`Microscopic' Theory of Superconductivity

A. J. Millis
Department of Physics
Columbia University

Department of Physics
Columbia University

Only a slight overstatement

Theory has been useless in the discovery of superconductors

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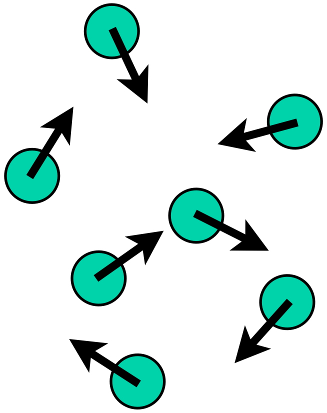
Example 1: Early 1900s

People realized: electrons constitute the ``conducting fluid" which carries electrical currents



Idea: every (conducting) solid contains a gas of electrons, all whizzing around in different directions. Applying an electric field biasses the motion, giving a net current.

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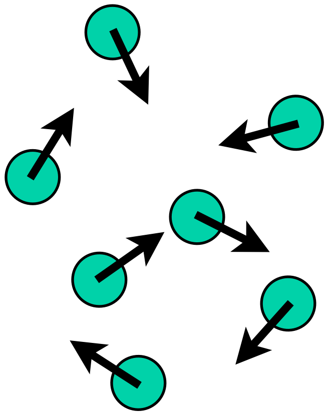
Example 1: Early 1900s

People realized: electrons constitute the ``conducting fluid" which carries electrical currents. Classical mechanic: motion from thermal agitation



As temperature goes to absolute zero, something strange should happen to the electrical conductivity

This reasoning was totally wrong, but the conclusion was correct and important

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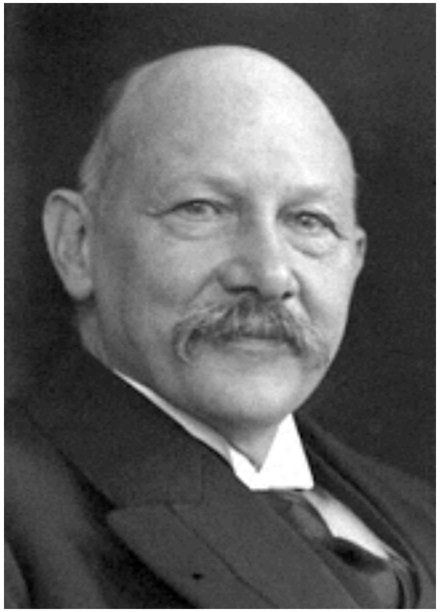
Heike Kamerlingh-Onnes



Wanted to see what happened to electron motion at very low temperatures

Initiated a major experimental effort in cooling materials to low temperatures, measuring properties

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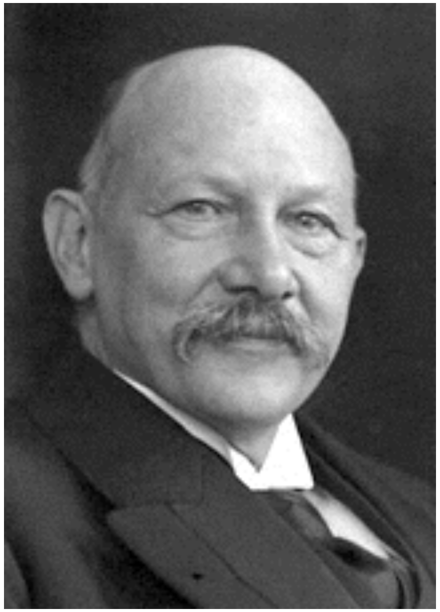
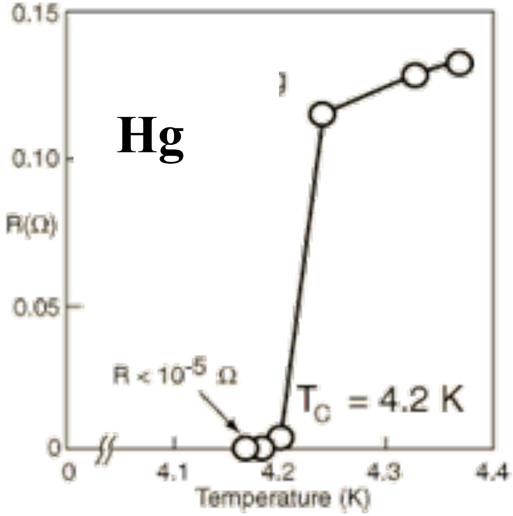
Heike Kamerlingh-Onnes

http://www.nobelprize.org/nobel_prizes/physics/laureates/1913/onnes-bio.html



Instead of finding that conduction ceased, he found superconductivity!!



H. K. Onnes, Commun. Phys. Lab. 12, 120 (1911) reproduced from http://hyperphysics.phy-astr.gsu.edu/hbase/solids/scex.html

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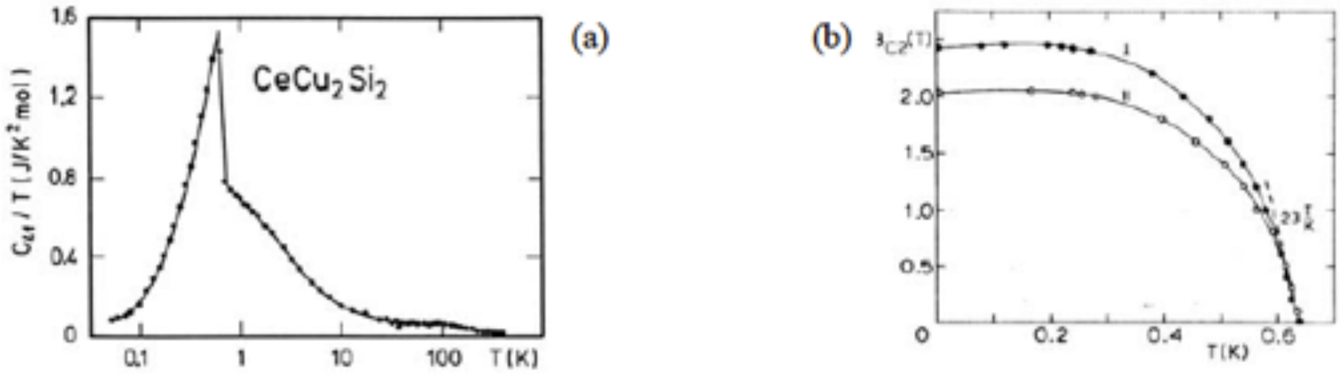
1979: Frank Steglich
Cerium Intermetallics with funny magnetic properties: Kondo lattice

$CeCu_2Si_2$

PRL 43 p 1892 (1979)



superconductivity with a transition temperature of abo
0.6K (not low relative to effective fermi energy)

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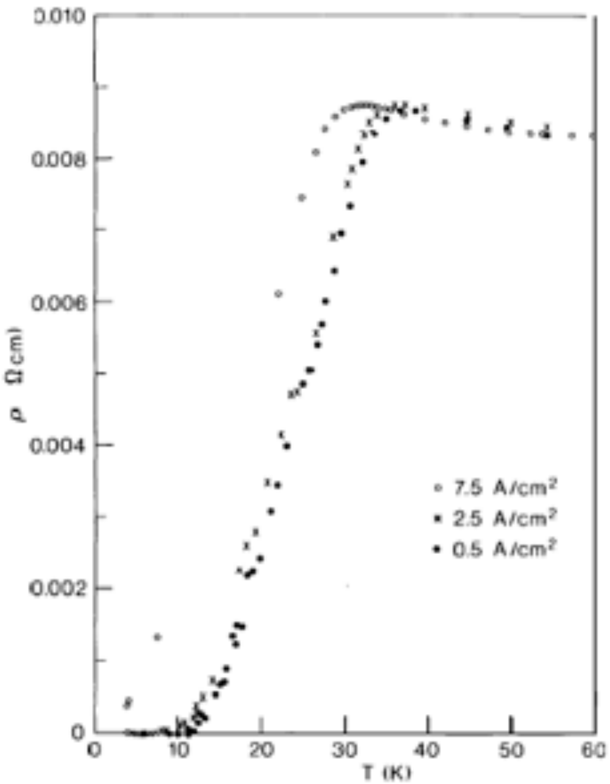
1985: Copper-oxide superconductors

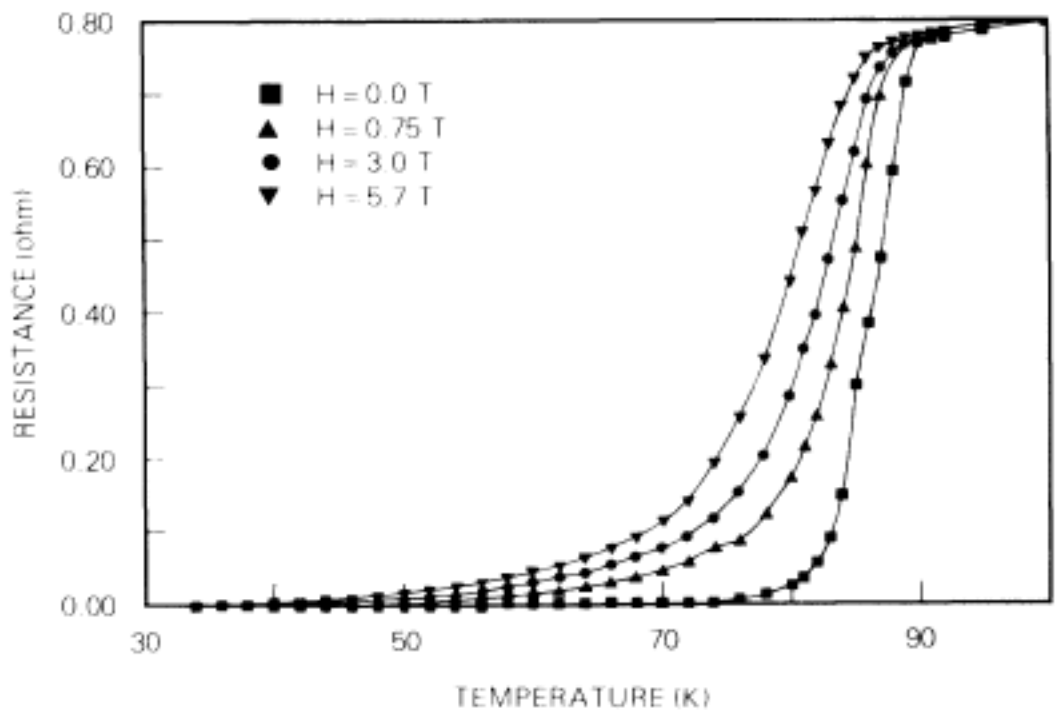
Bednorz and Mueller 1985

Z. Phys. B 64 189 1985



Paul Chu and MK Wu 1987

PRL 58 908 1987



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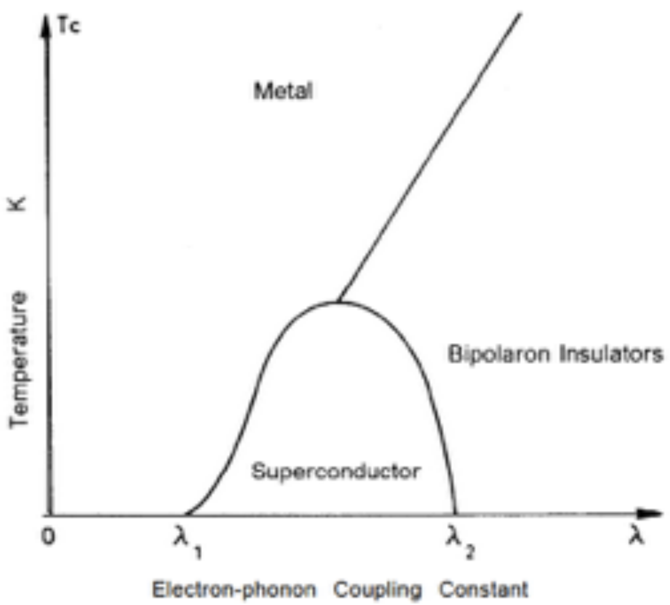
Mueller's motivation



2 wrong ideas:
(1) go all the way with phonon coupling--make it so strong you confine two electrons on same site: "bipolaron" (a small-size boson).

(2) La_2CuO_4 is nearly ferroelectric (it is not) and should be a good host for bipolarons (which ferroelectrics are not) and thus should be superconducting

This reasoning was totally wrong, but the conclusion was correct and important

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Understanding circa 2000

Conventional materials

*`Phonon mediated'
--light atoms
--wide (sp) bands
--cubic symmetry

*T_c<40K

*Underlying state `semiclassical'

High T_c

*Electronically mediated
--transition metal
--single narrow d-band
--nearby nontrivial insulator
--2D

*T_c>100K

*quantal fluctuations key

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2008: the Iron Age

Y. Kamihara, T. Watanabe, M. Hirano, and H. Hosono,
J. Am Chem. Soc. 130 3296 (2008)

These people were looking for a magnetic semiconductor with various useful properties.

What they found was a new family of high transition temperature superconductors

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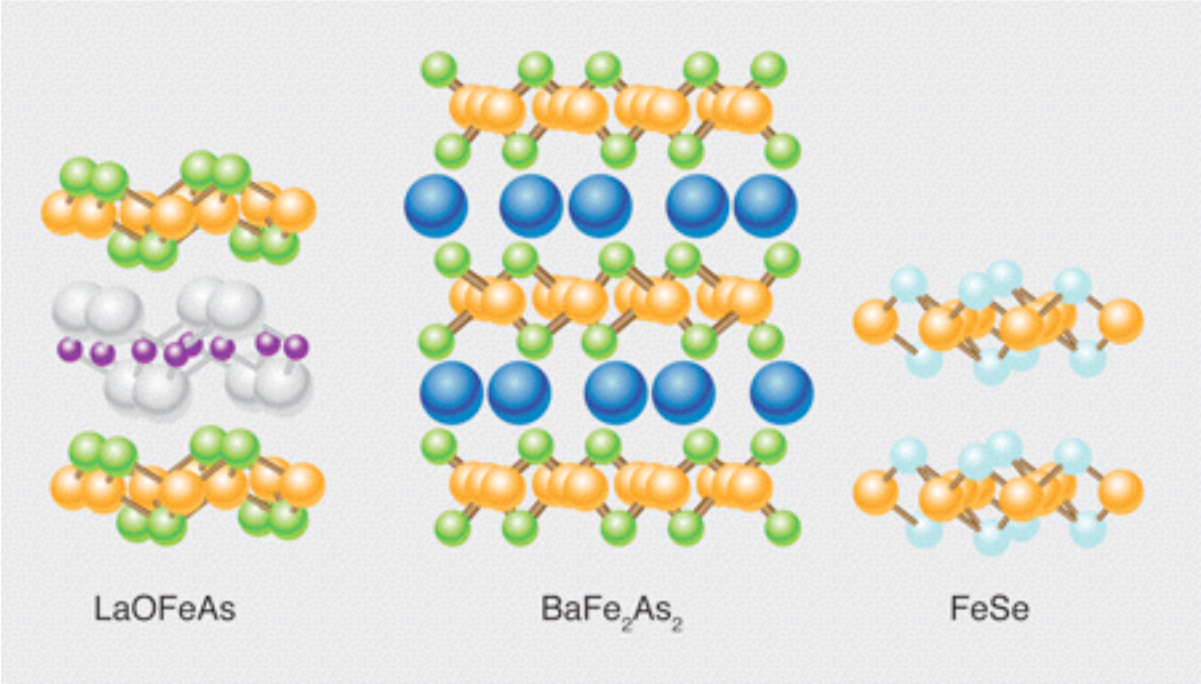
2008: the Iron Age

