Superconductivity and the Pseudogap in the 2D Hubbard Model: Results and implications for cuprates

Coda: slowly fluctuating density wave order in pnictides; ?implications? for cuprates

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Support: NSF-DMR-1308236

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Nan Lin
Columbia->Finance

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Two approaches to cuprate physics

Revel in the specifics

Identify the essentials

This talk: focus on (what I conceive of as) the essential behavior—

superconductivity and pseudogap

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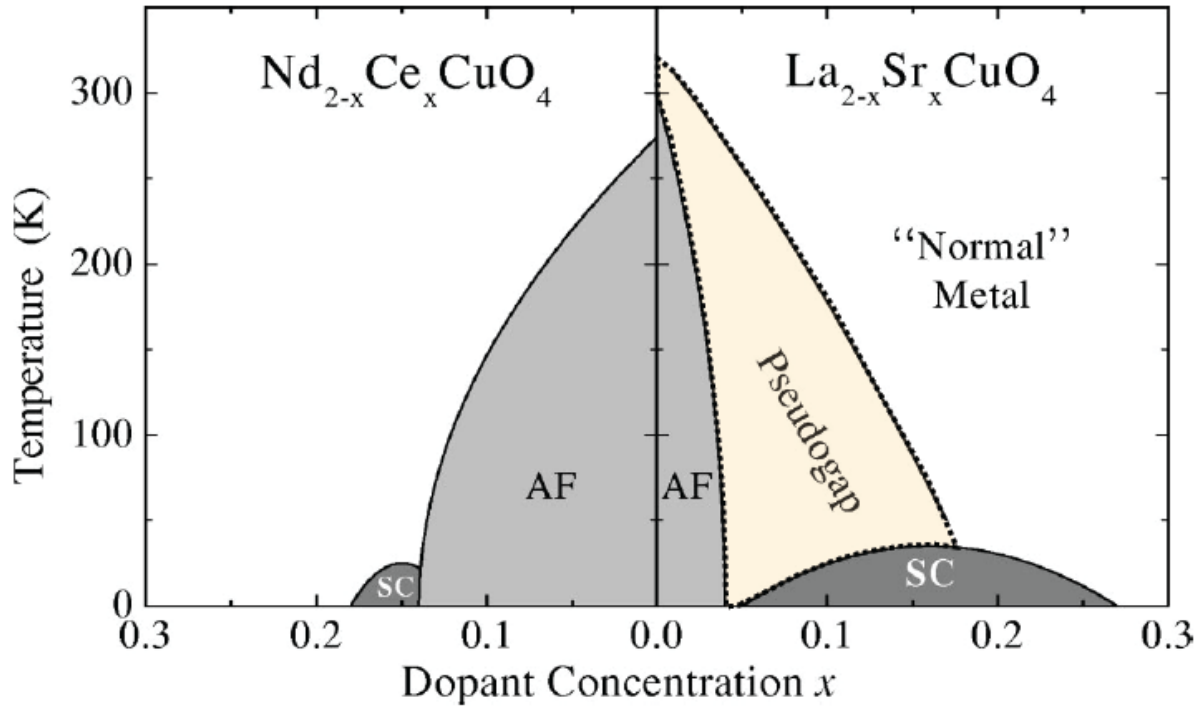
Key features of high-Tc cuprates

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



Mott insulating phase, giving rise (on hole but not electron doping) to an anomalous normal state characterized by important differences between zone-diagonal and zone face states, leading to a pseudogap unstable at lower T to a dx^2-y^2 symmetry superconducting state

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The Hubbard Model

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

1988: P.W. Anderson said

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

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

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More specifically

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We have reasonable confidence that

The 2d square-lattice Hubbard model has

- **momentum space differentiation (anisotropic scattering)**
- **dx^2-y^2 superconductivity in a superconducting dome with Tc 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

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We believe, but don't have complete and convincing evidence, that the 2d Hubbard model lacks, at least in any strong form

- **CDW order (independent of spin stripes)**
- **nematicity**

IMPLICATION: CDW order and nematicity are `epiphenomena': things that occur, and are interesting, but are not fundamental to the physics of the cuprates

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?Why do we believe this?

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References

- Emanuel Gull, Michel Ferrero, Olivier Parcollet, Antoine Georges, Andrew J. Millis, Phys. Rev. B82 155101 (2010)
- E. Gull, O. Parcollet and A. J. Millis, Phys. Rev. Lett. 110 216406 (2013)
- E. Gull and A. J. Millis, Physical Review B86 241106 (2012).
- Emanuel Gull, Andrew J. Millis. Phys. Rev. B88, 075127 (2013).
- E. Gull and A. J. Millis,Phys. Rev. B90, 041110 (2014).
- E. Gull and A. J. Millis, Physical Review B91, 085116 (2015).

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See also

Talks and papers by

Tremblay
Kotliar
Civelli
Parcollet

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A. Georges

Dynamical Mean Field Theory (DMFT)

G. Kotliar

DMFT: approximation to electron self energy

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

The $\mathbf{f^a(k)}$ determine the 'flavor' of DMFT

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

$\mathbf{N \to \infty}$ recovers exact solution

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Two approaches (related; both important)

Identify interesting physics and approximations that express it

Attempt to determine properties of N->infinity solution

Approach taken in this talk

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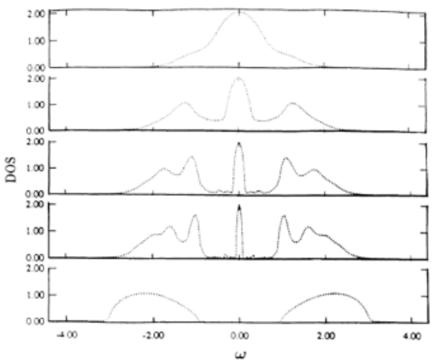
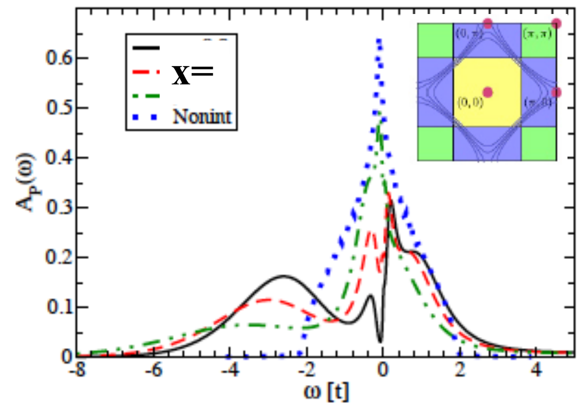
There is a long story about 'flavors' of DMFT and number of approximants (N) needed

N=1: extensive entropy midgap states



N=2,4: (over?)emphasis on singlet physics; PG just a DOS suppression



Here: present results which (we believe) are generic, representative of N->infinity limit

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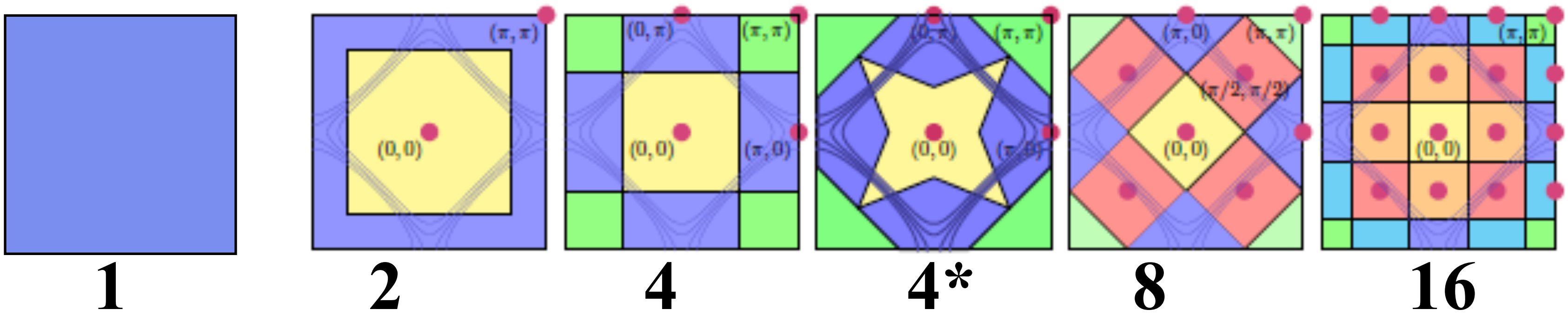
Momentum space version of DMFT

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



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

$\phi_{\mathrm{a}}(\mathrm{p}) = 1$ 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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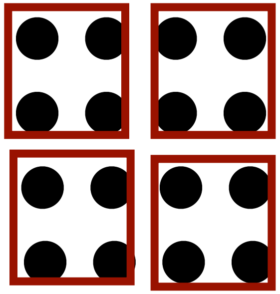
Obvious undesirable feature:

Momentum-space discontinuities

My view: interpolations that might smooth out the discontinuities are dangerous: potential for introducing new (and possibly wrong) physics.

