen, Hussain, RMP 75, 473 (2003)

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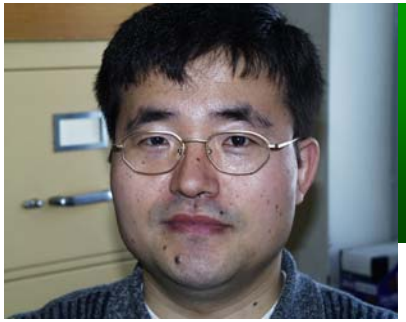

Pseudogap (CDMFT)

t' = -0.3 t, t'' = 0 t
U = 8t

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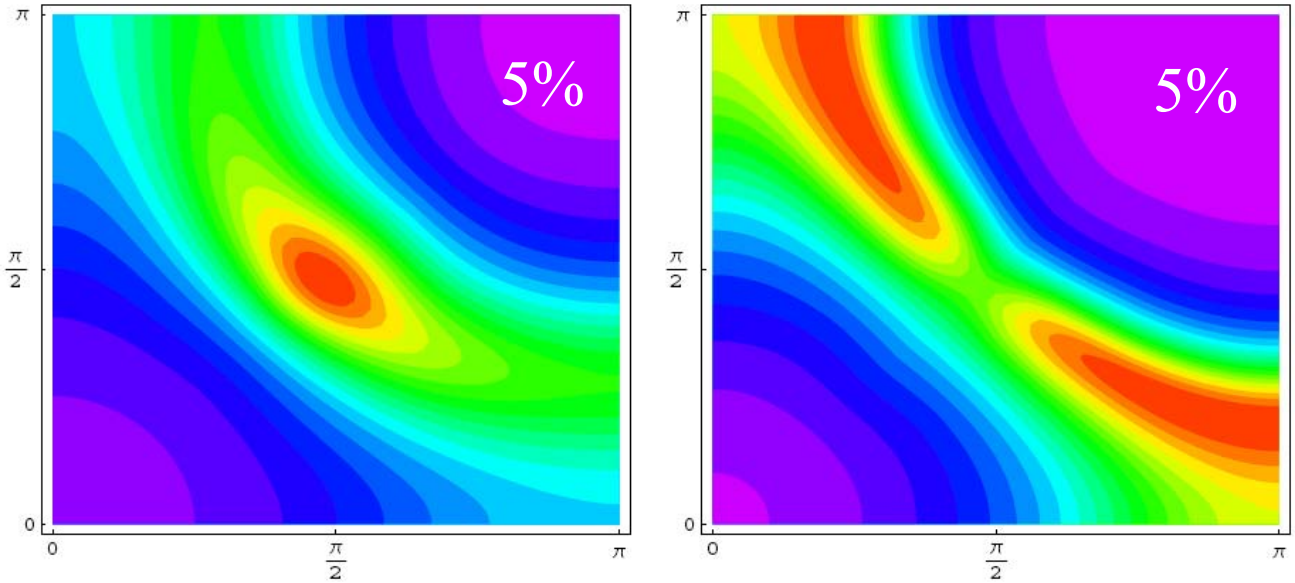

Kyung, Kancharla, Sénéchal, A.-M.S. T, Civelli, Kotliar PRB in press

FIG. 6: Density plot $A(\vec{k},0)$ in the $t-t'-U$ model with $U=8t$, $t'/t=-0.3$ for 5% hole- (left) and electron-doping (right). The current plots were obtained by taking the average of $A(\vec{k},\omega)$ in a $(-0.2t, 0.2t)$ window around the Fermi energy.

See also Sénéchal, AMT, PRL **92**, 126401 (2004).