Electronically two dimensional



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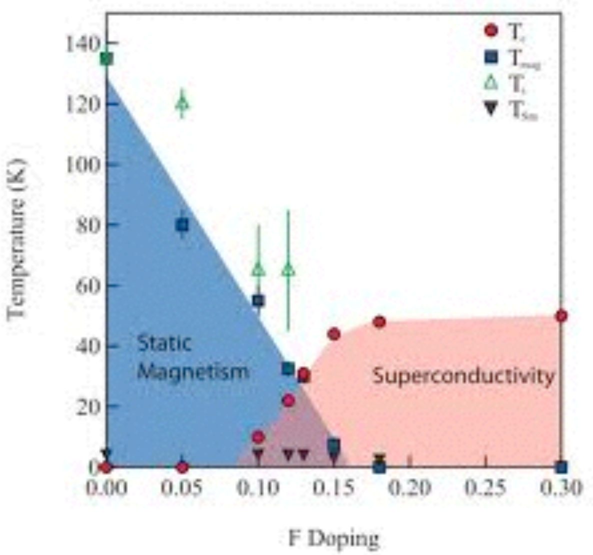
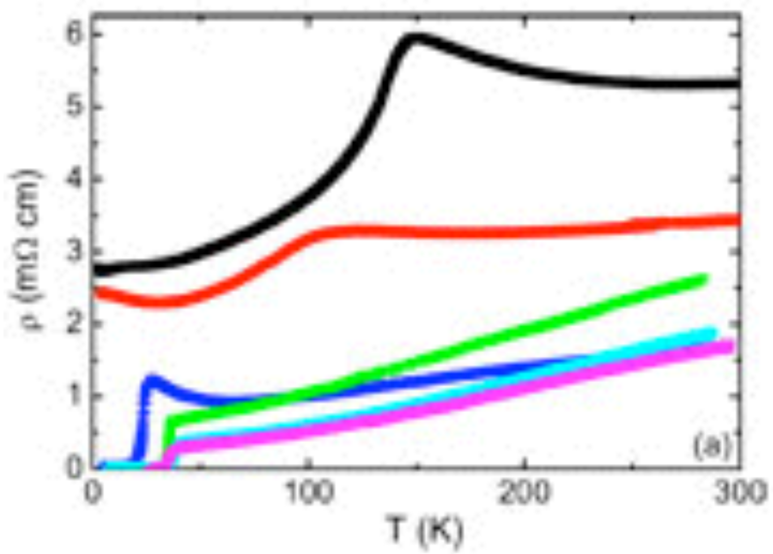
But no insulating phase nearby





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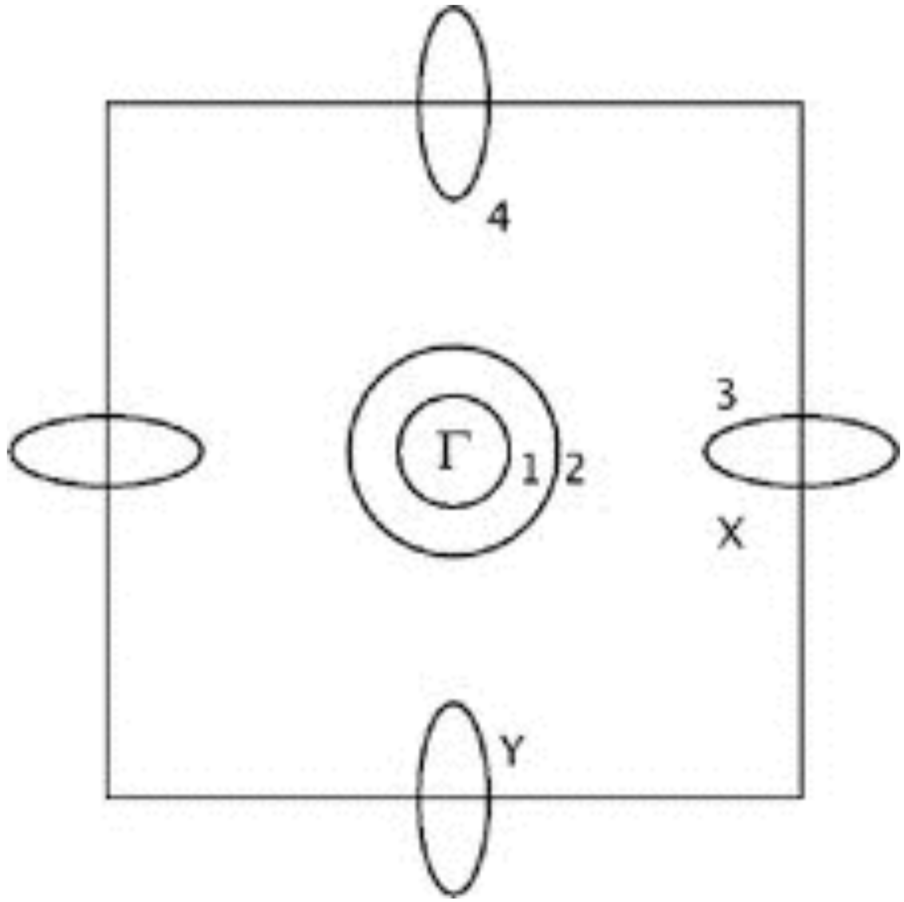
Multiple bands



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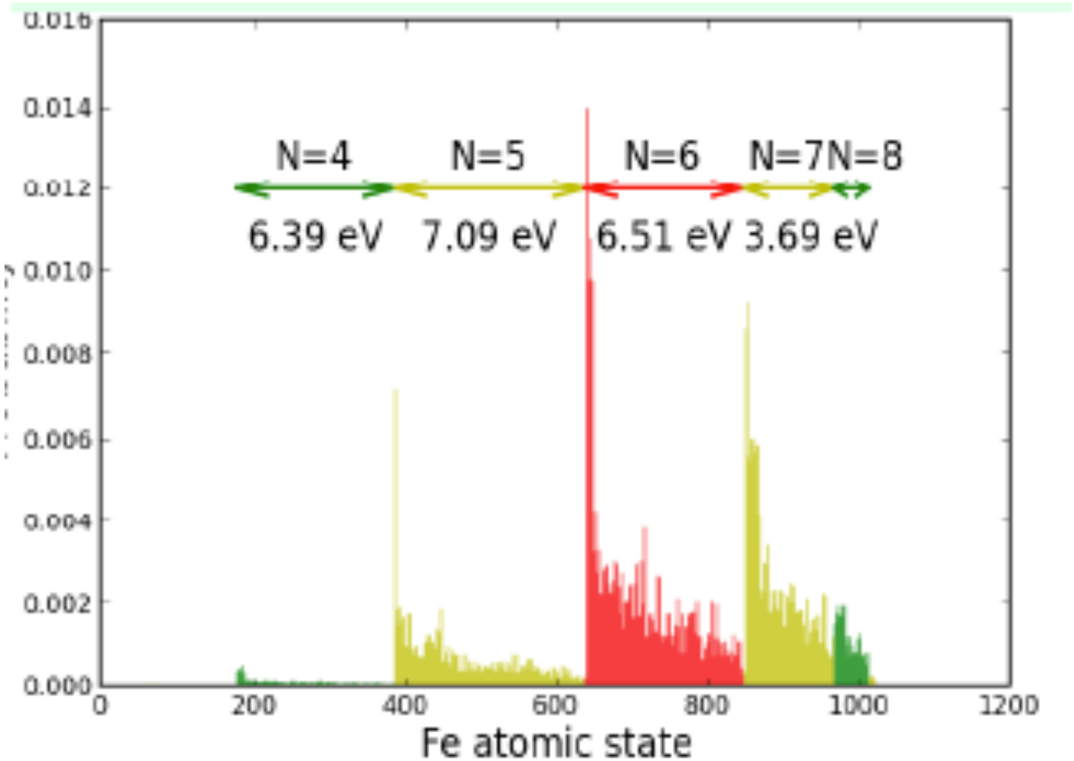
Large local moment (S=2) on Fe site



Kotliar/Haule; also Georges

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Understanding circa 2013

Conventional materials

*`Phonon mediated'
- --light atoms
- --wide (sp) bands
- --cubic symmetry

*$T_c<40K$

*Underlying state `semiclassical'

Cu-O High T_c

*Electronically mediated
- --transition metal
- --single narrow d-band
- --Near nontrivial insulator
- --2D

*$T_c>100K$

*Nontrivial quantal fluctuations

Fe-As High T_c

*Electronically mediated
- --transition metal
- --multiple d-bands
- --2D
- --physics of large-spin local moment

*$T_c>50K$

*quantal fluctuations not crucial.

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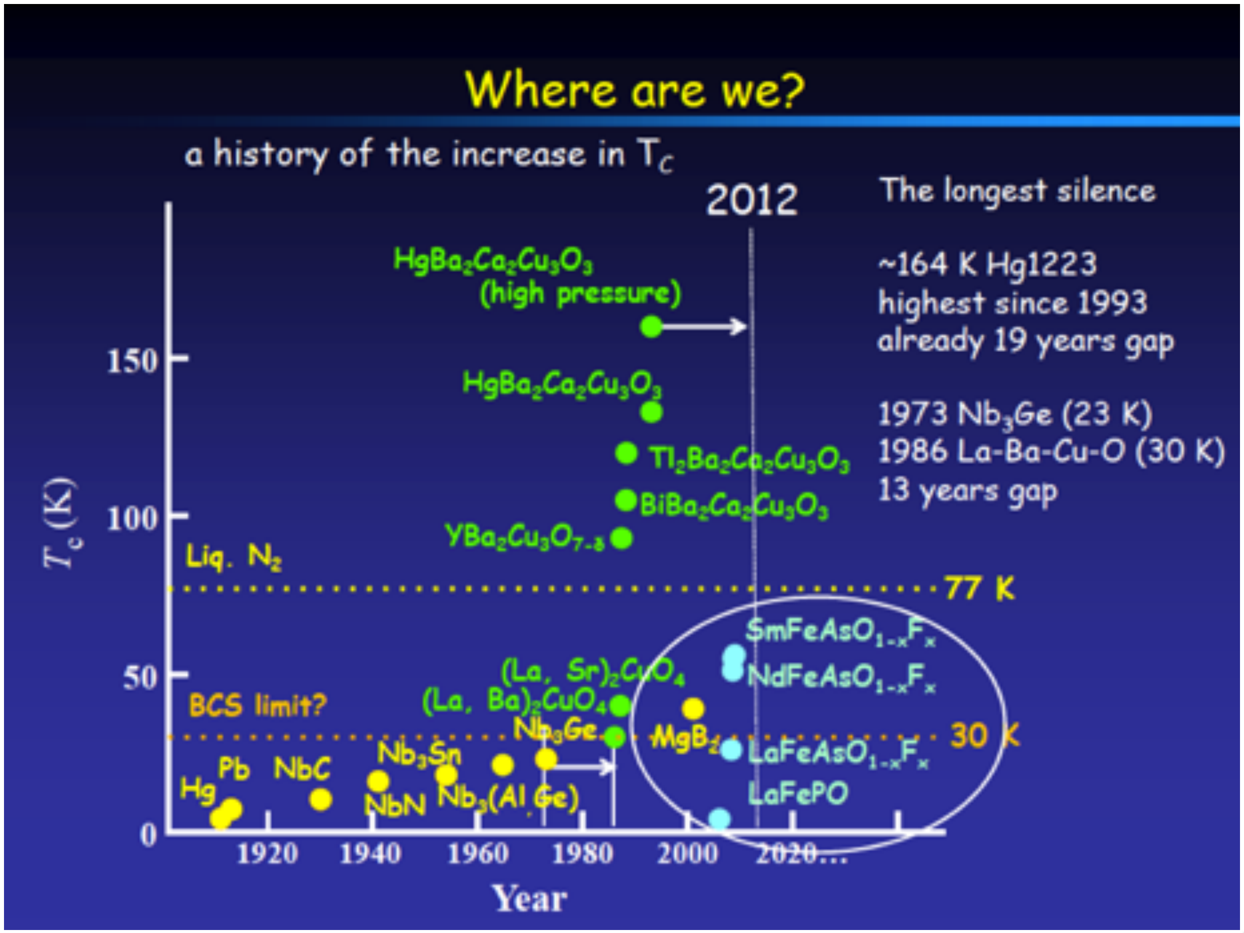
Many different superconductors known wide range in transition temperature



H. Takagi: SCES 2012 conference

How do we understand this?

How high is Tc going to get?

What are the good materials to look for?

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References—an incomplete list

1. Fermi Liquid Theory

—Abrikosov, Gorkov, Dzyaloshinskii, Methods of Quantum Field Theory in Statistical Physics
—R. Shankar, Rev Mod Phys 66, p 129 1994
—J Polchinski arxiv/hep-th/9210046

2. Migdal-Eliashberg Theory of Superconductivity

—Phonons: Scalapino, Schreiffer, Wilkins PR 148 264 (1966)
D J. Bergmann and D. Rainer, Z. Phys. 263, 59 (1973)
—Spin fluctuations: Millis, Sachdev, Varma PRB37 4975 (1988)
Monthoux and Lonzarich PRB59, 14598 (1999)
Monthoux, Lonzarich, Pines, Nature 450 1177
Abanov, Chubukov Schmalian, EPL 55 p 369

3. Other topics (also see refs in these articles)

—Hubbard Model: Raghu and Kivelson, Phys. Rev. B 83, 094518 (2011)
Gull, Parcollet and A Millis, PRL 110 216406
—SrTiO3: van der Marel, Melchov and Mazin Physical Review B 84, 205111 (2011)
—C-60 +other organics: M. Capone, RMP 81 p. 943

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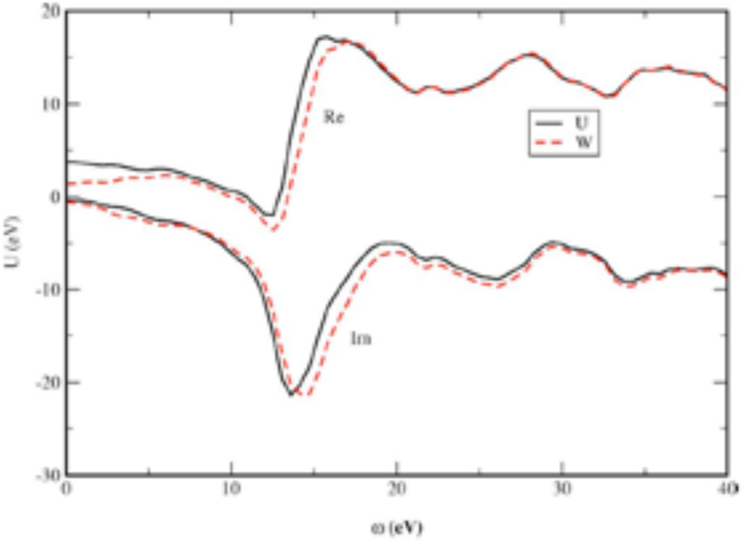
Example: Screened U $SrVO_3$



Aryasetiawan et al.
PRB74 125106 (2006)

Key point: most of the screening of the on-site interaction is done by an ``all electron" plasmon at an energy ~15 eV.