But see T. Maier and T. Schulthess: DCA+
Phys. Rev. B 88, 115101 (2013)



Alternative (CDMFT) approach: break translational invariance. `Periodization' needed. Kotliar, Tremblay. Civelli. Sakai

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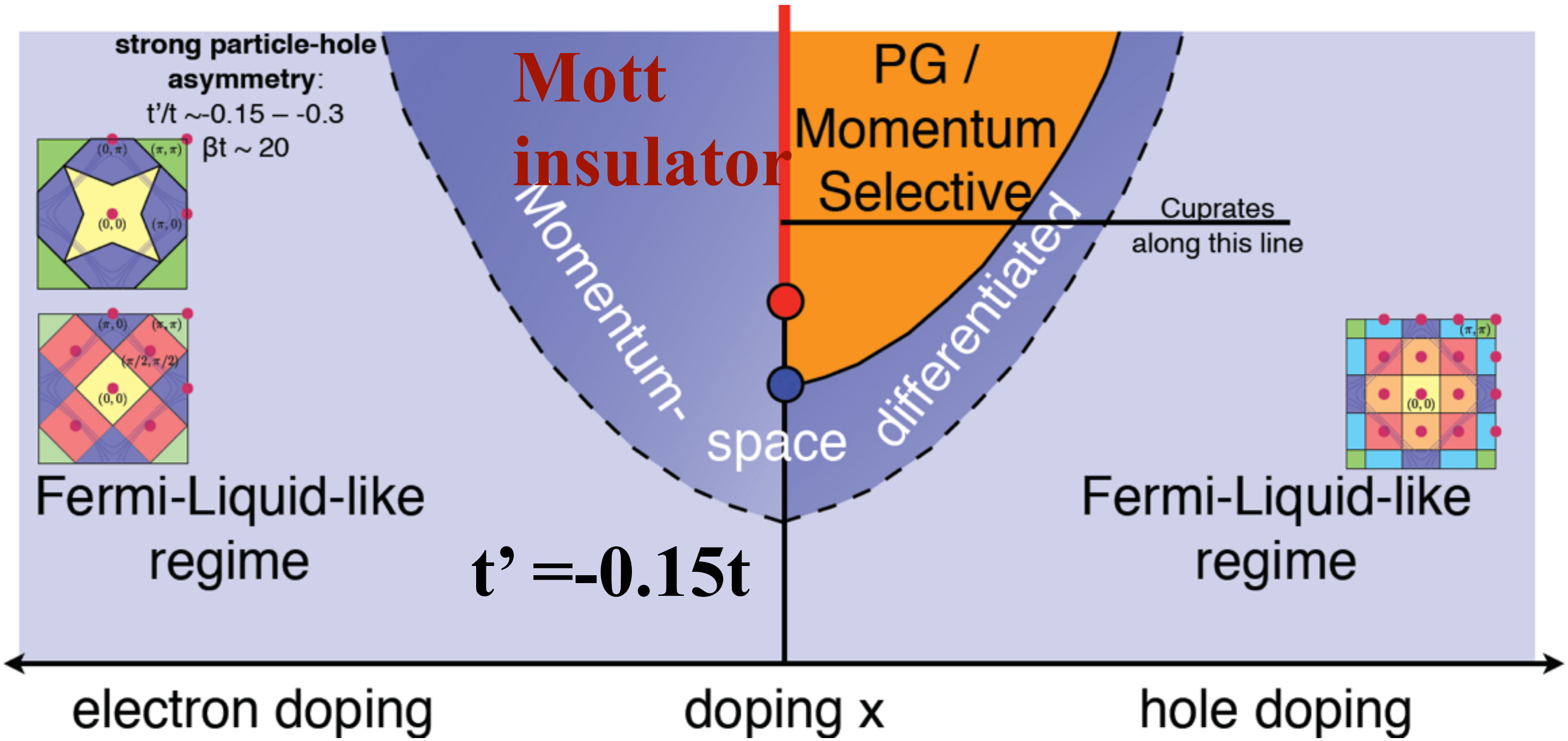
Phase diagram: Mott insulator separated from fermi liquid by pseudogap for hole but not electron doping



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).

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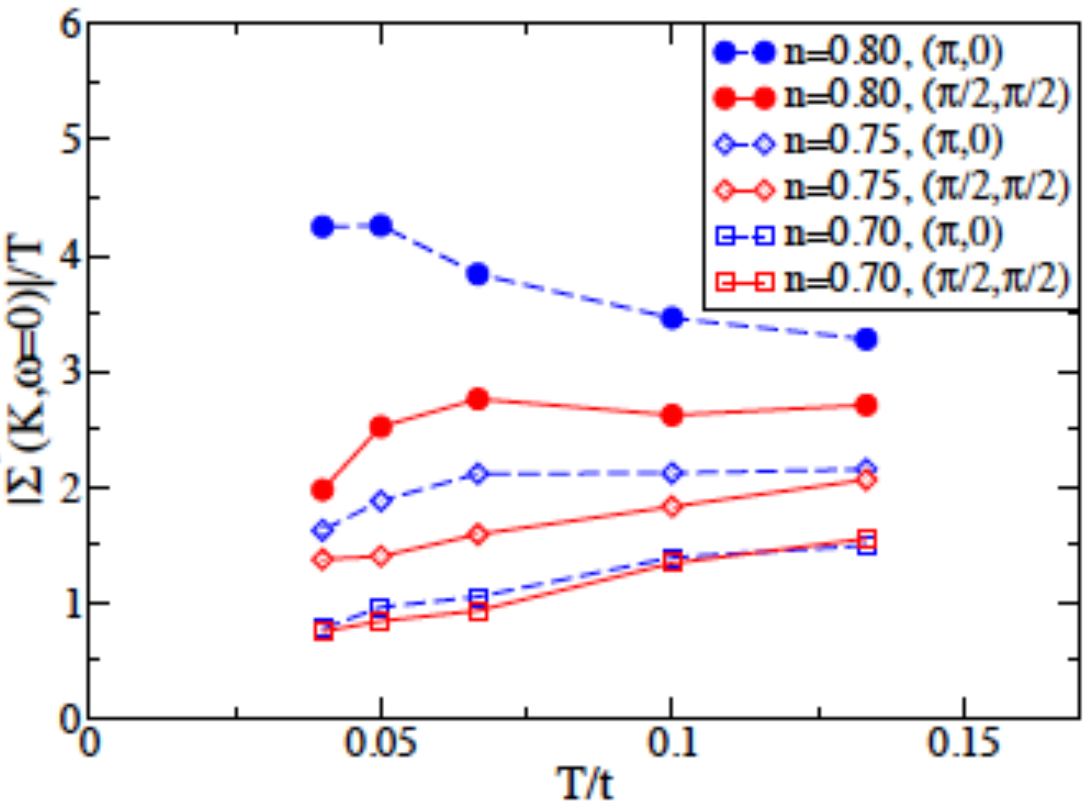
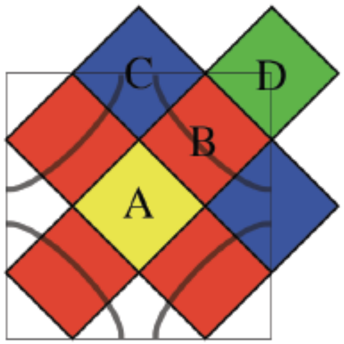
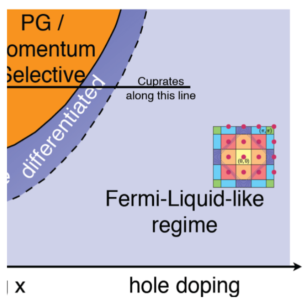
differentiated phase