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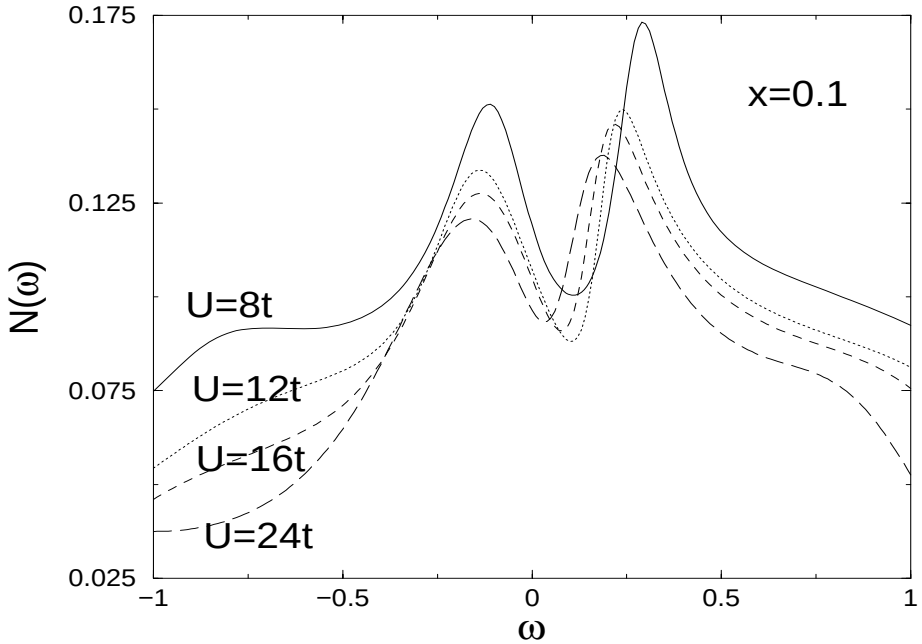
Other properties of the pseudogap



Effect of *U*

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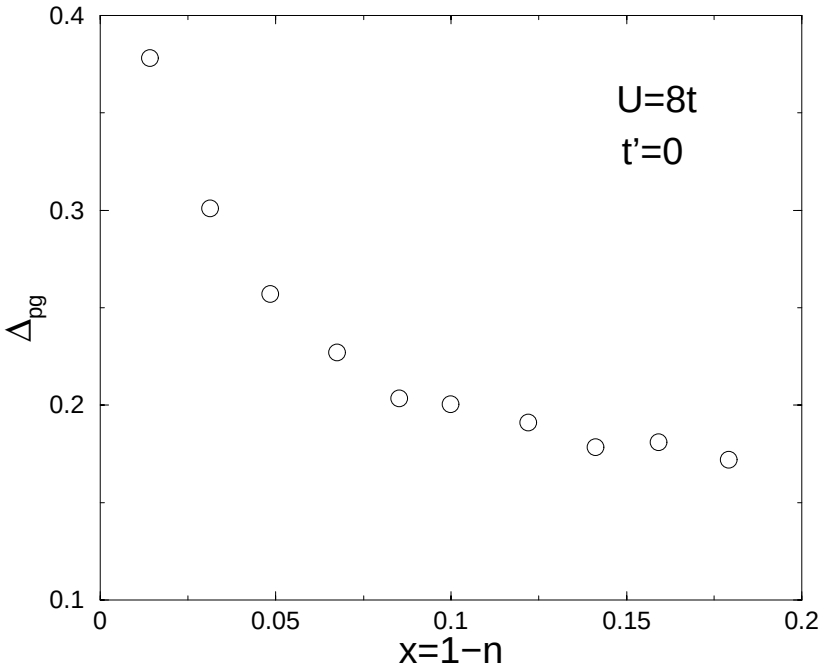

Pseudogap size function of doping

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See also Sénéchal, AMT, PRL **92**, 126401 (2004).

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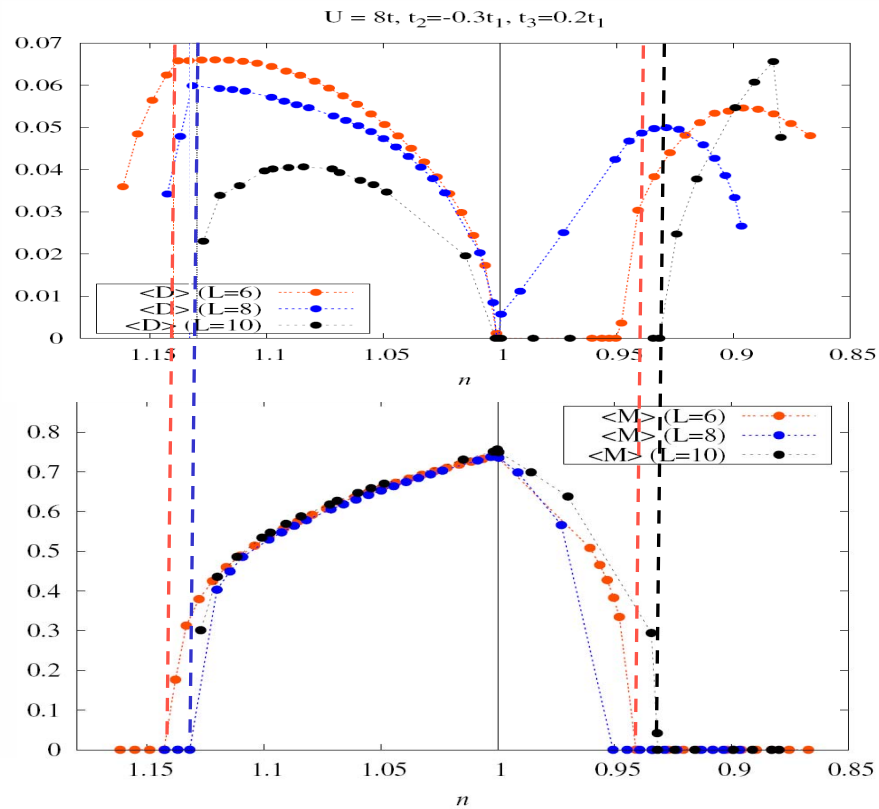
Summary - Conclusion