In general, below this plasmon scale, for most purposes metals are characterized by an interaction that is short ranged and of the order of unity

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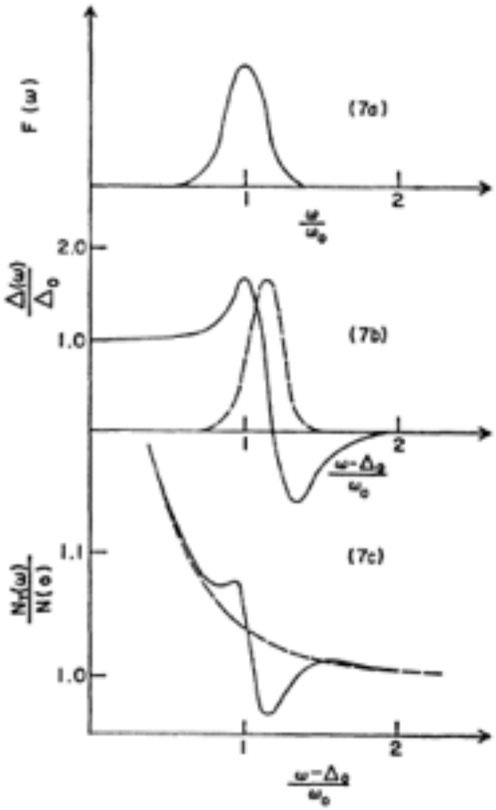
Superconducting gap function



Distribution of phonons and couplings (model)

Gap function (not anomalous self energy)

Tunnelling density of states

Scalapino, Schreiffer Wilkins PR 148 264 (1966)

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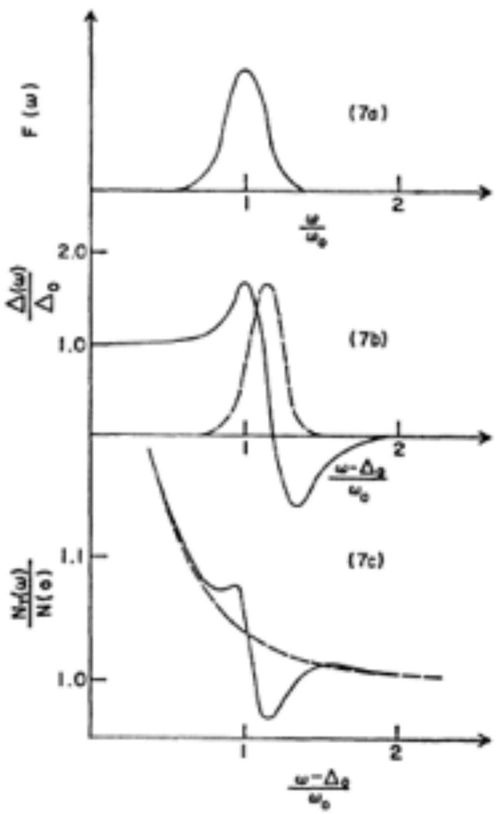
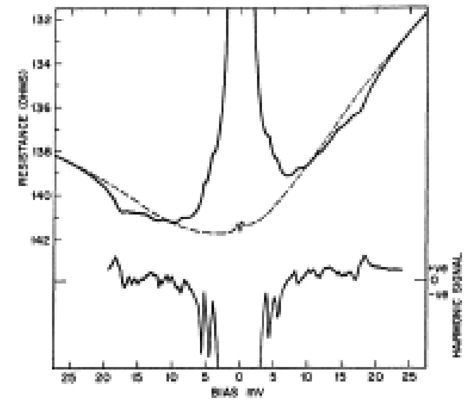
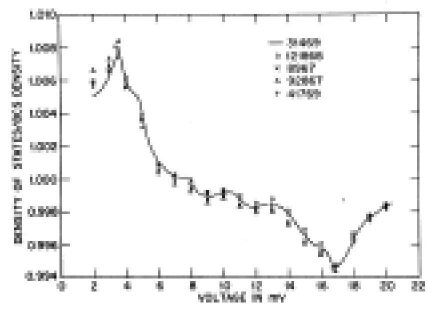
and tunnelling data

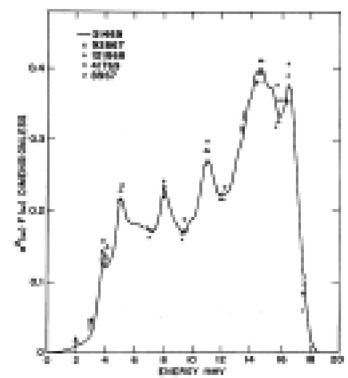


Scalapino, Schreiffer Wilkins PR 148 264 (1966)



Sn: Rowell et al PRB 3 1971





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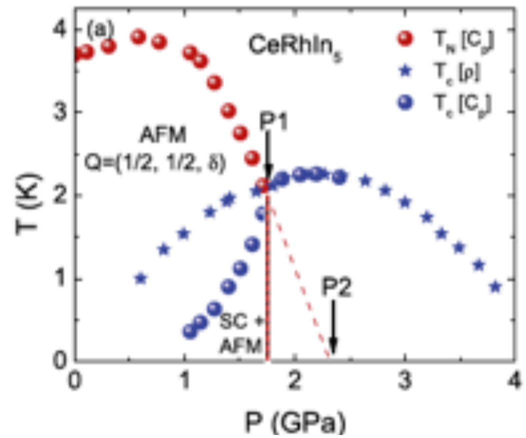
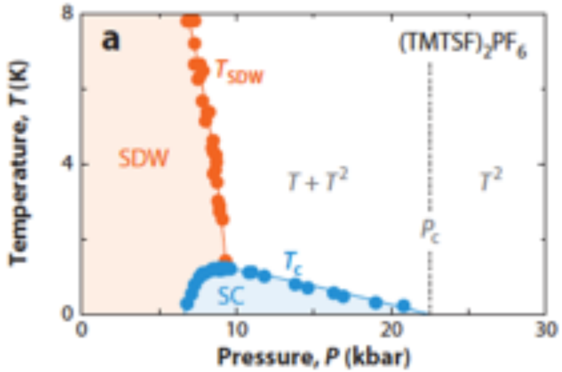
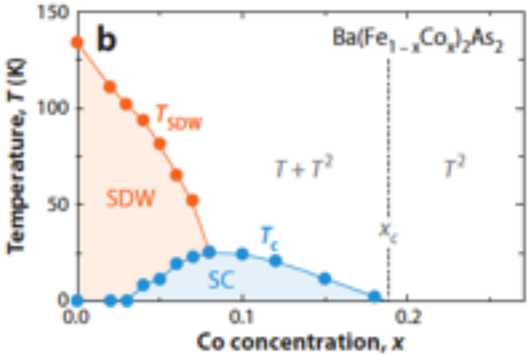
Non-phonon-mediated SC

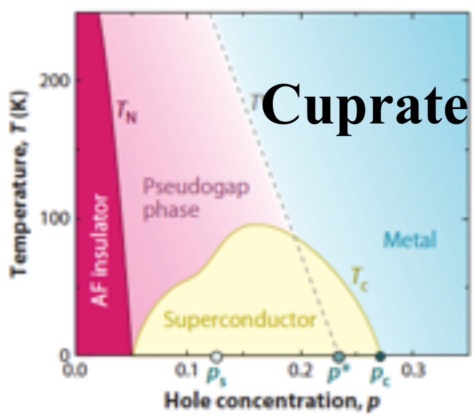
example:





Clear association, across many different systems, of proximity of superconductivity to antiferromagnetic phase





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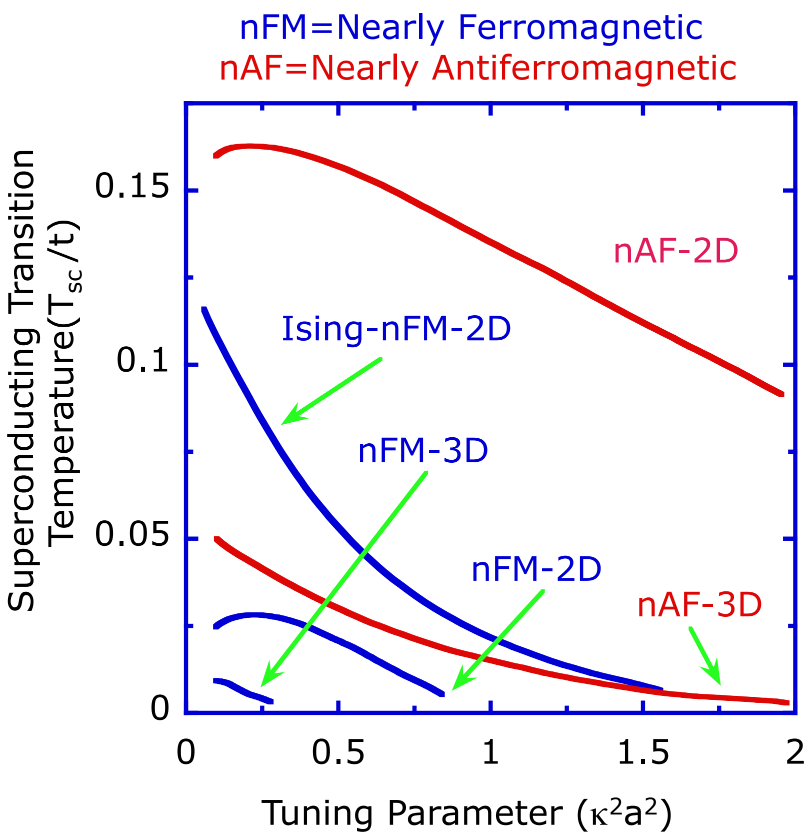
Eliashberg calculations: spin fluctuations



2D antiferromagnetic fluctuations are special

Monthoux and Lonzarich PRB59, 14598 (1999)

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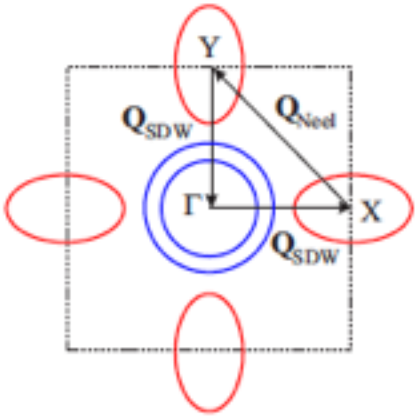
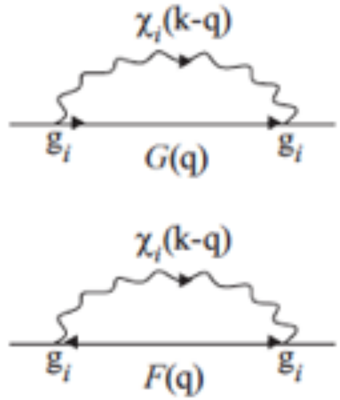
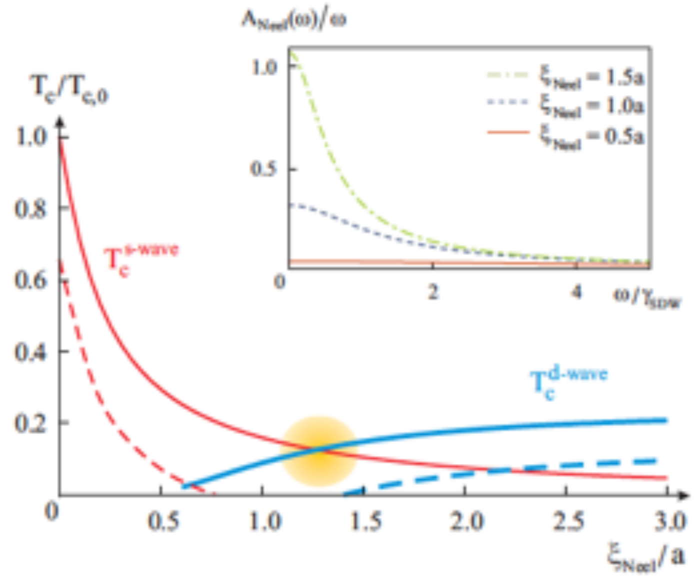
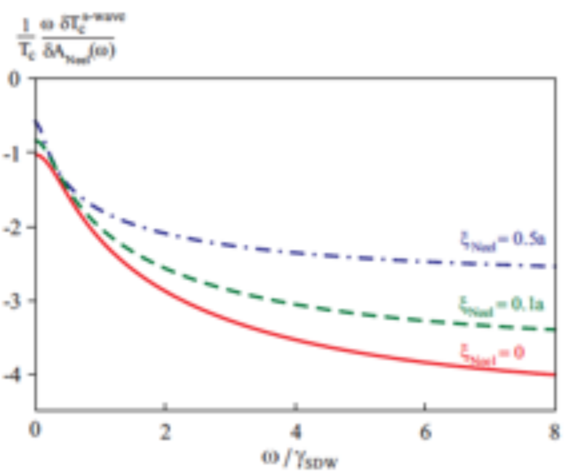
Pnictides: 2 kinds of spin flucts







Phys. Rev. Lett. 110, 117004 (2013)



Strong pair breaking effect of \`wrong' kind of spin flucts

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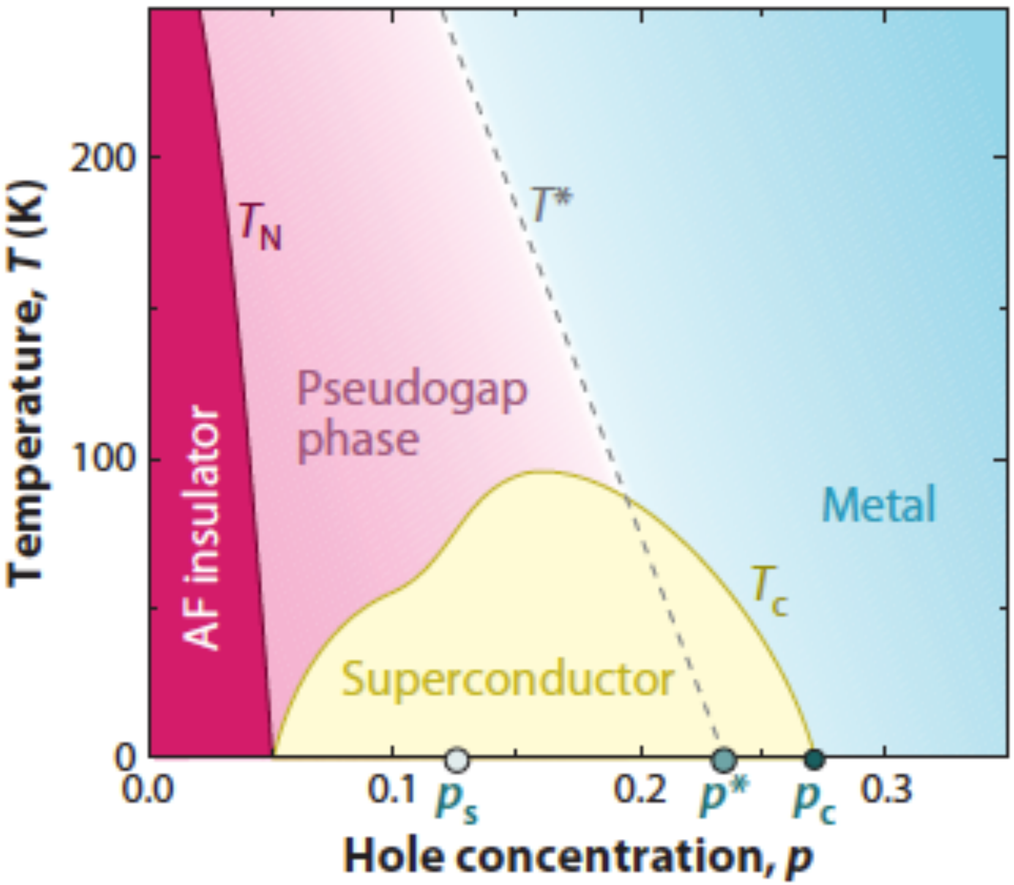
Copper Oxide Superconductivity the Mott Insulator and the Pseudogap



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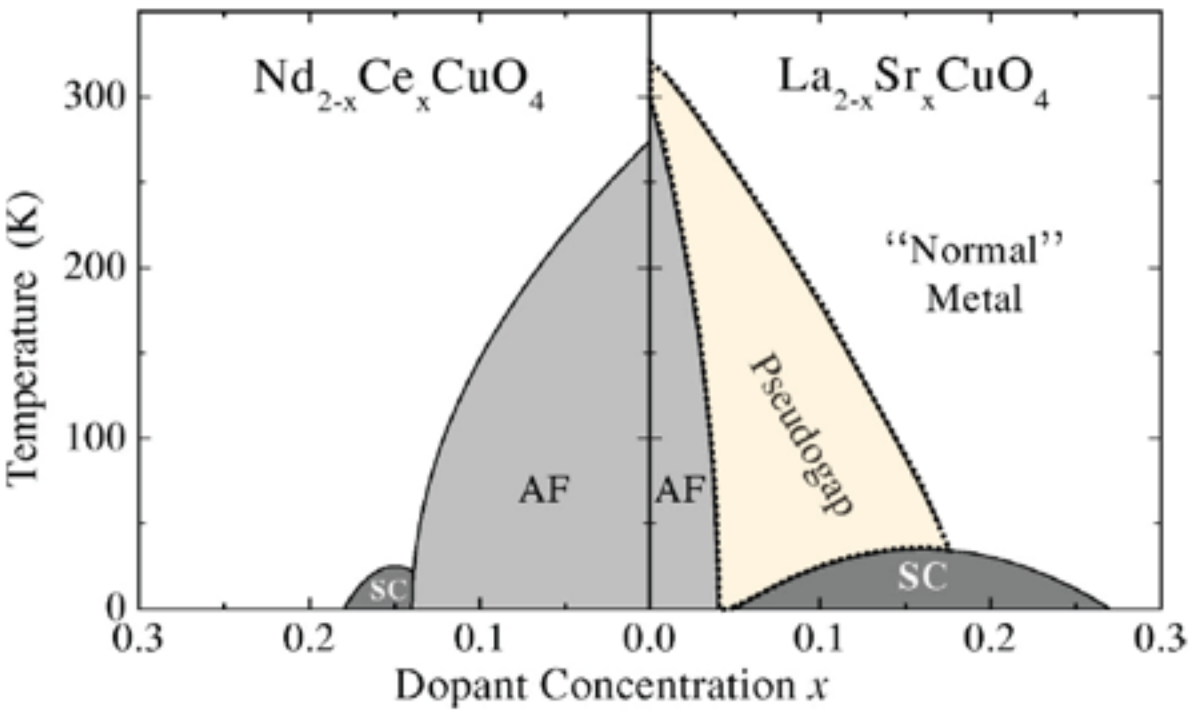
The Pseudogap: a phenomenon of hole doped cuprates