Electron scattering rate by sector







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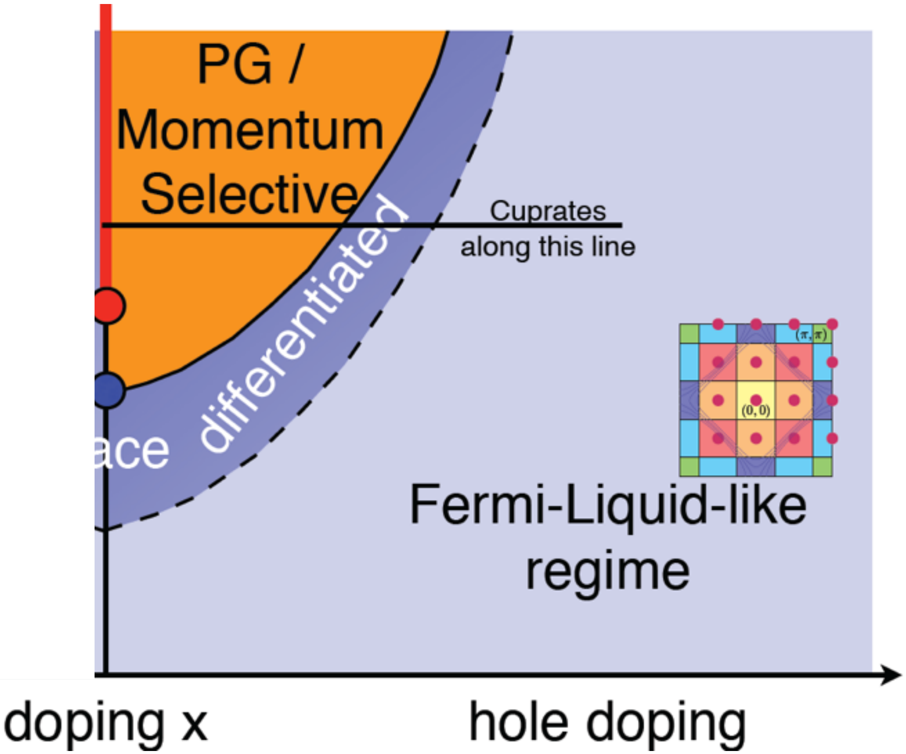
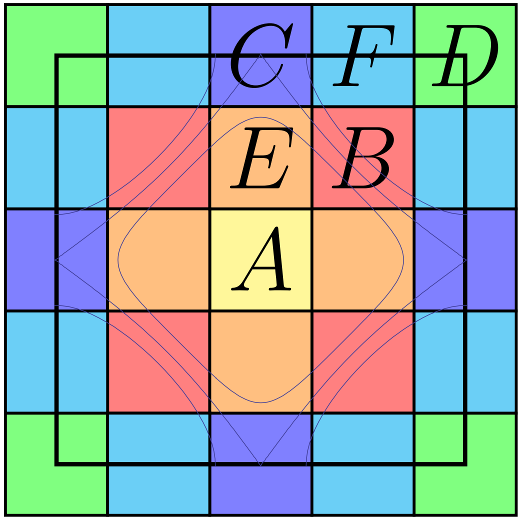
Momentum selective phase: partially gapped fermi surface





We see: gap opens in momentum sector C but not in B

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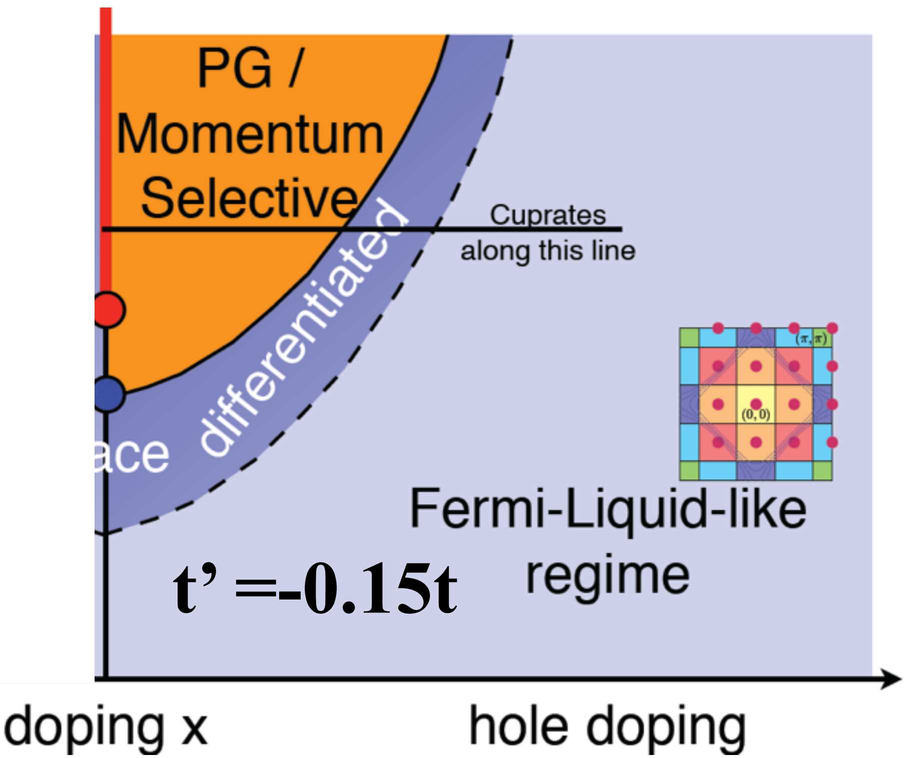