- Ground state of CuO_2 planes (h-, e-doped)
  - V-CPT, (C-DMFT) give overall ground state phase diagram with *U* at intermediate coupling.
  - Effect of *t'*.
- Non-BCS feature
  - Order parameter decreases towards $n = 1$ but gap increases.
  - Max dSC scales like *J*.
  - Emerges from a pseudogaped normal state (Z) (scales like *t*).



Sénéchal, Lavertu, Marois, A.-M.S.T., PRL, 2005

Kancharla, Civelli, Capone, Kyung, Sénéchal, Kotliar, A-M.S.T. cond-mat/0508205

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Conclusion

- The Physics of High-temperature superconductors is in the Hubbard model (with a very high probability).
- We are beginning to know how to squeeze it out of the model!
- Numerical solutions … DCA (Jarrell, Maier) Variational QMC (Paramekanti, Randeria, Trivedi).
- Role of mean-field theories : Physics
- Lot more work to do.

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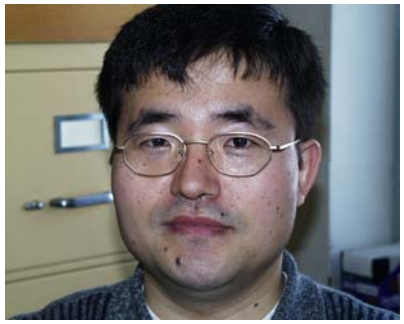

Bumsoo Kyung

David Sénéchal

Sarma Kancharla

Marc-André Marois

Pierre-Luc Lavertu

UNIVERSITÉ DE SHERBROOKE

Outside collaborators

Gabi Kotliar

Marcello Civelli

Massimo Capone

Mammouth, série

Réseau Québécois de Calcul de Haute Performance

Éducation, Loisir et Sport Québec

Canada Foundation for Innovation
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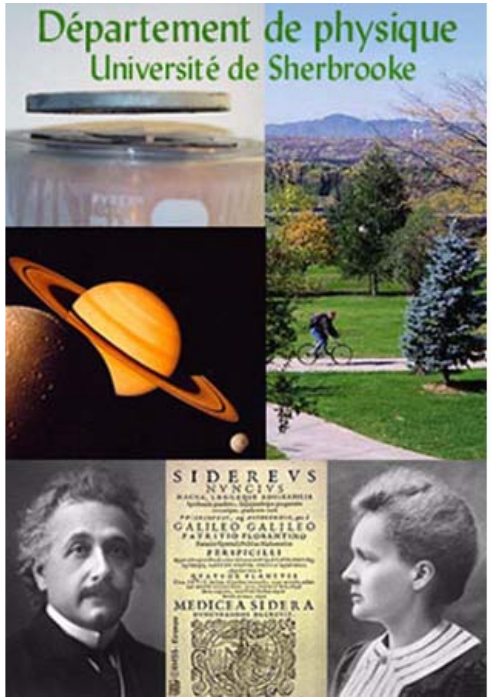

André-Marie Tremblay

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Some Recent Review Articles

- A.-M.S. Tremblay, B. Kyung and D. Sénéchal, cond-mat/0511334
- T. Maier, M. Jarrell, T. Pruschke, and M. H. Hettler, Rev. Mod. Phys. **77**, 1027 (2005)
- G. Kotliar, S. Y. Savrasov, K. Haule, V. S. Oudovenko, O. Parcollet, and C.A. Marianetti, cond-mat/0511085 v1 3 Nov 2005

C'est fini...

Thank you