Damascelli *et al.*, Rev. Mod. Phys 75, 2 (2003)



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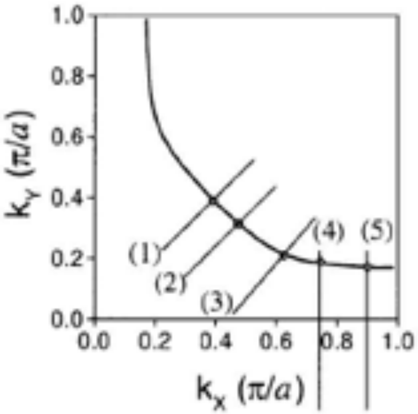
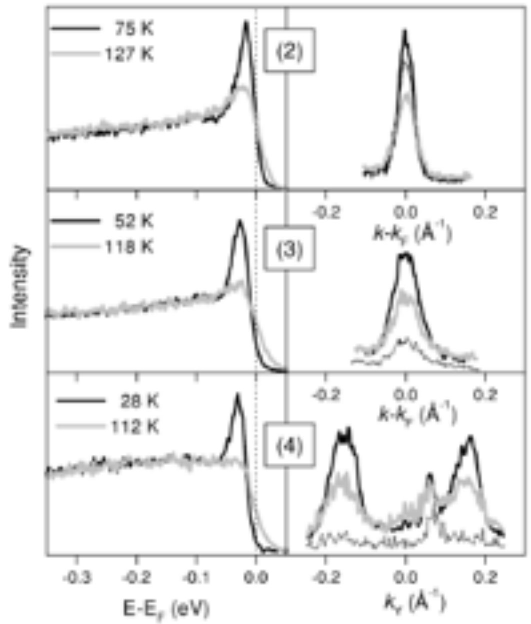
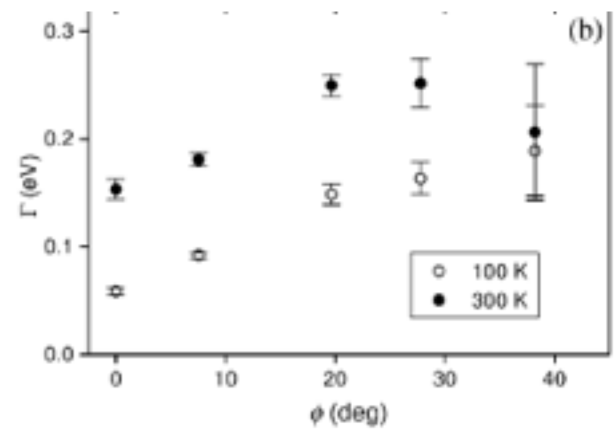
Key features of the pseudogap

Momentum space differentiation: ARPES







Valla et al PRL 2000

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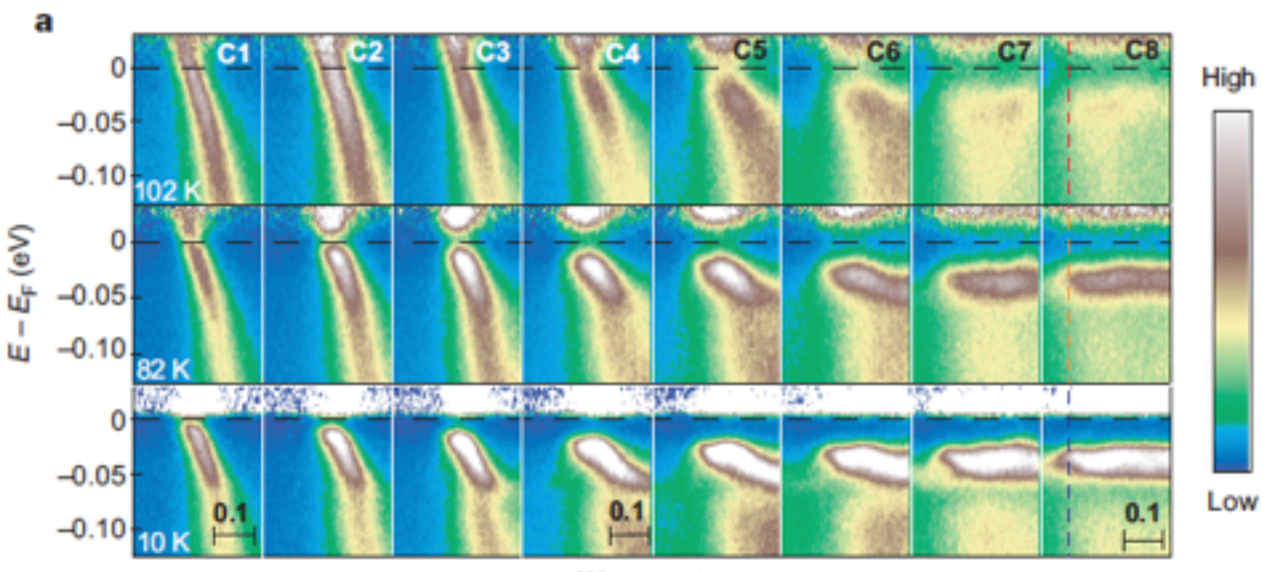
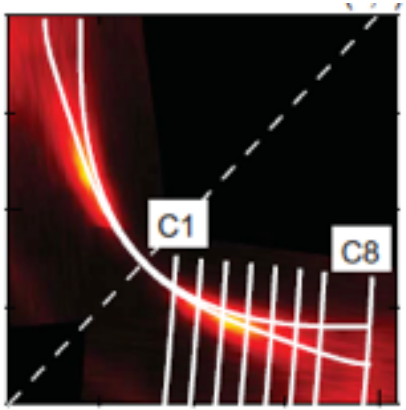
Key features of the pseudogap

Momentum space differentiation (optimally doped) evolves to pseudogap (underdoped)





S. Lee et al, Nature 450, p. 81 (2007)

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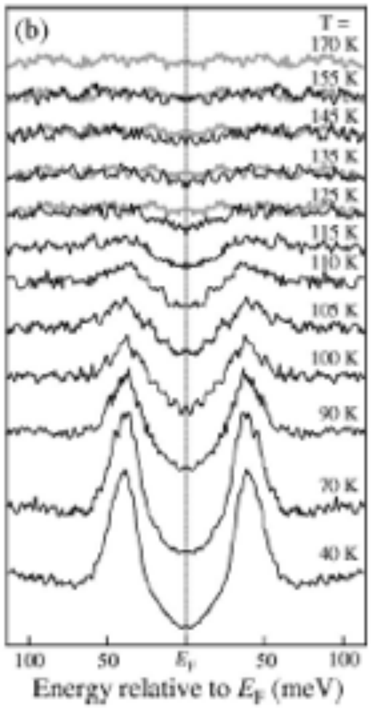
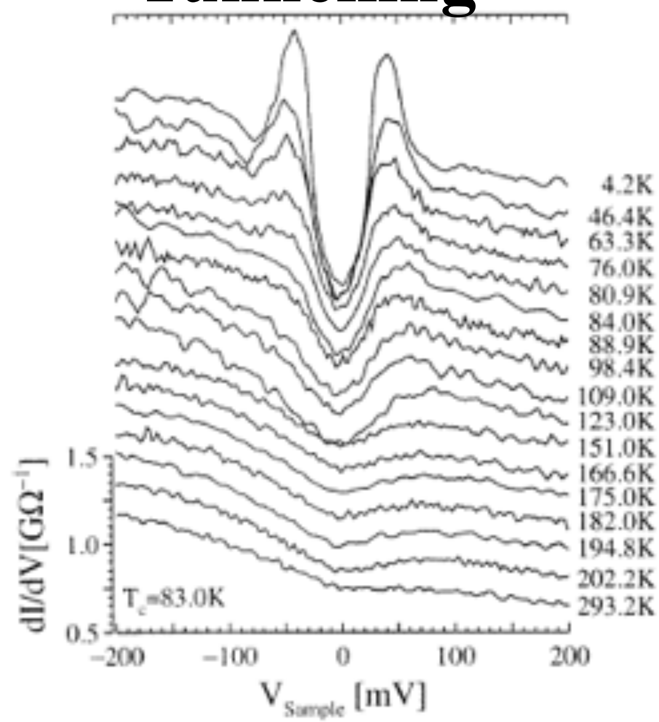
PG Signatures in ARPES and tunneling not so strong

ARPES



Sato et al PRL 89 067005 (2002)

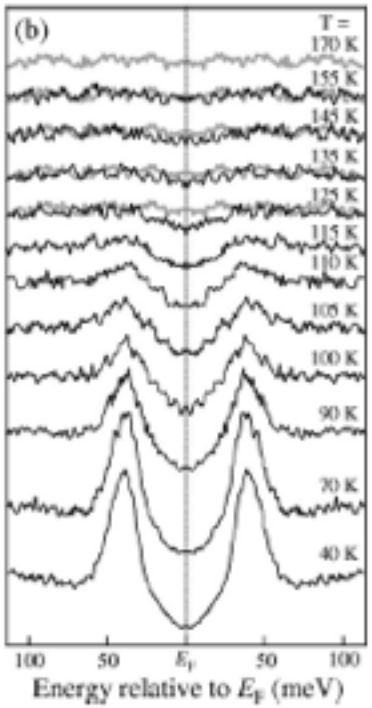
Tunnelling



Renner et al PRL 80 149 (1998)

DOS Maximum in PG becomes minimum in SC state

ARPES



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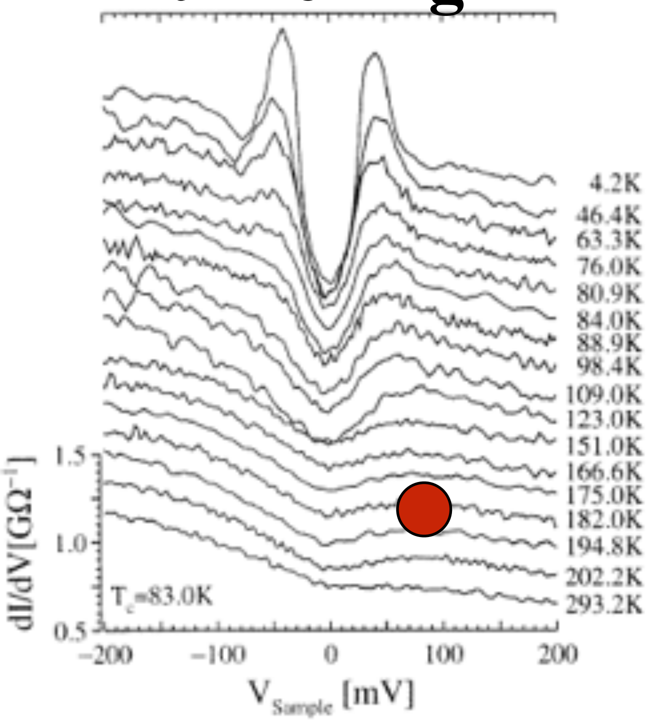

Renner et al PRL 80 149 (1998)

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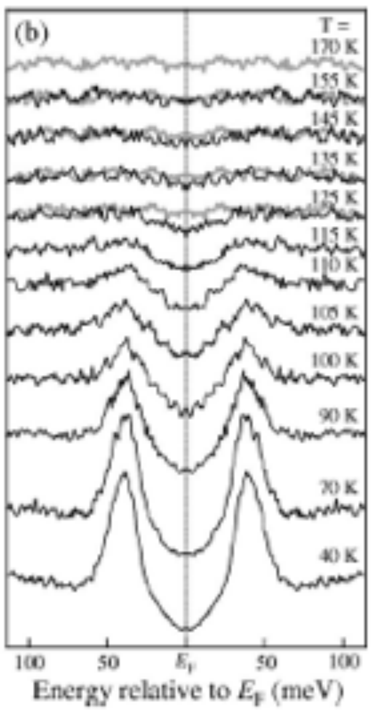
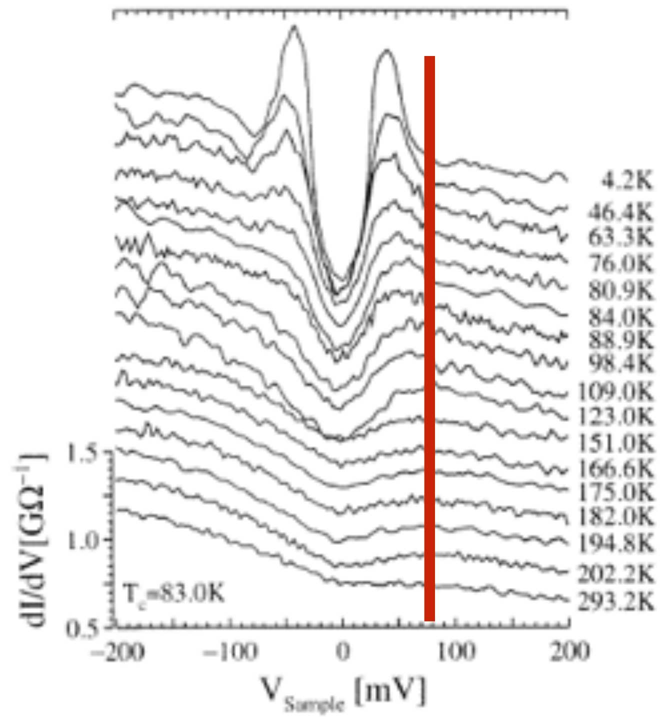


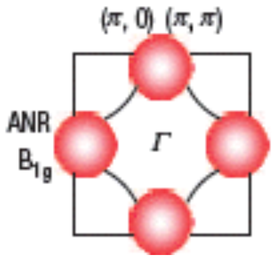
Sato et al PRL 89 067005 (2002)