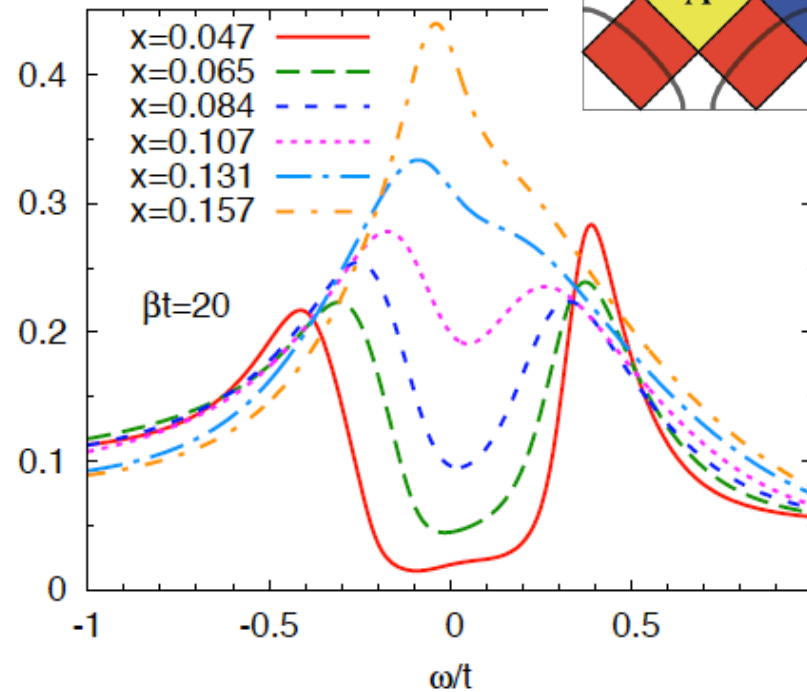

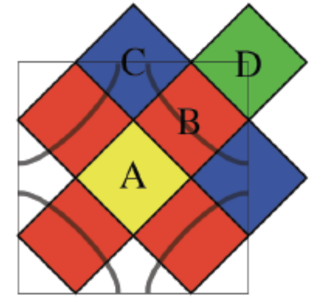

gap opens around zone face

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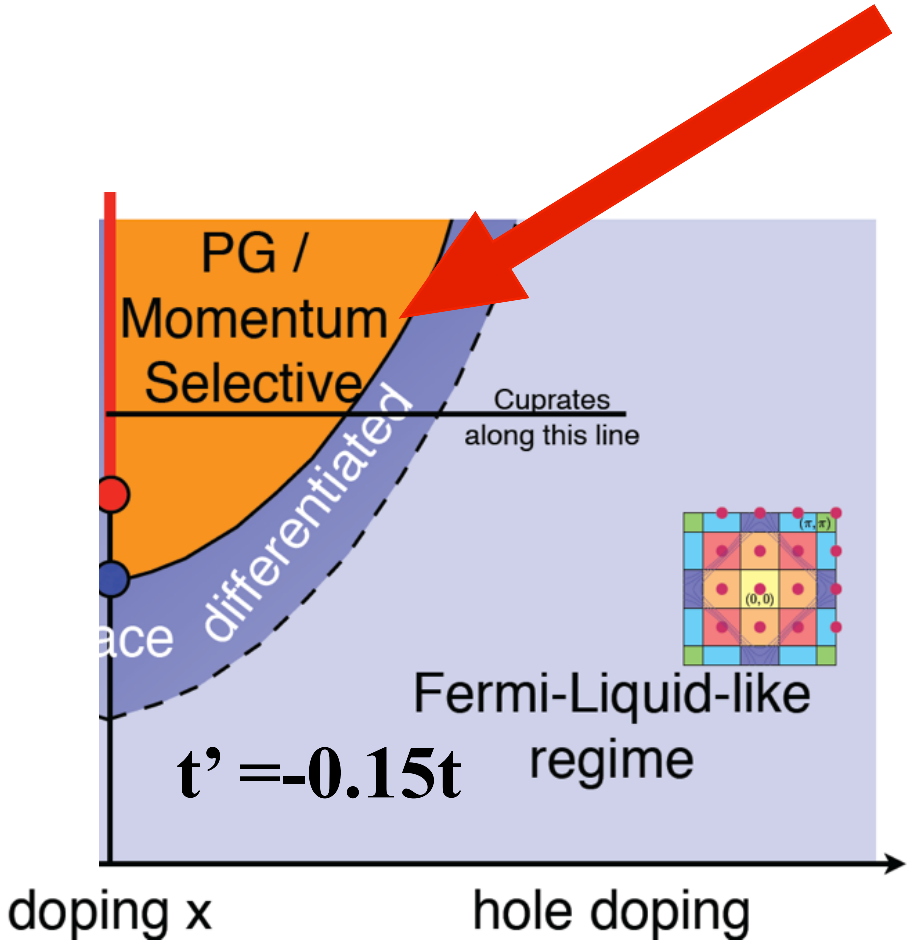
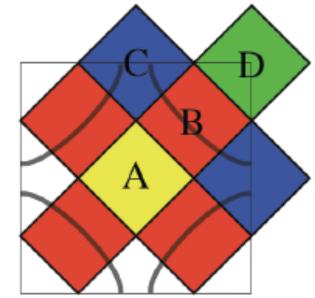
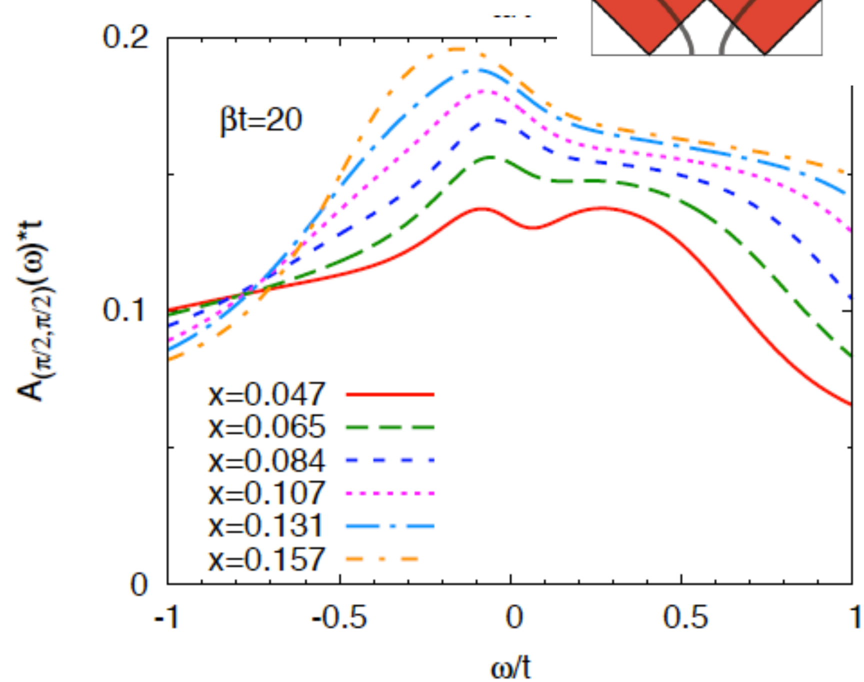
Intermediate phase: partially gapped fermi surface







but not along zone diagonal

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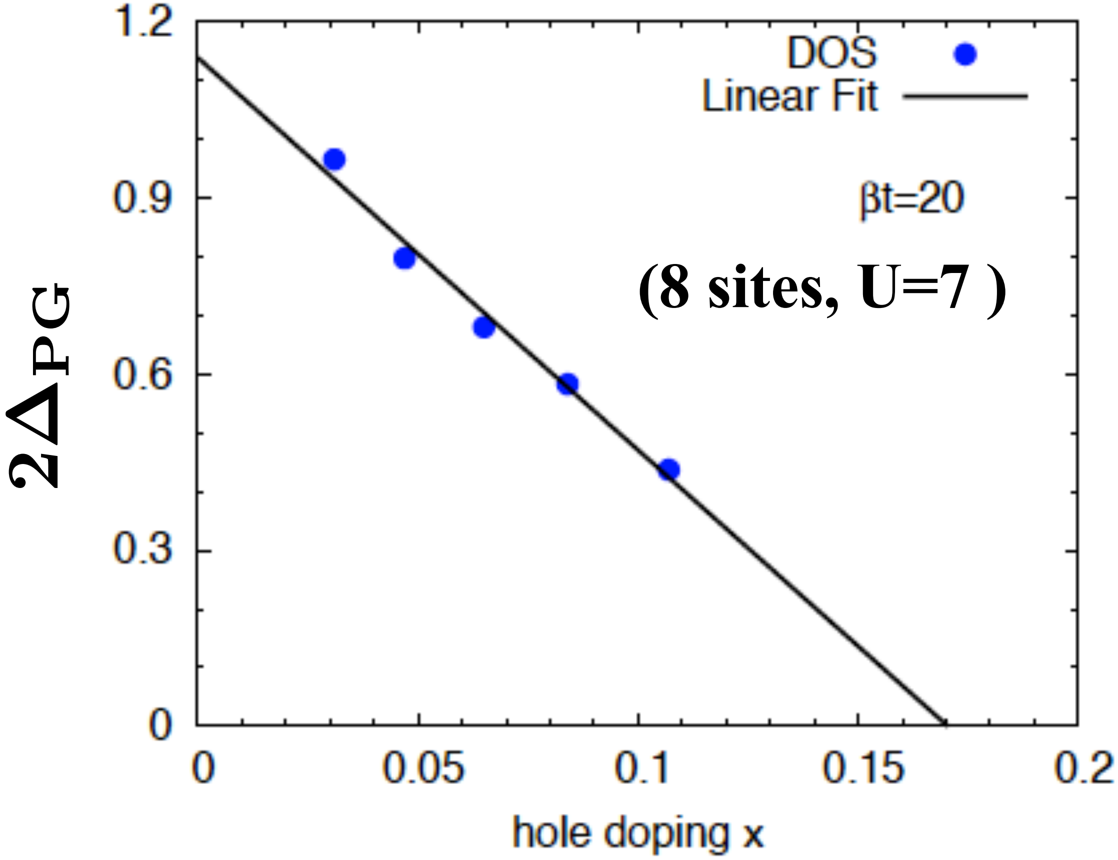
The pseudogap does NOT connect smoothly to the Mott gap