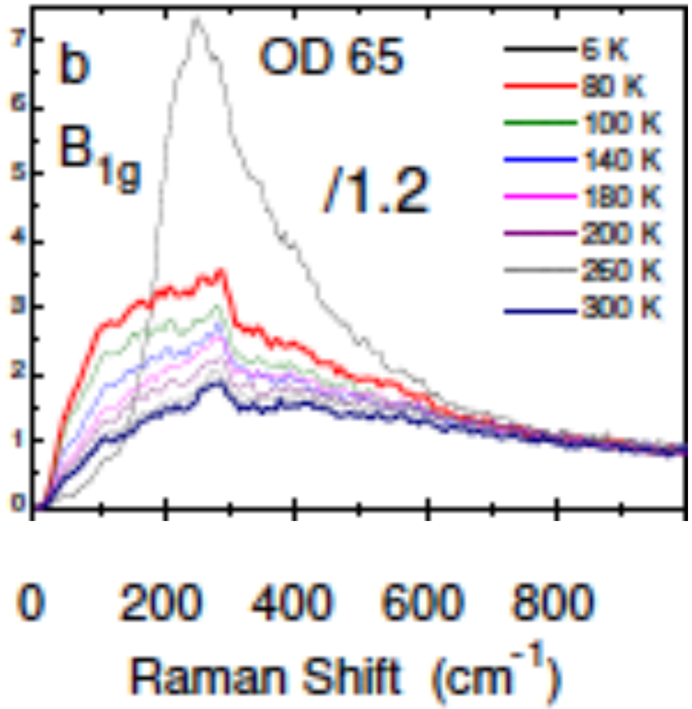
Tunnelling

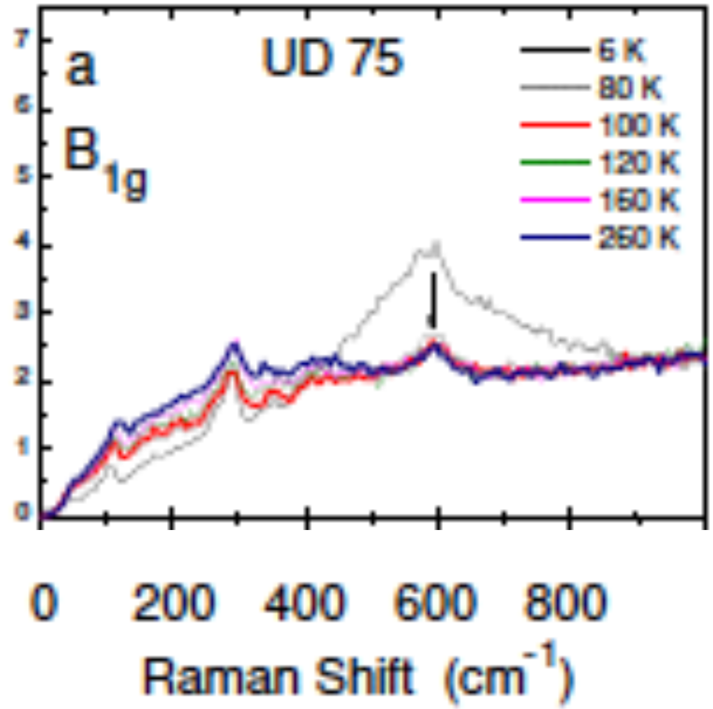


Renner et al PRL 80 149 (1998)

PG also in 2 particle probes: e.g. B_{1g} Raman Scattering



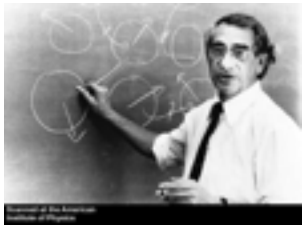




A. Sacuto et al arXiv:1209.3171

Theory: The 2D `Hubbard model'

$$\mathbf{H} = -\sum_{ij} t_{i-j} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$



P.W. Anderson said

The 2d Hubbard model captures the physics of high-Tc superconductivity

Last decade: dynamical mean field theory solution of Hubbard model

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A. Georges

DMFT

G. Kotliar

Electron self energy: infinite x infinite matrix

$$\Sigma^{\alpha_1\alpha_2}(\omega) = \sum_{a} f_a^{\alpha_1\alpha_2}\ \Sigma^a_{DMFT}(\omega)$$

DMFT: approximate as sum of small number a=1…N of functions

Determined from auxiliary quantum impurity model with self-consistently determined hybridization function

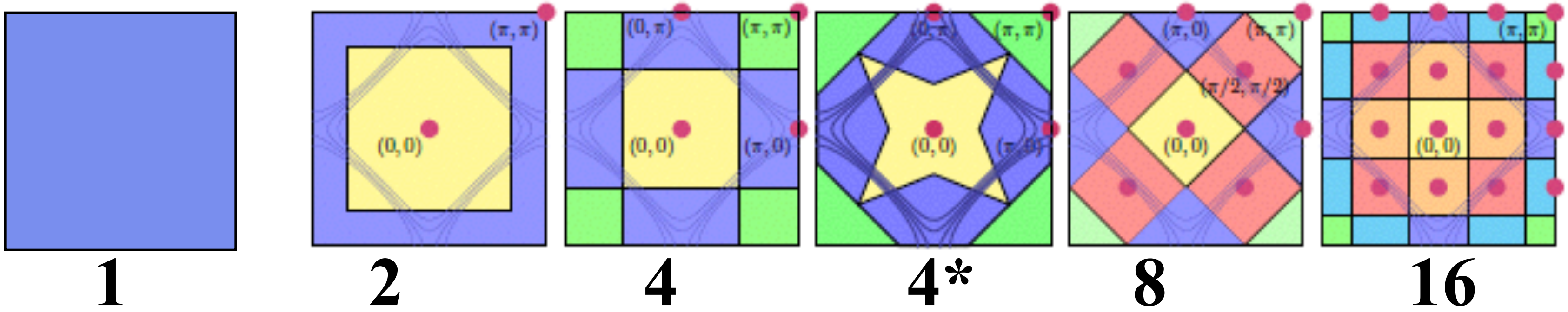
different choices of f: different 'flavors' of approximation.

N->infinity: recover original model

Momentum space version of DMFT

M. H. Hettler, M. Mukherjee, M. Jarrell, and H. R. Krishnamurthy
Phys. Rev. B **61**, 12739 (2000)

tile Brillouin zone: choose N momenta K_a, draw an equal area patch around each one



$$\Sigma_{\mathbf{p}}(\omega) \rightarrow \Sigma_{\mathbf{p}}^{\mathbf{approx}}(\omega) = \sum_{\mathbf{a}} \phi_{\mathbf{a}}(\mathbf{p})\Sigma_{\mathbf{a}}(\omega)$$

$\phi_{\mathbf{a}}(\mathbf{p}) = 1$ **if p is in the patch containing K_a and is 0 otherwise**

Find Σ_a from N-site quantum impurity model + self consistency condition

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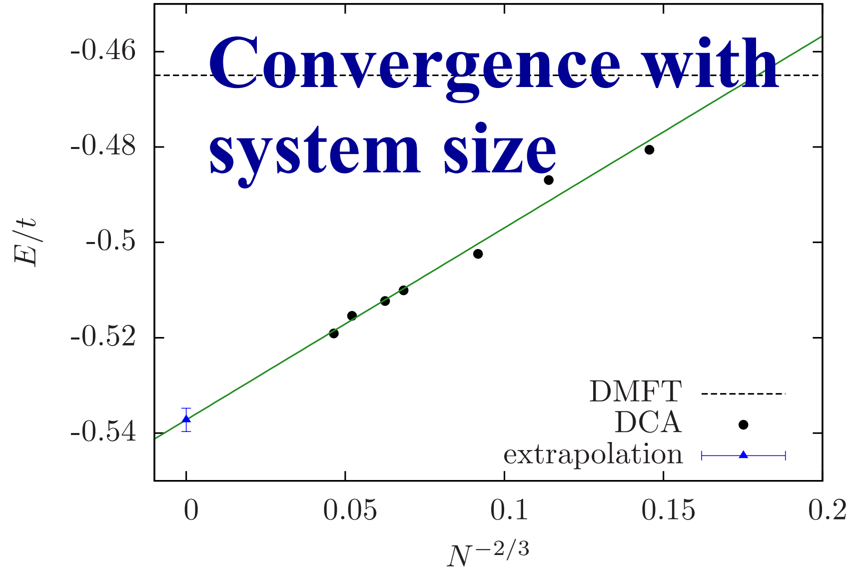
Status: high T, N~100 accessible.

3D Hubbard. U=8t, n=1



Temp=0.4t

Fuchs, **Gull**, et al PRL 106 030401 (2011)

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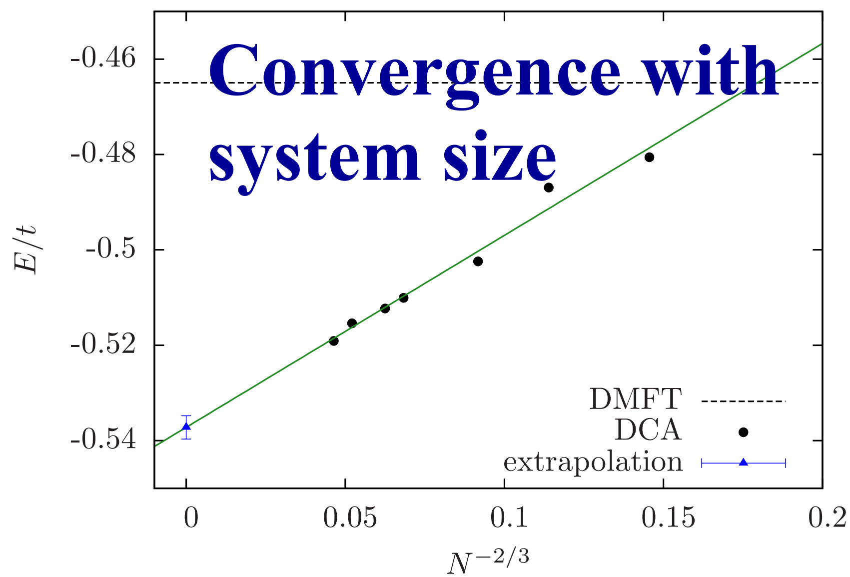
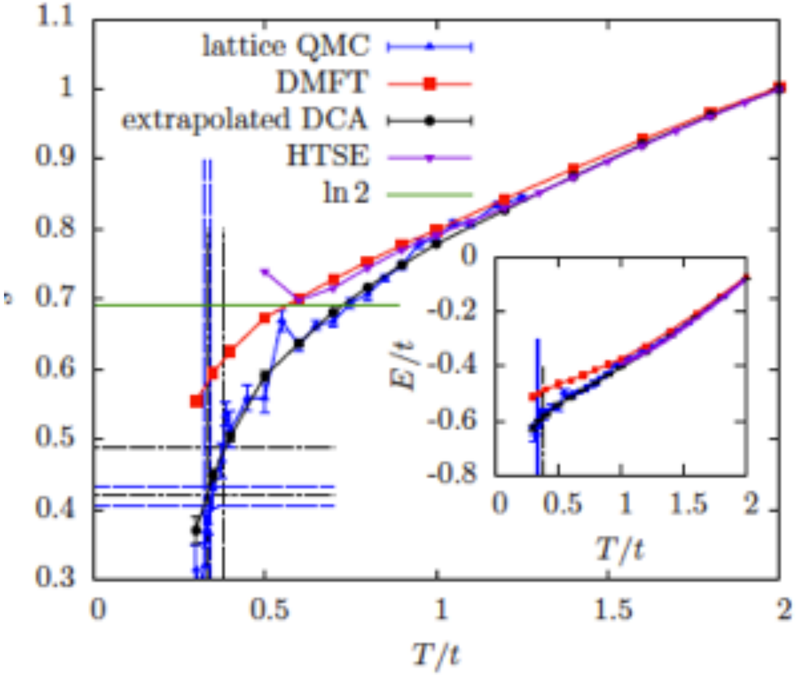
Status: high T, N~100 accessible.

3D Hubbard. U=8t, n=1





Temp=0.4t

Fuchs, **Gull**, et al PRL 106 030401 (2011)

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In 'interesting' $U \sim U_{Mott}$, low T regime

We can do:

Clusters up to N~16
U~7t
T~t/60
(surveys: 8 site--spot checks, N=16)

Comparisons up to N=16: ~25% accuracy

E. Gull, O. Parcollet, P. Werner, and A.J.M, Phys. Rev. B80, 245102 (2009).

N Lin, E. Gull, and A. J. M, Phys. Rev. B82, 045104 (2010).

E. Gull, M. Ferrero, O. Parcollet, A. Georges, A. J. M, Phys. Rev. B82 155101 (2010).

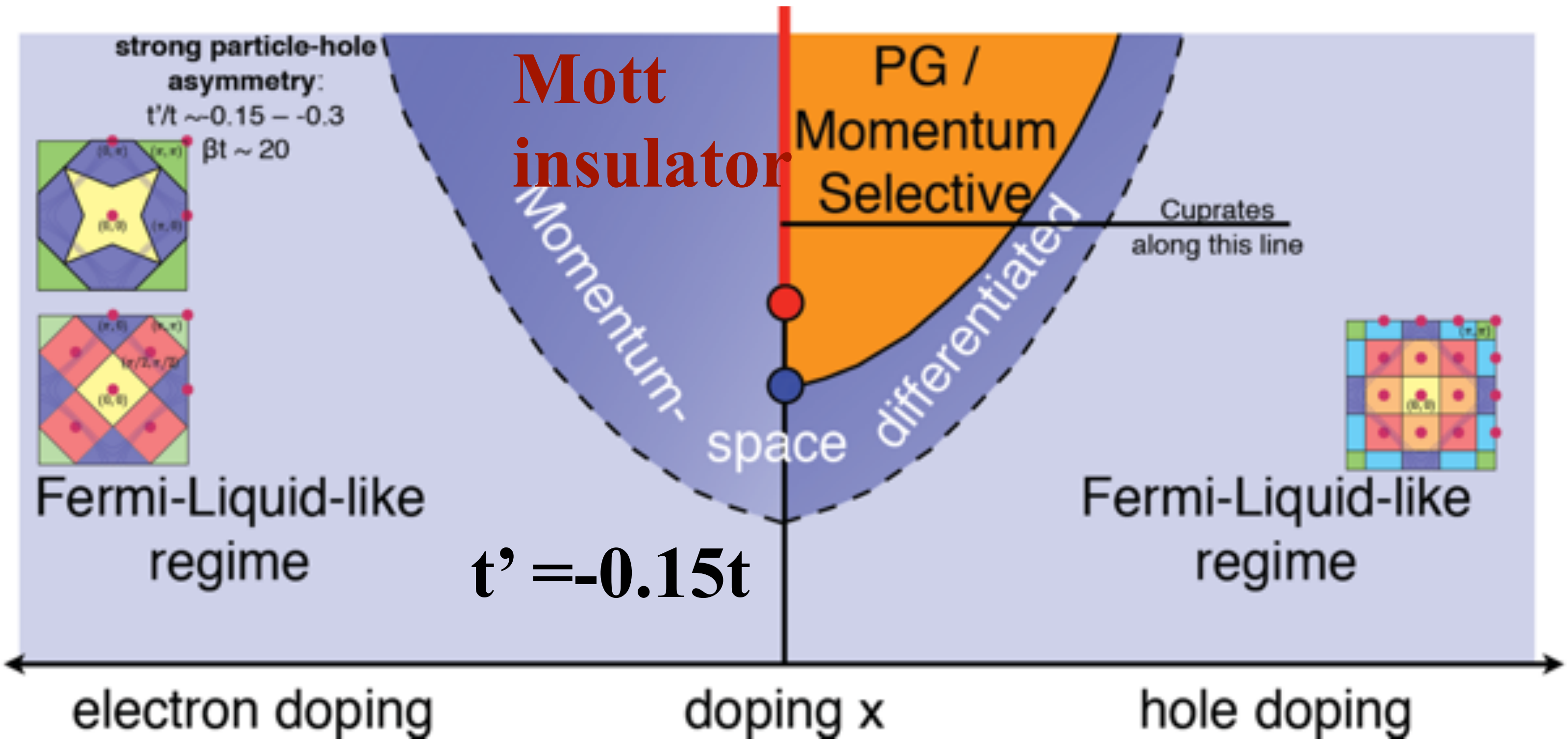
Analogy:

Density functional <=> 'Luttinger Ward functional

Kohn-Sham equations <=> quantum impurity model

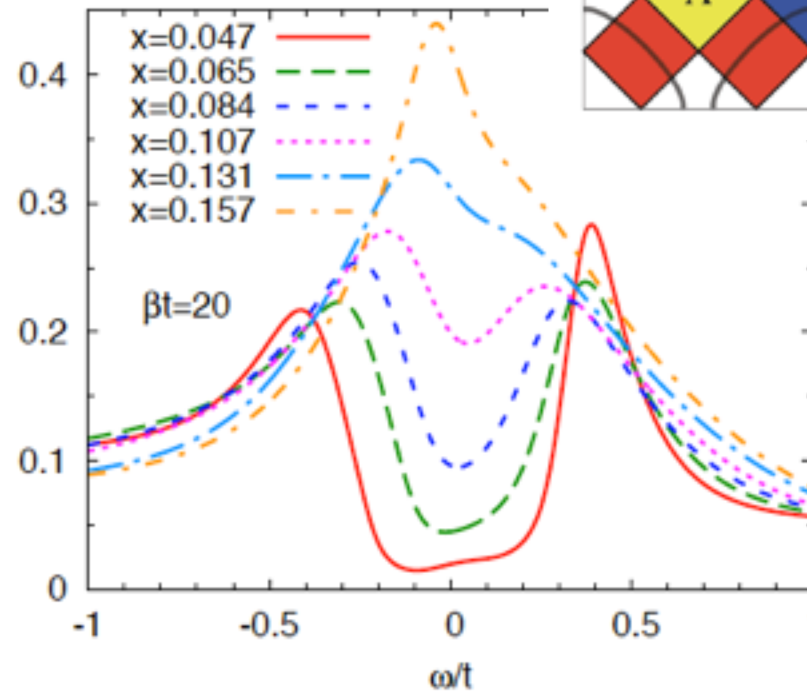
Particle density <=> electron Green function

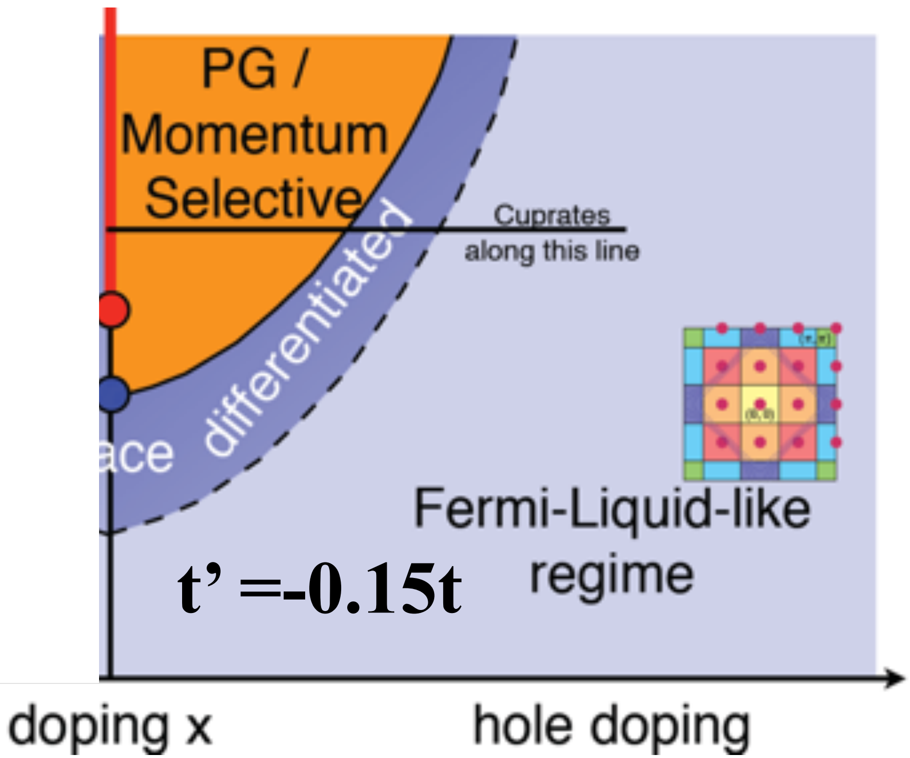
Phase diagram: Mott insulator separated from fermi liquid by pseudogap for hole but not electron doping



P. Werner, E. Gull, O. Parcollet and A. J. Millis, Phys. Rev. B 79, 045120 (2009)
E. Gull, O. Parcollet, P. Werner, and A. J. Millis, Phys. Rev. B 80, 045120 (2009).
Emanuel Gull, Michel Ferrero, Olivier Parcollet, Antoine Georges, Andrew J. Millis, Phys. Rev. B82 155101 (2010).

Intermediate phase: partially gapped fermi surface

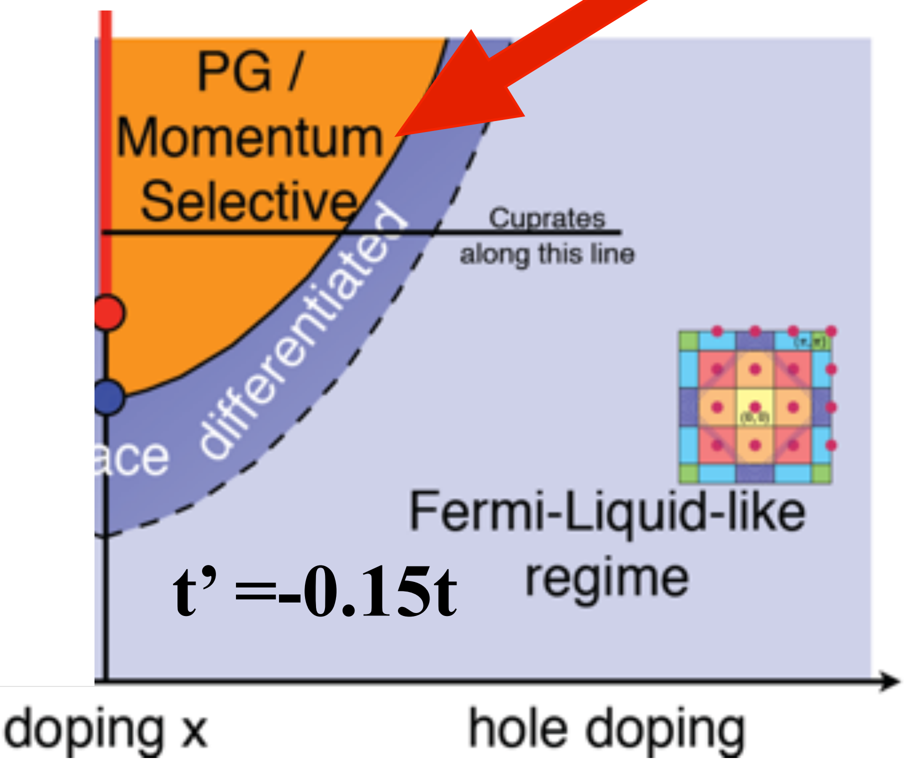


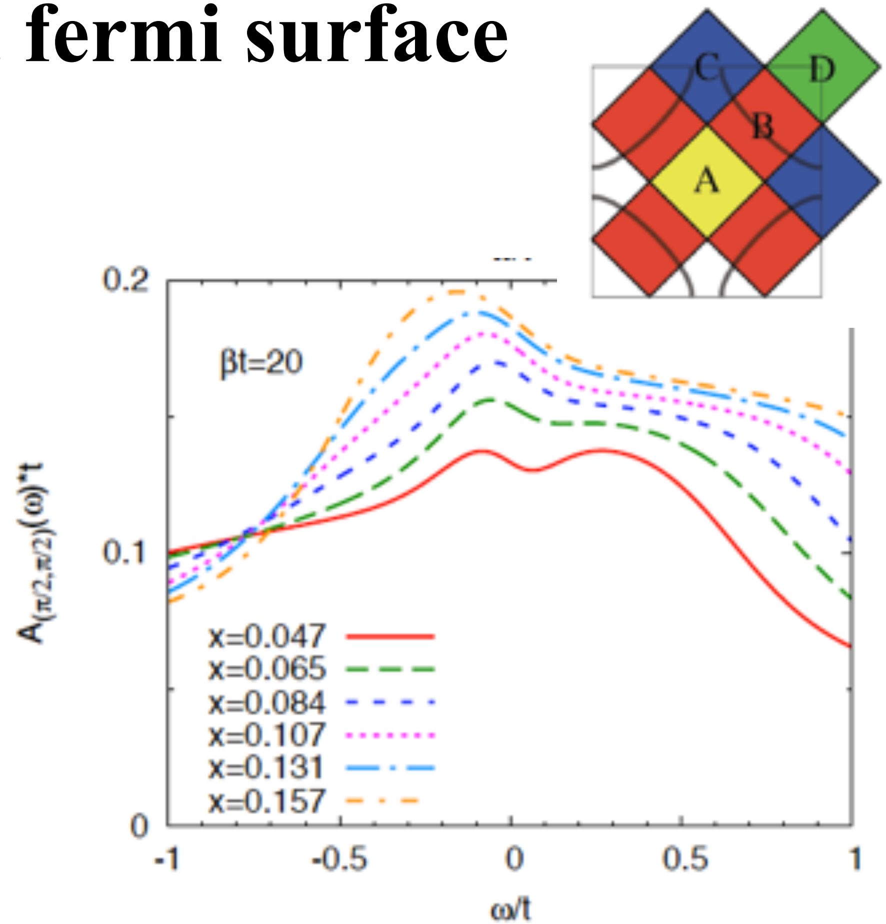


t' =-0.15t

gap opens in momentum sector C

Intermediate phase: partially gapped fermi surface





but not in B

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SC in DMFT

Pioneeers: (2x2 cluster)

--Lichtenstein, Katsnelson PRB 62, R9283 (2000).
--Maier, Jarrell, Pruschke, Keller, PRL **85**, 1524 (2000).

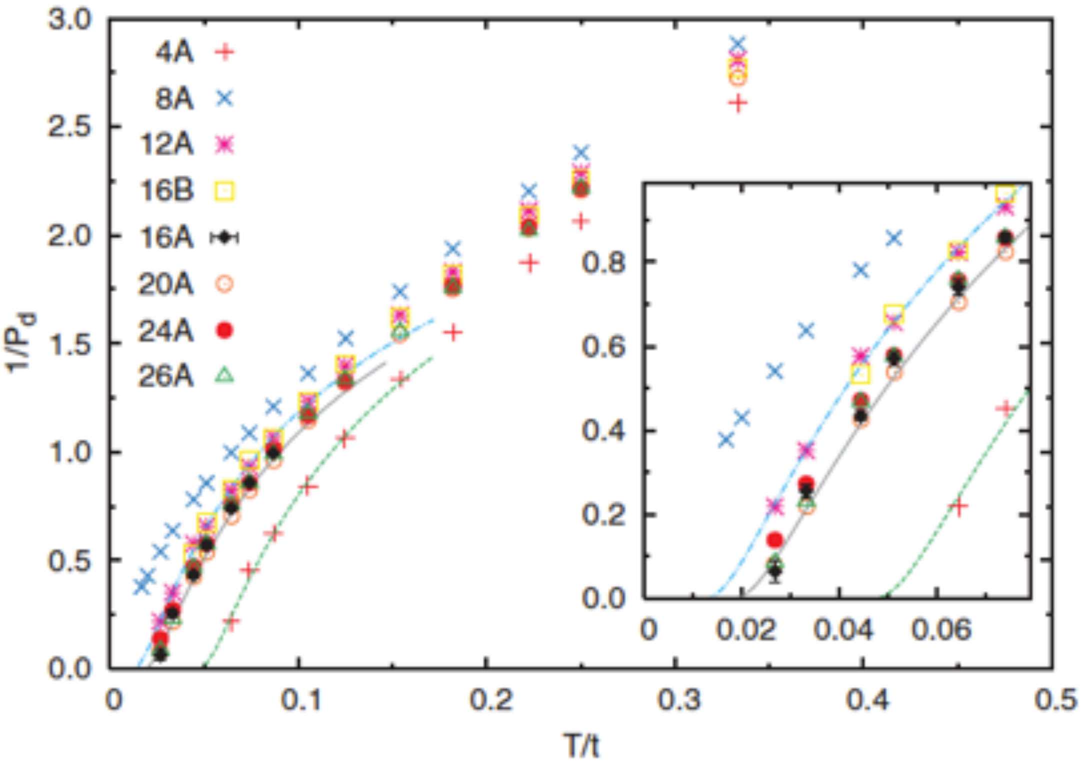
Lots of other work (mainly 2x2 clusters):

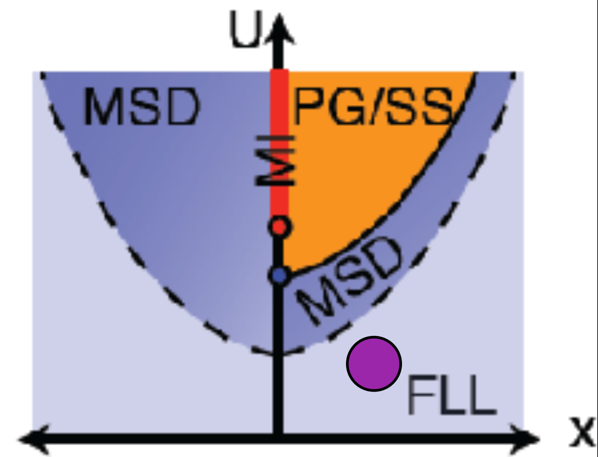
--S. S. Kancharla, B. Kyung, D. S´en´echal, M. Civelli, M. Capone, G. Kotliar and A.-M. S. Tremblay, Phys. Rev. B 77, 184516 (2008).
--T. A. Maier, D. Poilblanc, and D. J. Scalapino, Phys. Rev. Lett. 100, 237001 (2008).
--M. Civelli, M. Capone, A. Georges, K. Haule, O. Parcollet, T. D. Stanescu, and G. Kotliar, Phys. Rev. Lett. 100, 046402 (2008).
--M. Civelli, Phys. Rev. Lett. 103, 136402 (2009).
--G.Sordi,P. Śemon,K.Haule,andA.-M.S.Tremblay, Phys. Rev. Lett. 108, 216401 (2012).

Large clusters: Superconductivity established

T. A. Maier, M. Jarrell, T. Schultheiss, P. Kent and J. White, Phys. Rev. Lett. 95, 237001 (2005)

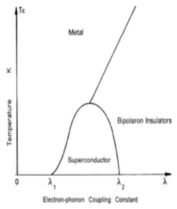
High T susceptibility: clusters up to N=26 at x=0.1 U=4t (too small for Mott phase)