as $x \to 0$

$2\Delta_{PG} \to 1$

but

$2\Delta_{Mott} \approx 2$



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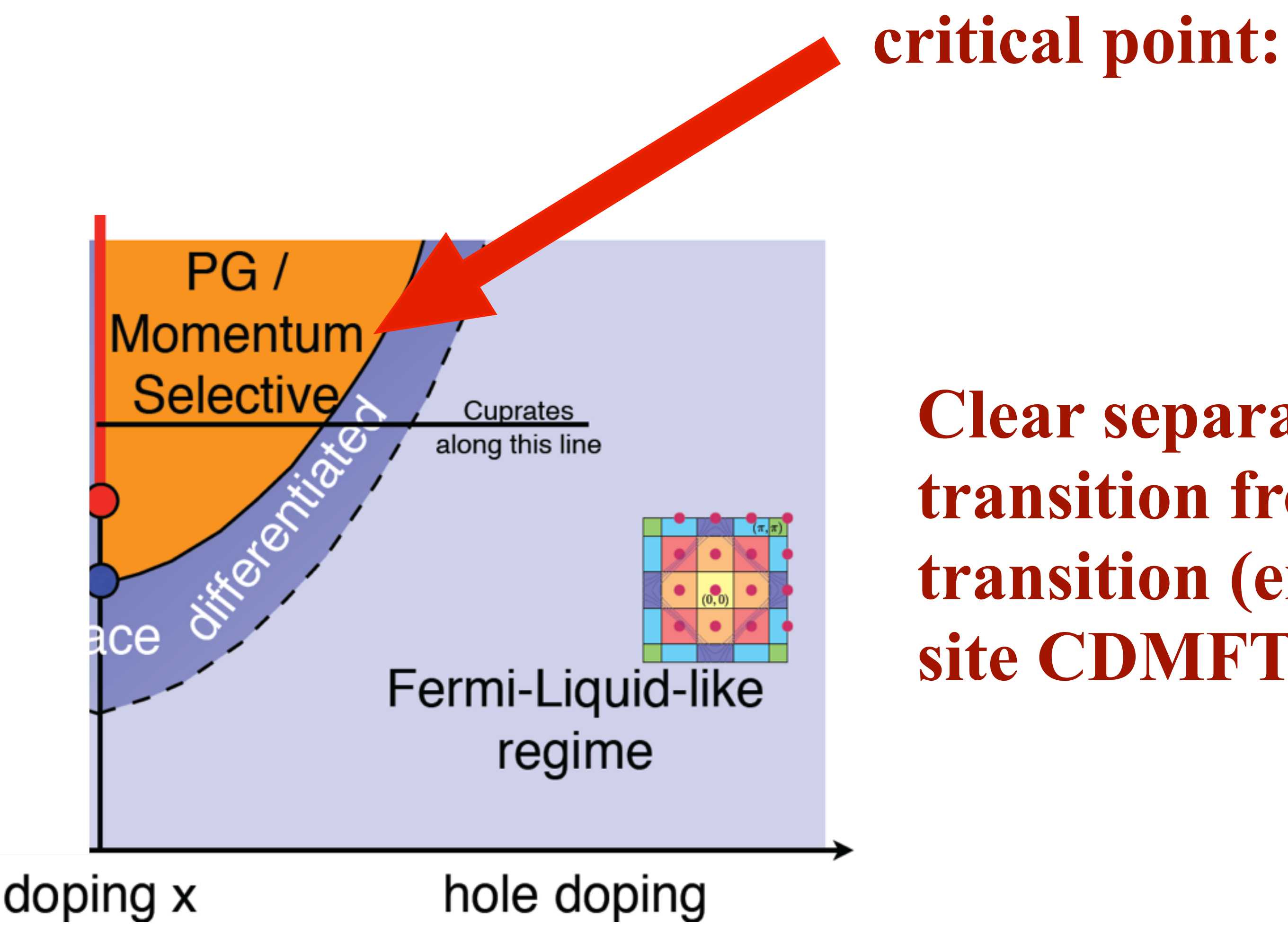
Momentum selective phase: partially gapped fermi surface



Clear separation of PG transition from Mott transition (except in 4 site CDMFT)

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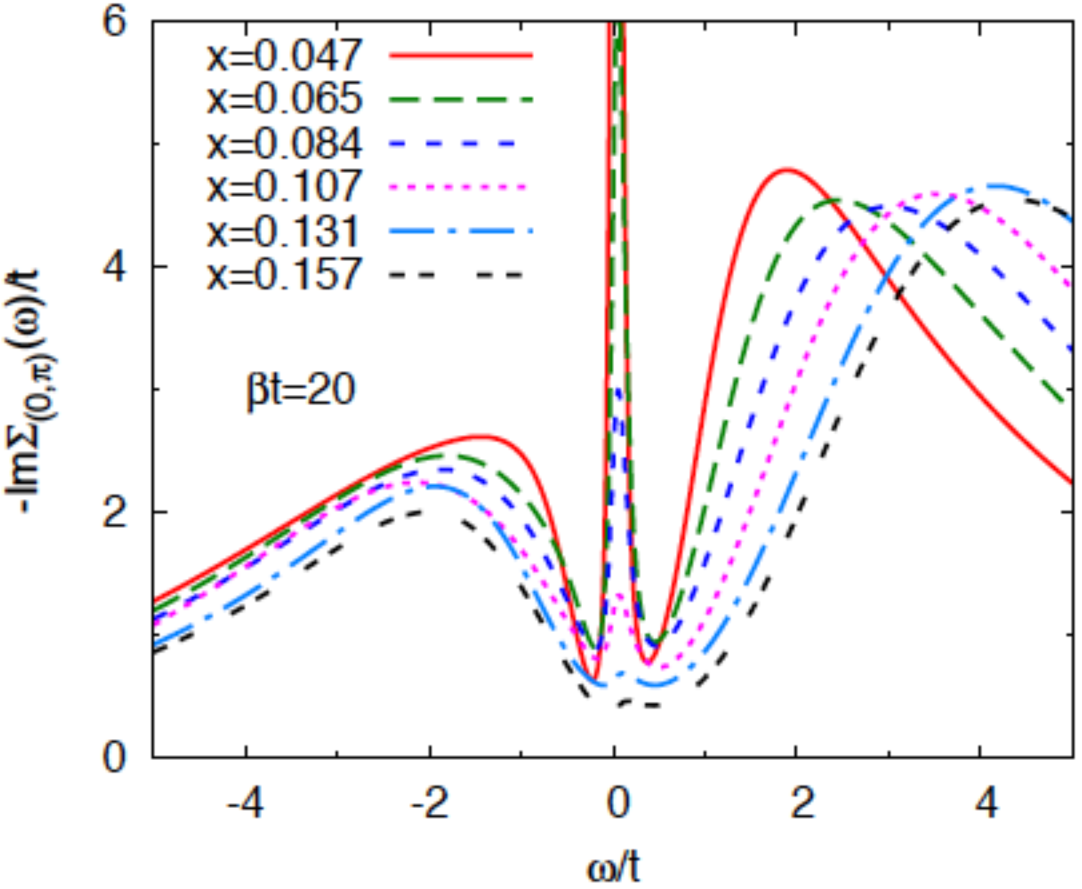
Pseudogap: marked by appearance of pole in self energy (N>4)



Phys. Rev. B 82, 045104 (2010)

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.

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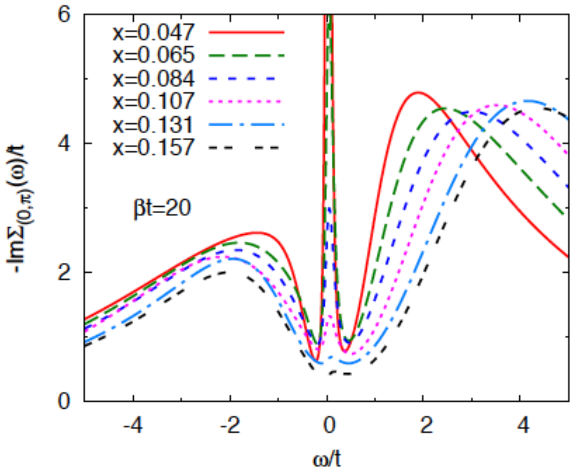
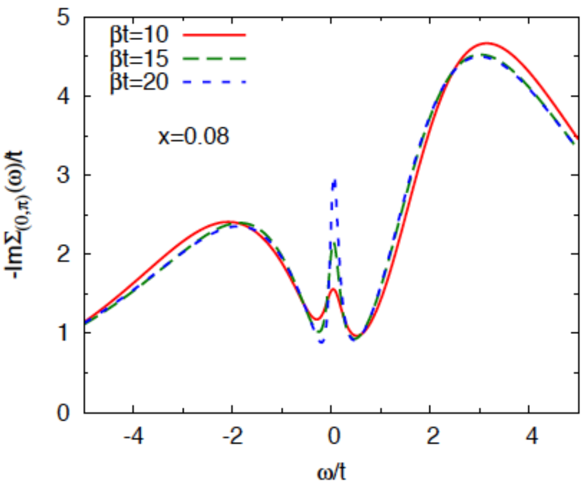
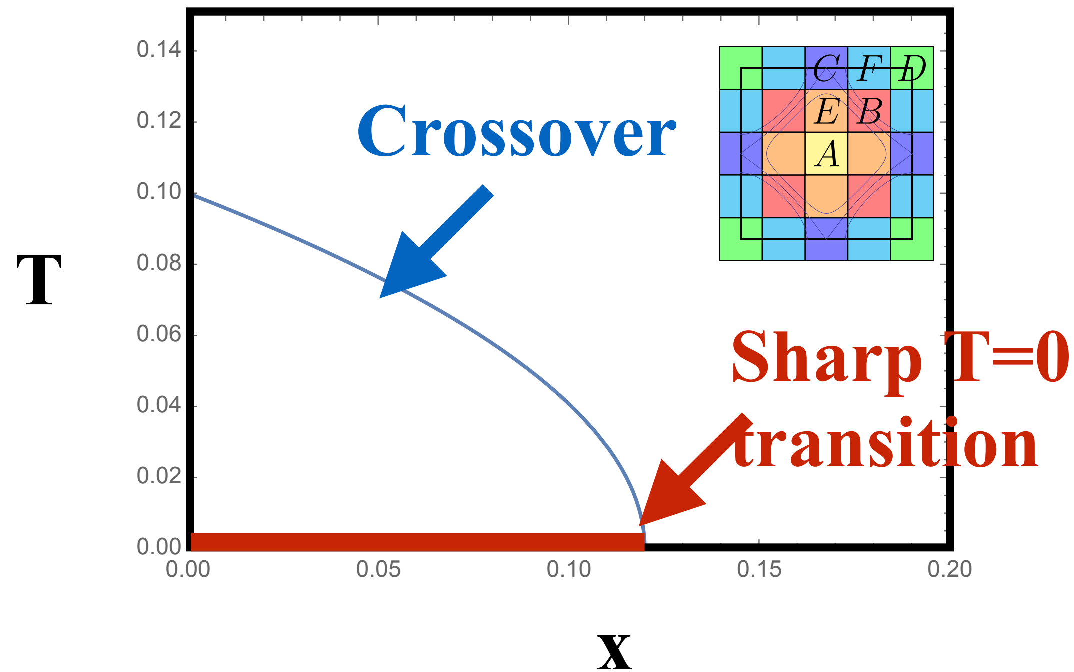
Order parameter: gap in (0,Pi) sector sharply defined only at T=0