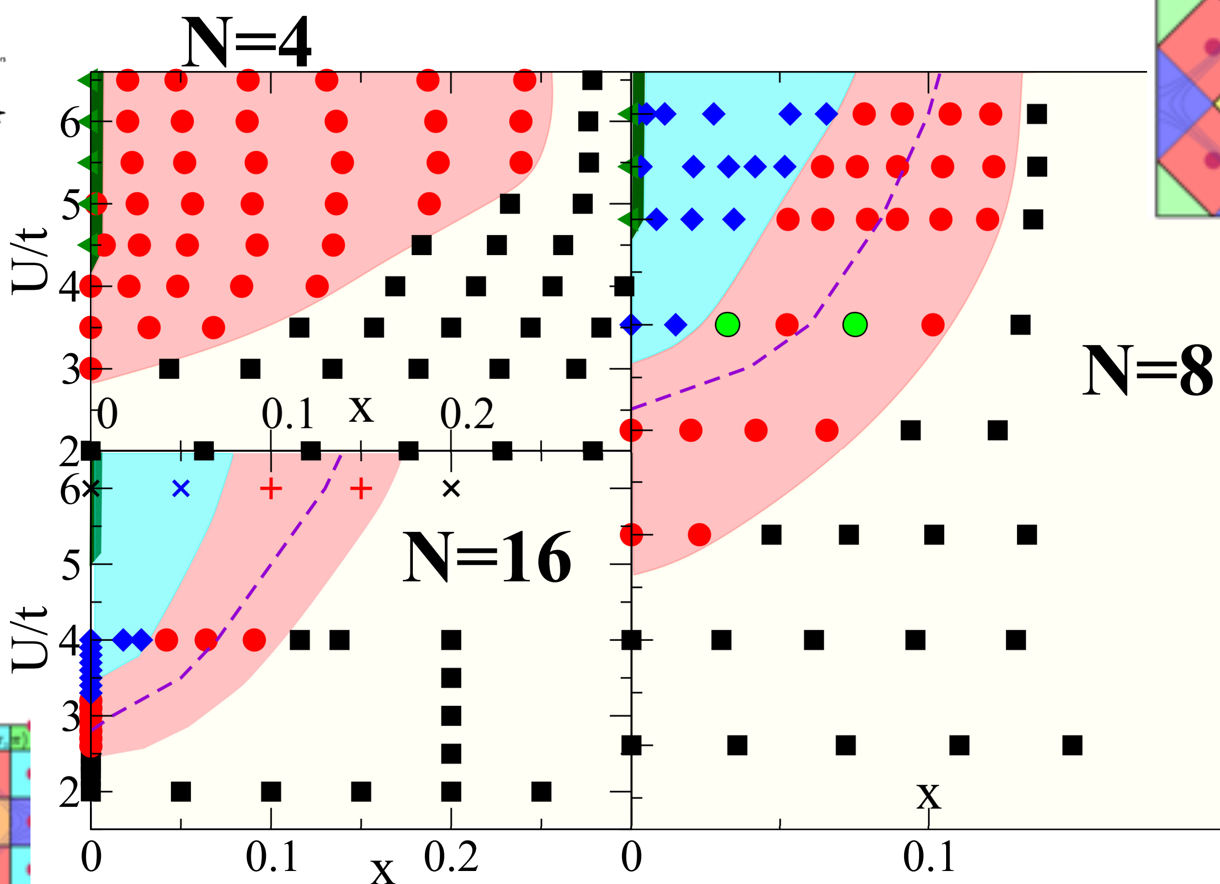


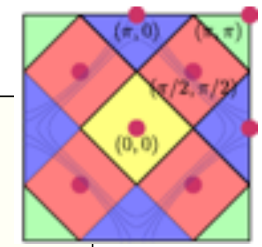


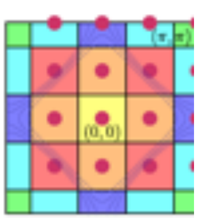
● **MJSKW point**

Phase diagram, different clusters









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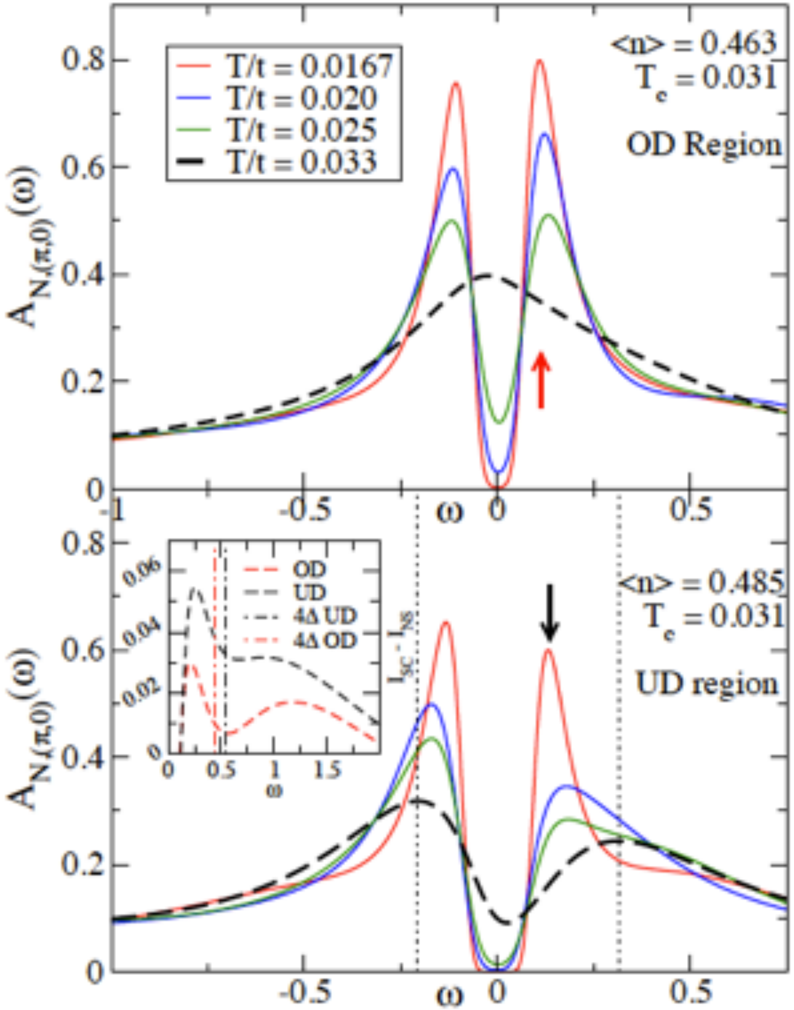
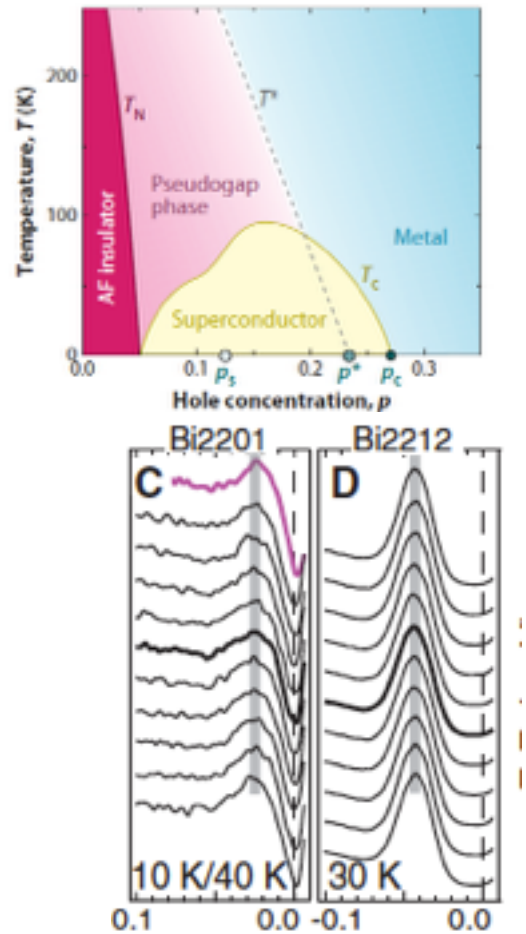
Superconductivity and the pseudogap





SC Gap smaller than PG

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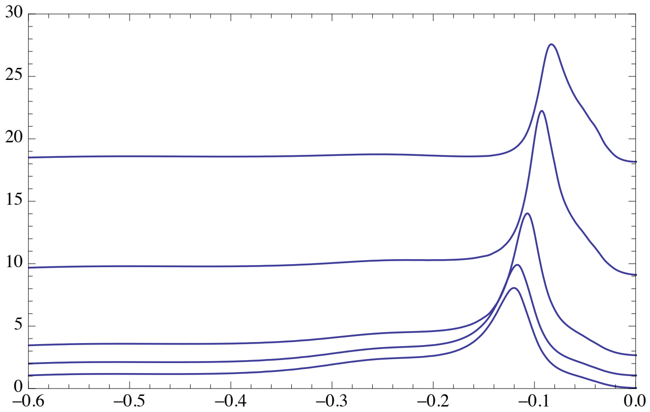
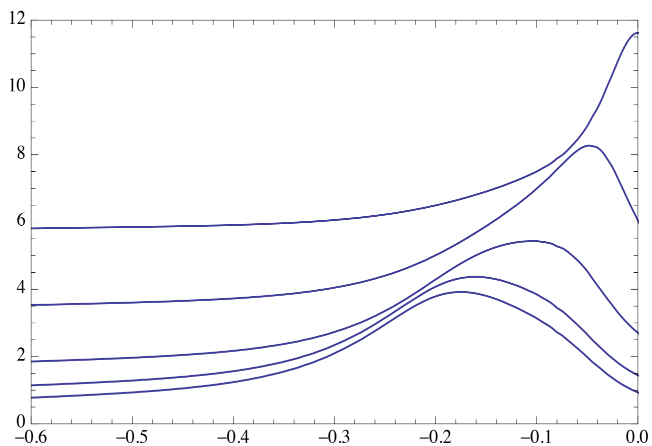
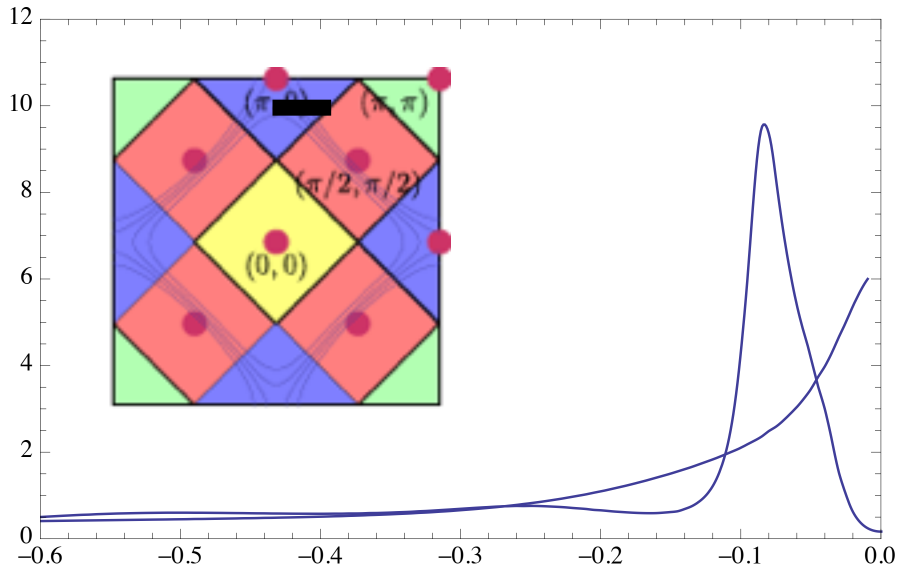
Simulated ARPES: Overdoped







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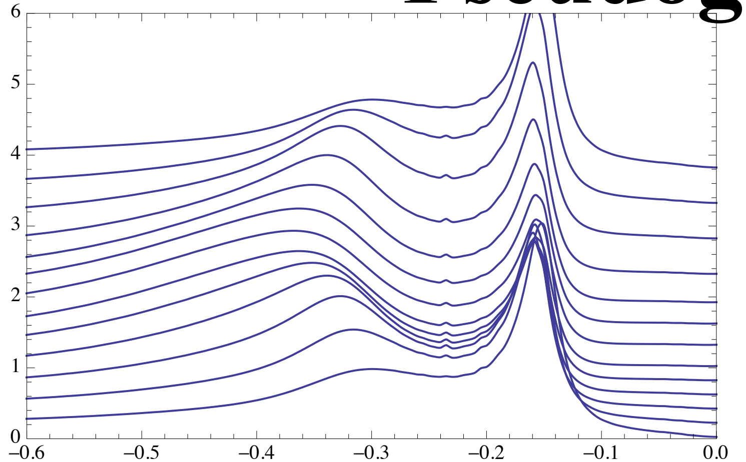
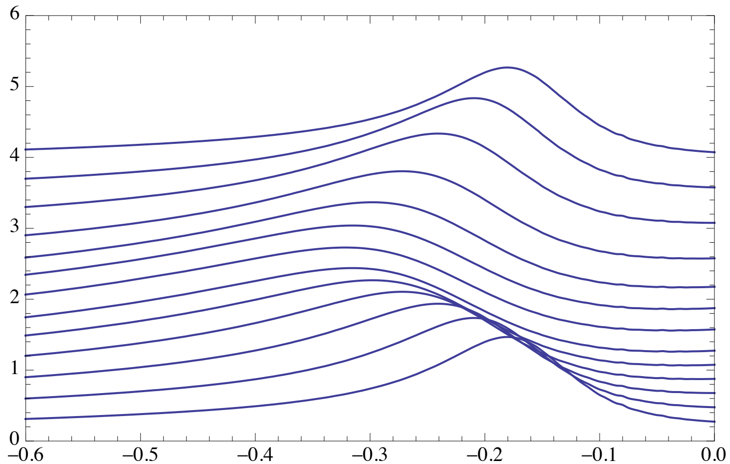
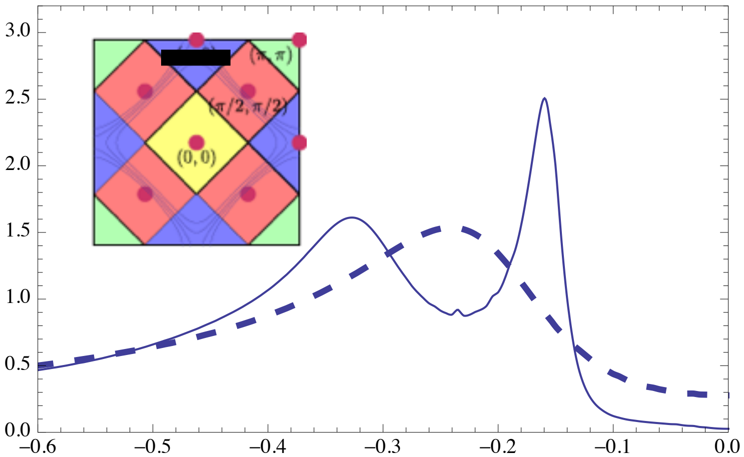
Simulated ARPES Spectra: Pseudogap regime







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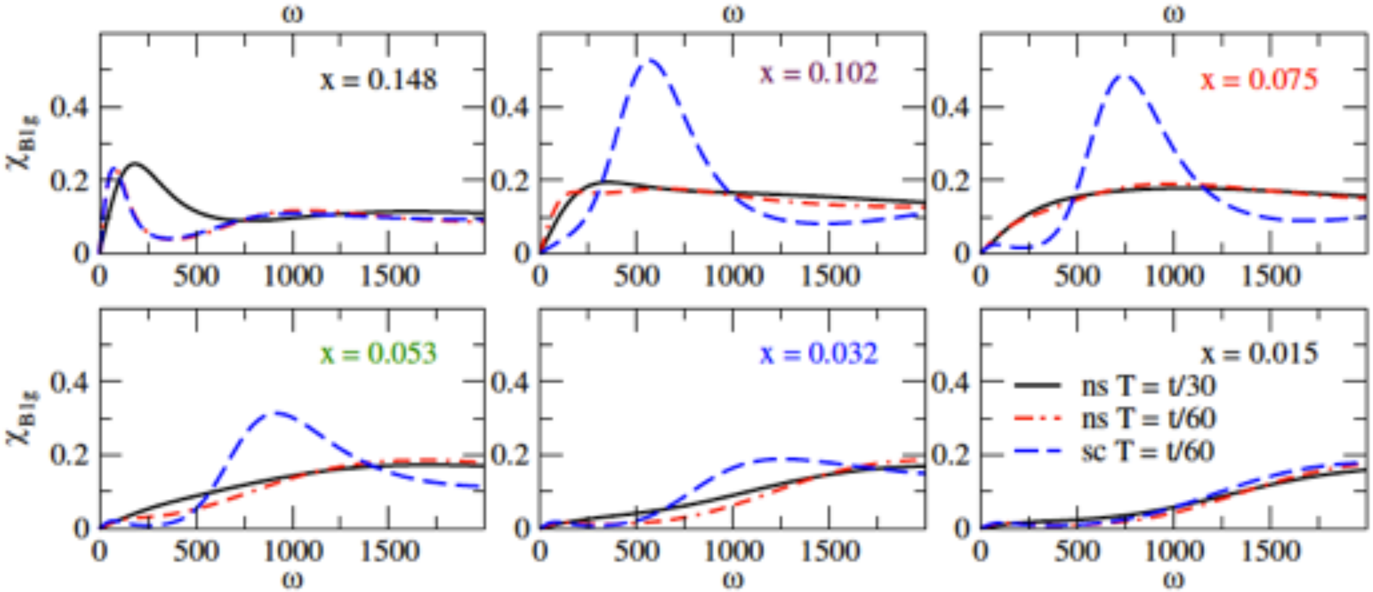
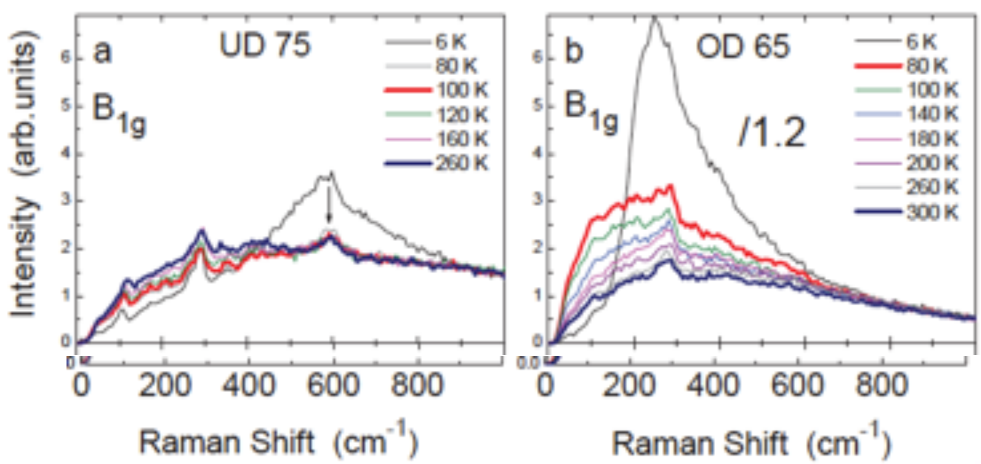
Raman scattering