T=0: sharp transition

T>0: crossover



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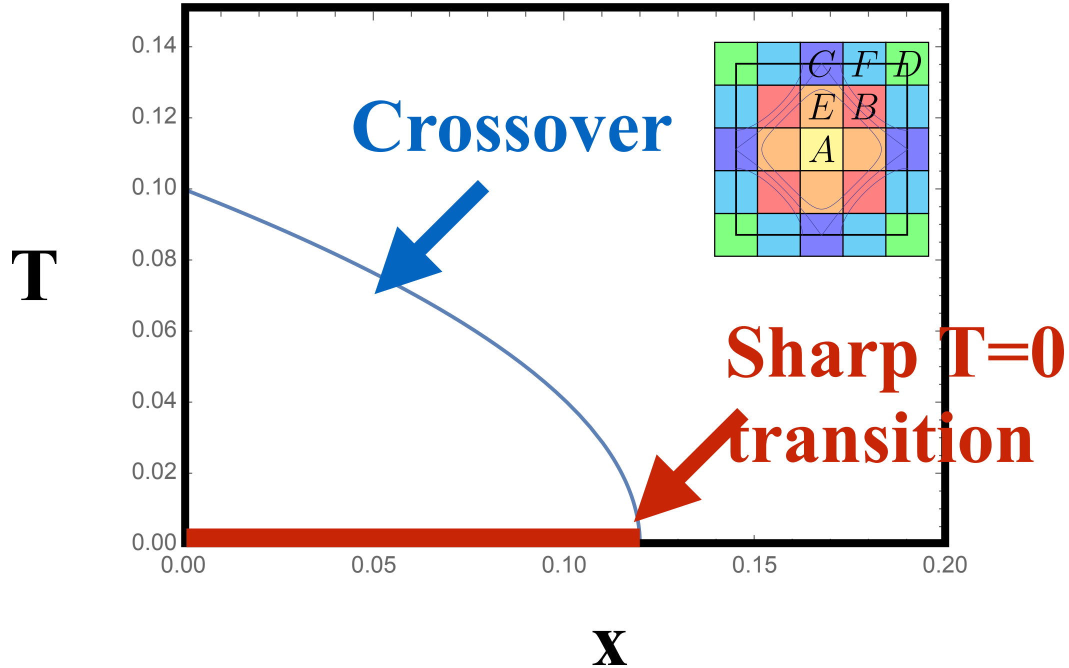
Order parameter: gap in (0,Pi) sector sharply defined only at T=0

Crossover: reasonably sharp change in physical properties.

T=0: sharp transition
T>0: crossover

We find that the T=0 transition is second order for N>4. If it were weakly first order, nothing important would change



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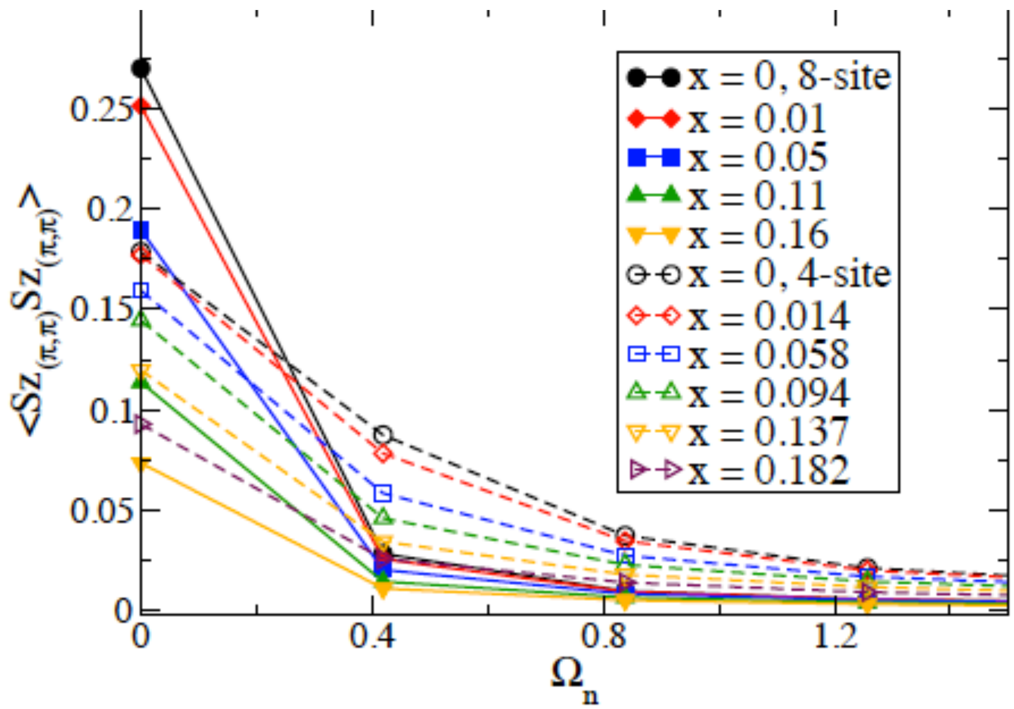
Pseudogap associated with enhanced antiferromagnetic spin correlations



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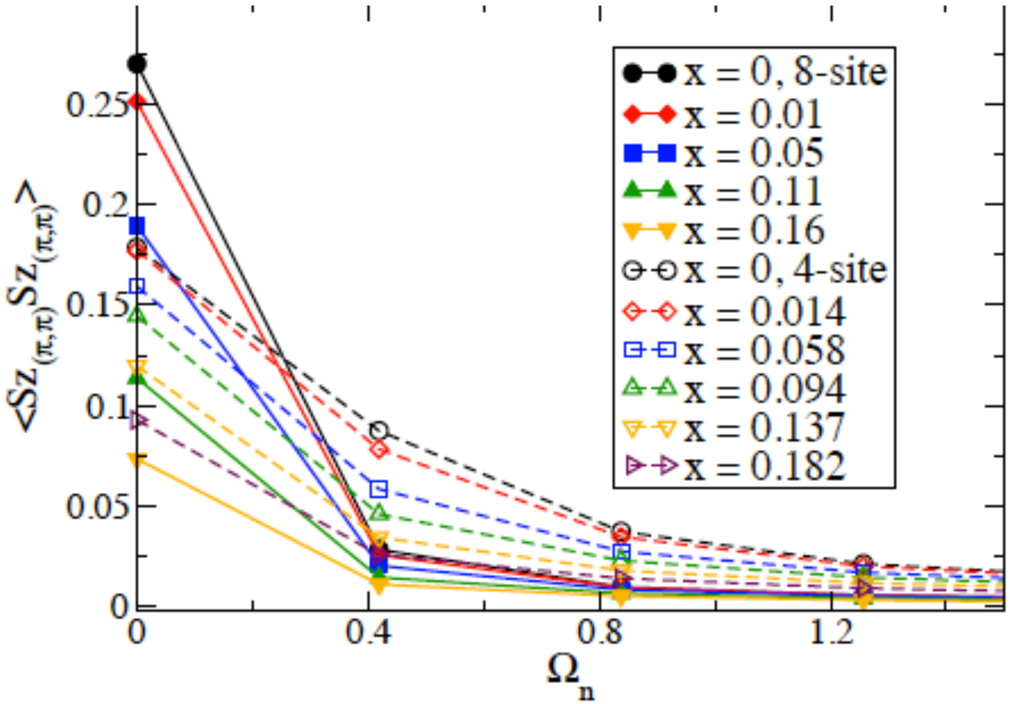
Pseudogap associated with enhanced antiferromagnetic spin correlations



These are equal-time impurity-model correlations. We are working on getting the real dynamical correlations (vertex corrections needed).

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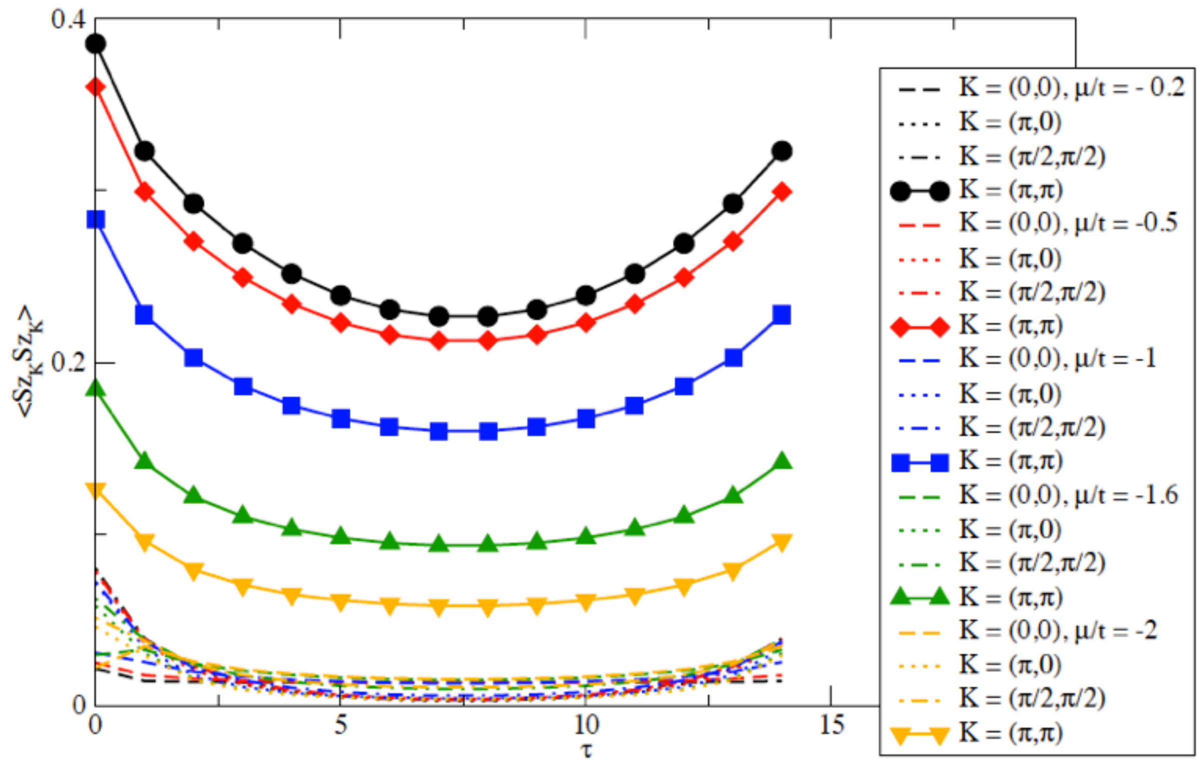
Spin correlations at other wavevectors not enhanced



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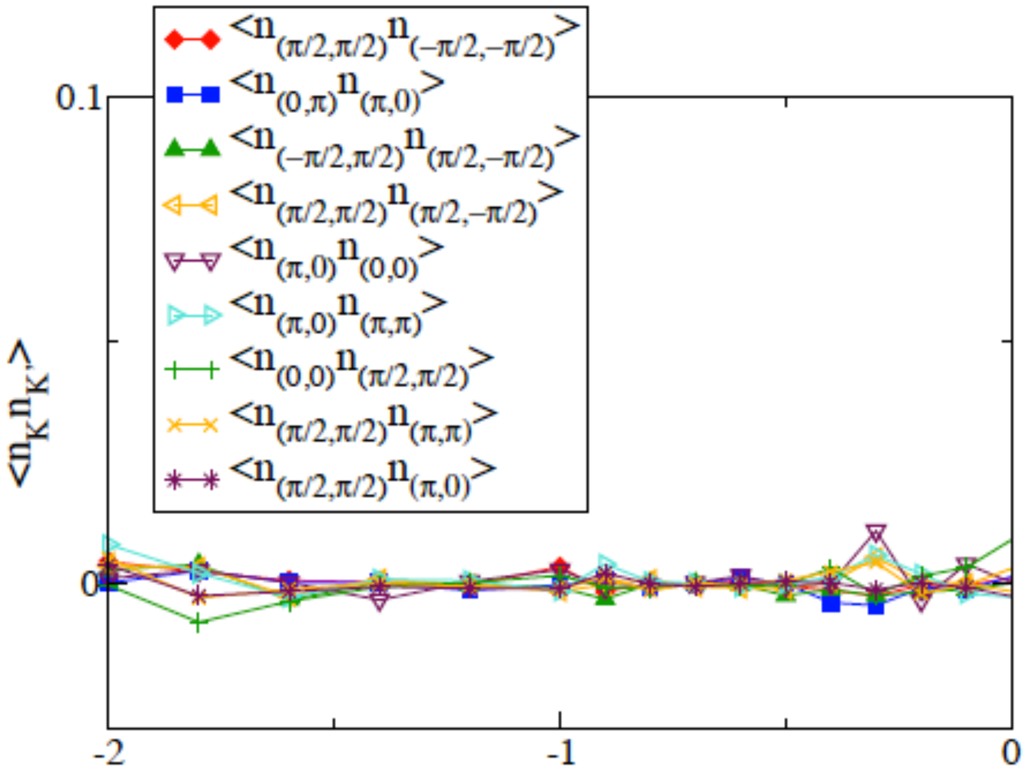
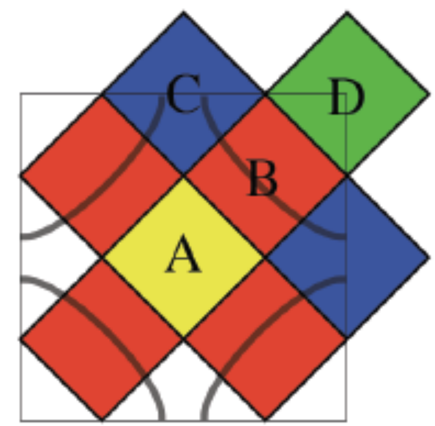
No charge `nematicity’





NO enhancement of inter-patch density fluctuations is visible

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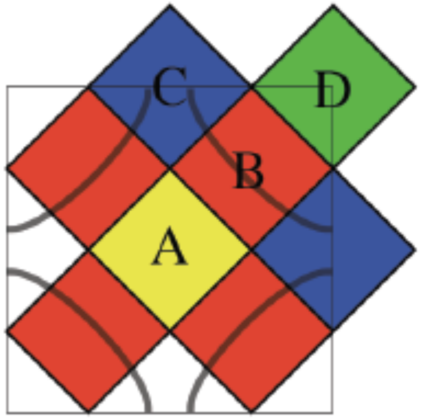
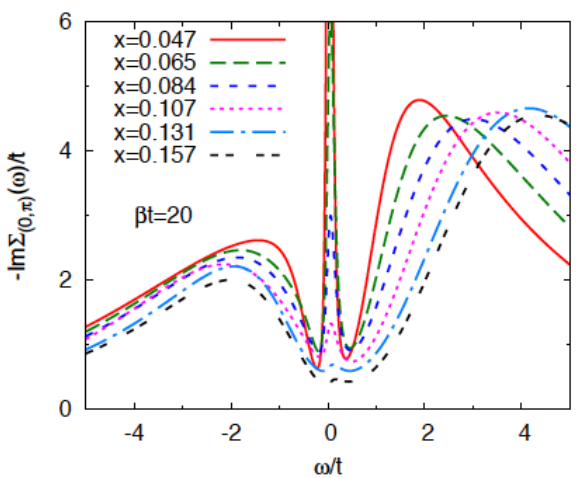
However, sensitivity to breaking C4 symmetry



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



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

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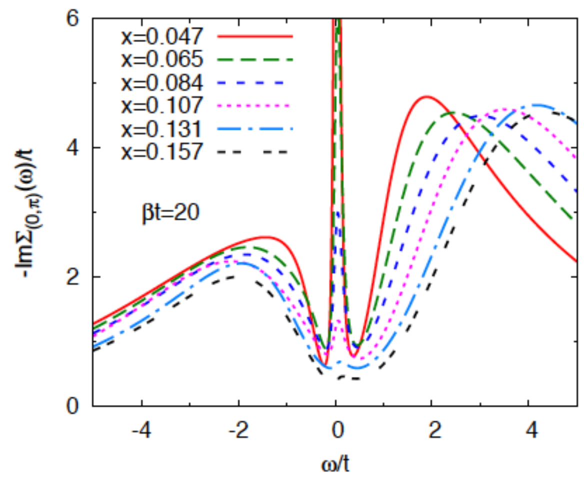
Pseudogap Summary

- 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



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Now: superconductivity

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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 subsequent 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).