Calculation



Data
Sacuto et al

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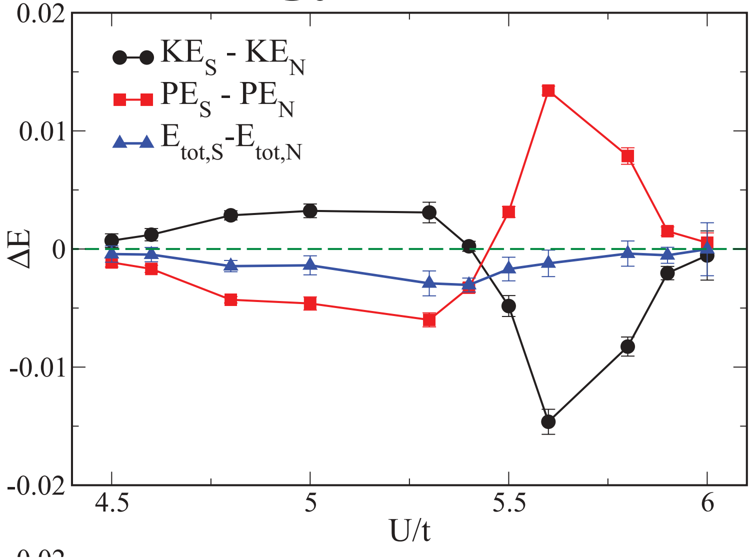
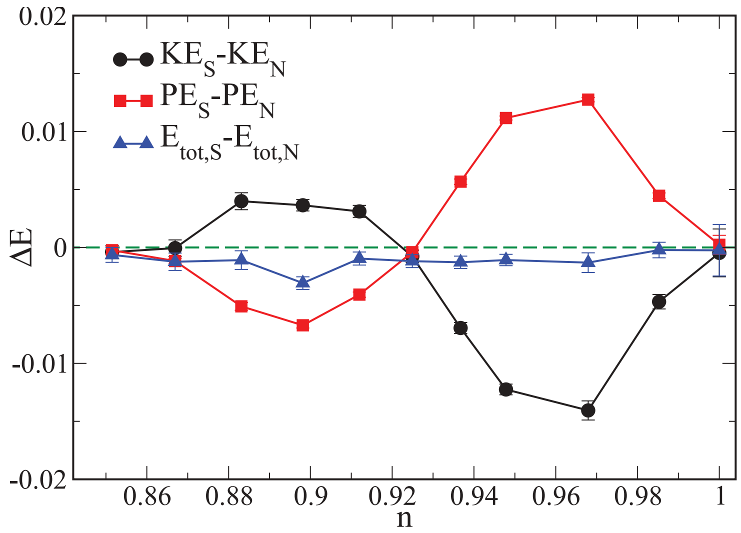
energetics of superconductivity

Energy of U



Energy vs n



In the pseudogap regime, superconductivity is associated with a decrease of kinetic energy

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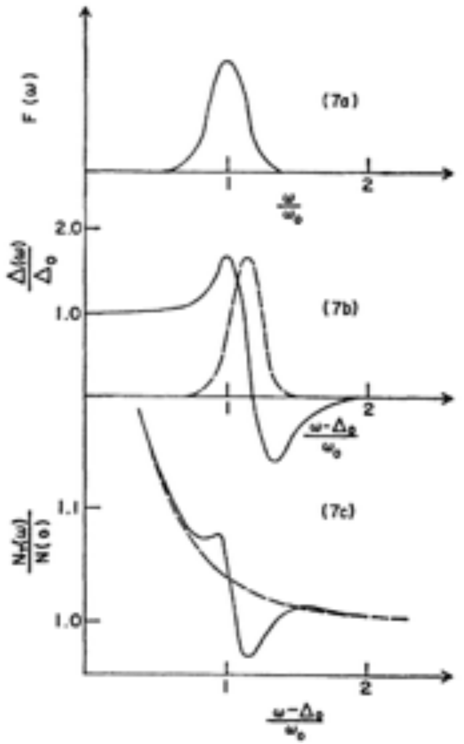
Pairing Mechanism

Lead



Conventional superconductors: look at frequency dependence of complex gap function

$$\Delta(\omega) = \frac{\Sigma^{A}(\omega)}{1 - \frac{\Sigma^{N}(\omega)}{\omega}}$$

Scalapino, Schreiffer,
Wilkins, PBR 148 263 1966

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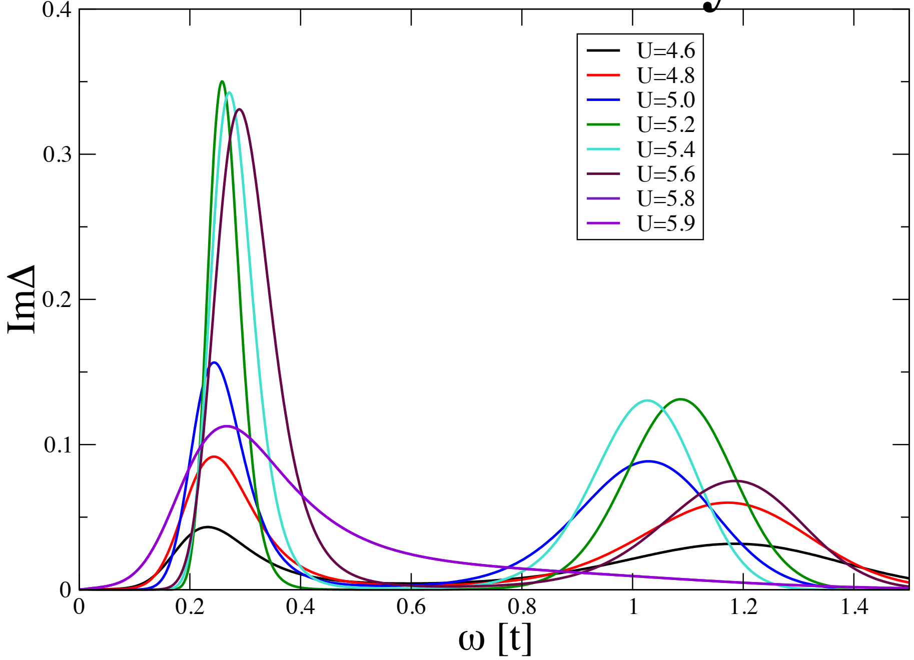
Pairing Mechanism: Hubbard Model

$$\Delta(\omega) = \frac{\Sigma^{A}(\omega)}{1 - \frac{\Sigma^{N}(\omega) - \Sigma^{N}(-\omega)^{\star}}{2\omega}}$$

Half Filled: vary U



Continue $\Delta(i\omega_n)$
find $\Delta''(\omega > 0) \geq 0$

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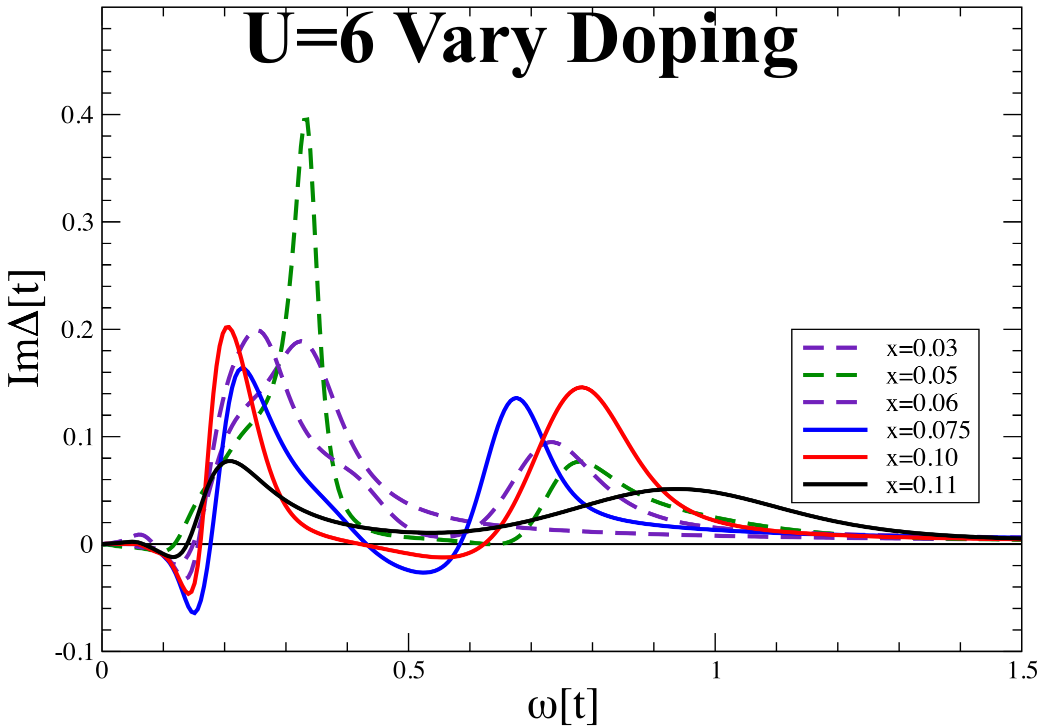
Pairing Mechanism: Hubbard Model

$$\Delta(\omega) = \frac{\Sigma^{A}(\omega)}{1 - \frac{\Sigma^{N}(\omega) - \Sigma^{N}(-\omega)^{\star}}{2\omega}}$$

Thanks to Doug Scalapino for discussion



Nonzero only for w<t.
Peak at low frequency unusual.

Negative values: continuation errors in self energies.

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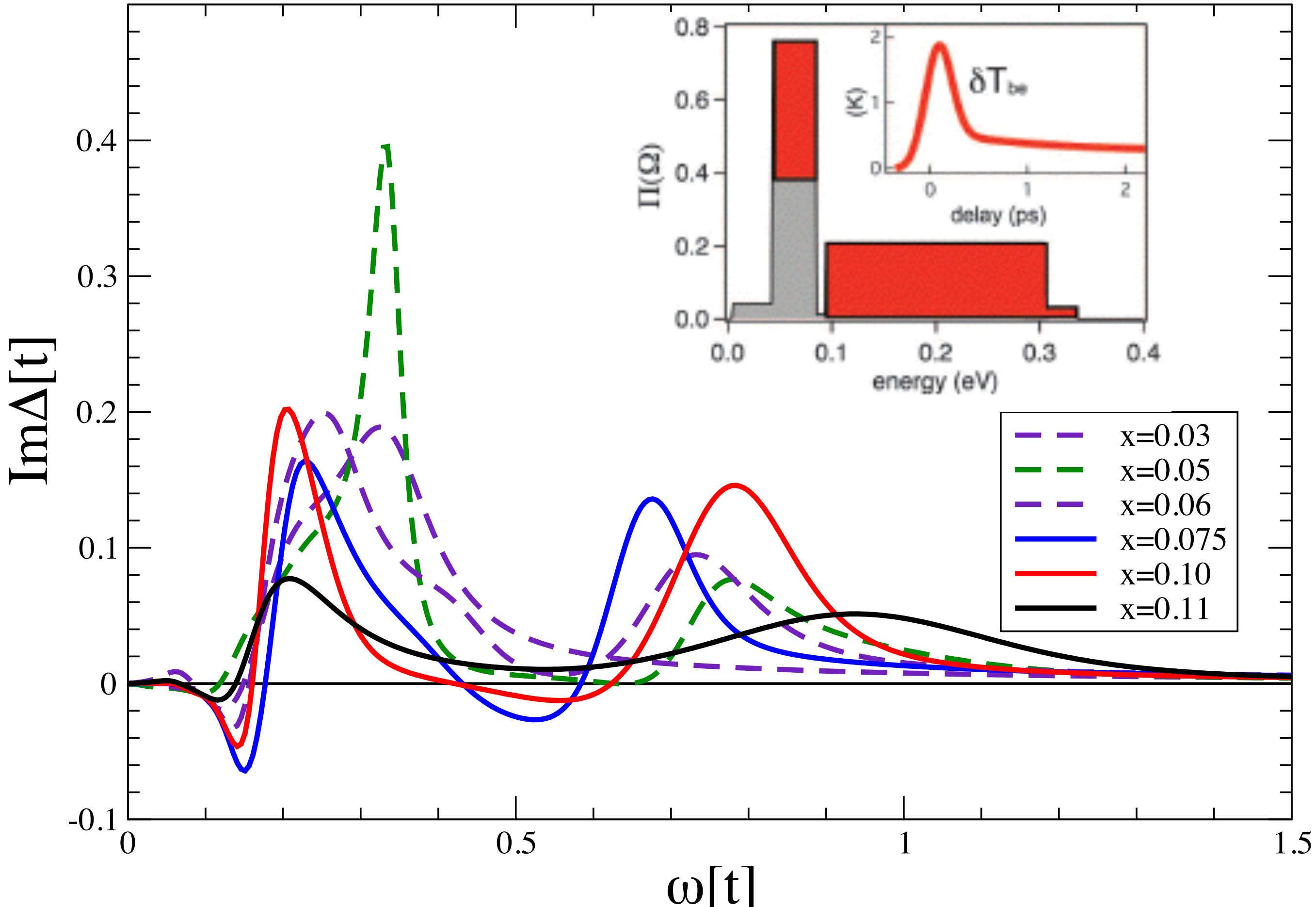
?Coincidence?



Inset: experimental estimate of pairing boson spectral function
Dal Conte et al, Science, 335 6067 (2012)

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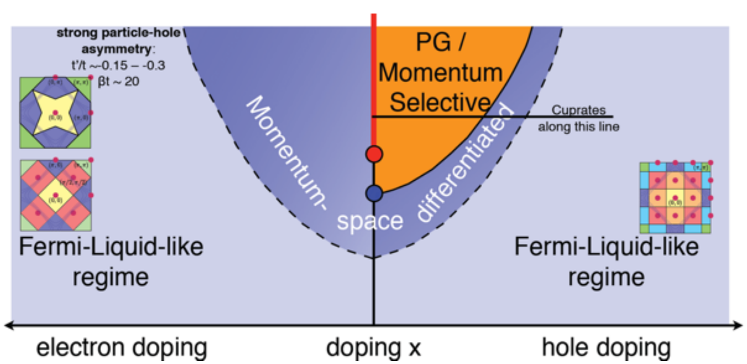
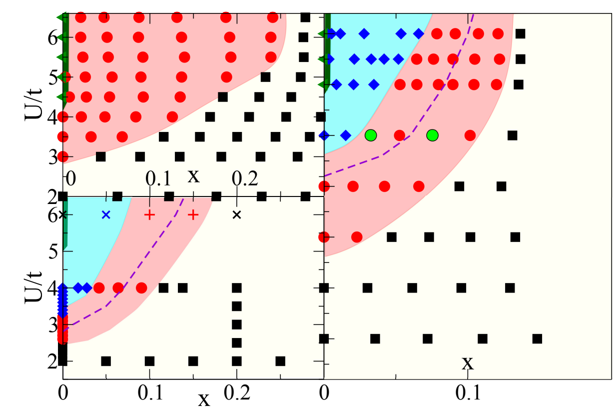
Summary: Hubbard model

—Superconductivity, found via numerical solution (no assumption re which modes are important).
—maximized near PG phase boundary and due to Unconventional 'pairing glue'
—Scale of SC is <<U



$\Delta_{PG} > \Delta_{SC}$



Now can ask: what is missing from the Hubbard model? How do we optimize Tc?

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