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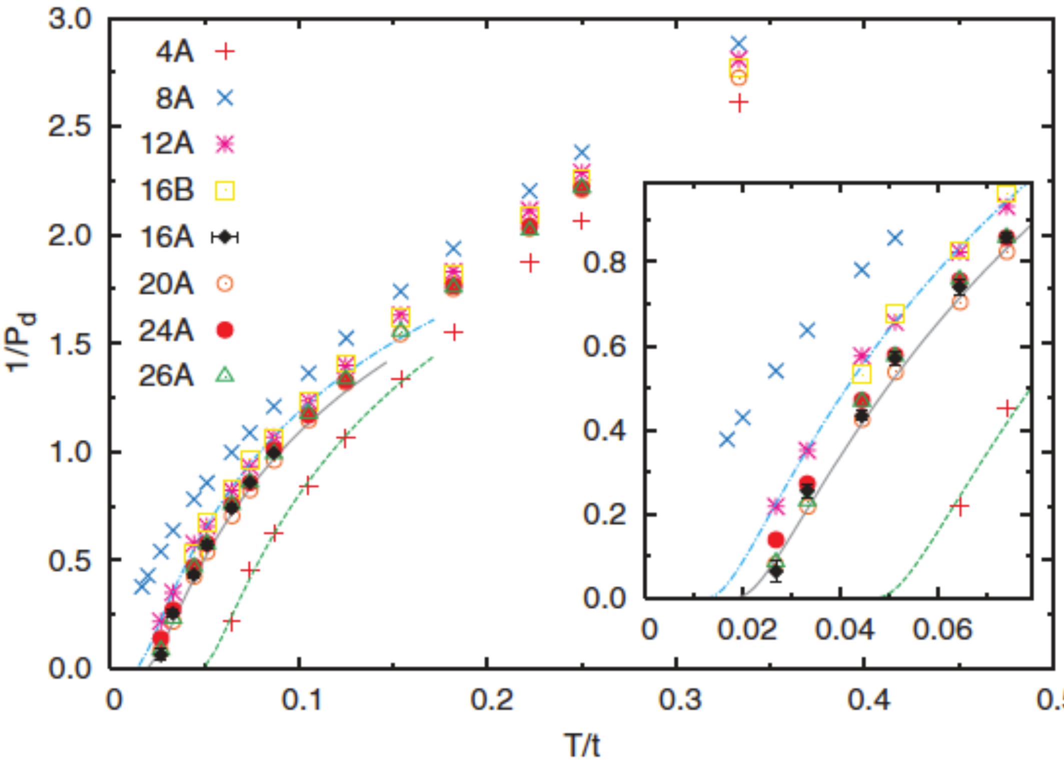
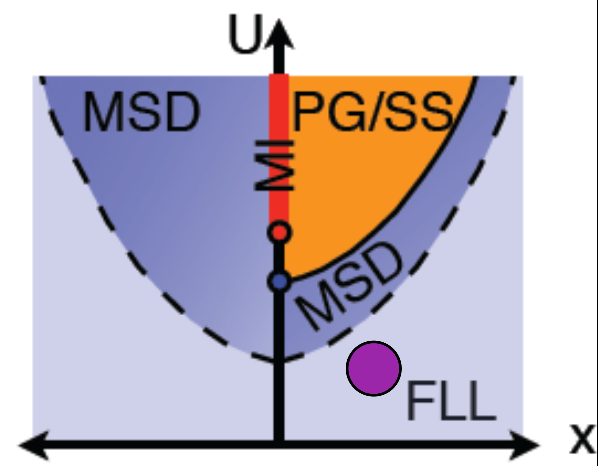
Large clusters: Superconductivity established

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

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Our work: construct the sc state and determine some properties

- E. Gull, O. Parcollet and A. J. Millis, Phys. Rev. Lett. 110 216406 (2013)
- E. Gull and A. J. Millis, Physical Review B86 241106 (2012).
- Emanuel Gull, Andrew J. Millis. Phys. Rev. B88, 075127 (2013).
- E. Gull and A. J. Millis,Phys. Rev. B90, 041110 (2014).
- E. Gull and A. J. Millis, Physical Review B91, 085116 (2015).

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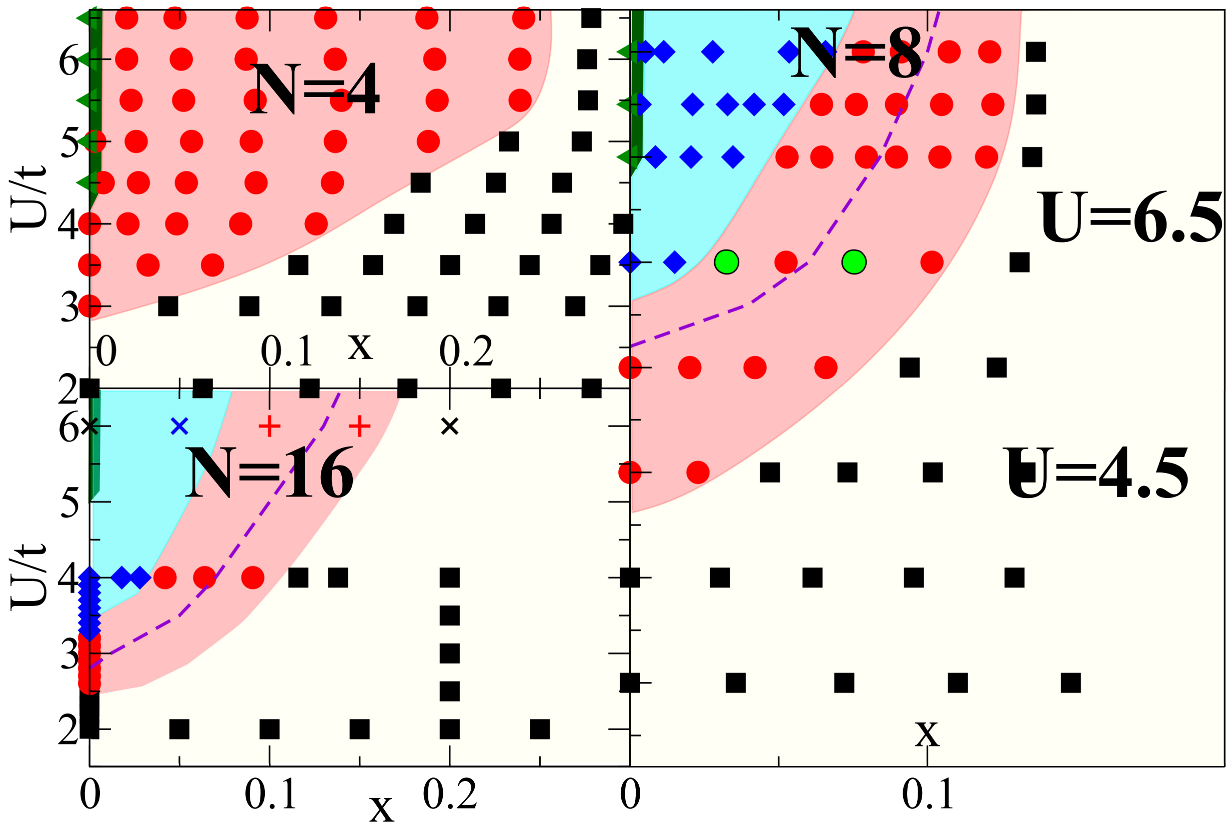
Phase diagram, different clusters
T=t/40



superconductivity **only** near **insulator**, cut off by **pseudogap**

N=4 a bit of an outlier. 8 and 16 differ at small U but have similar doping dependence at larger U

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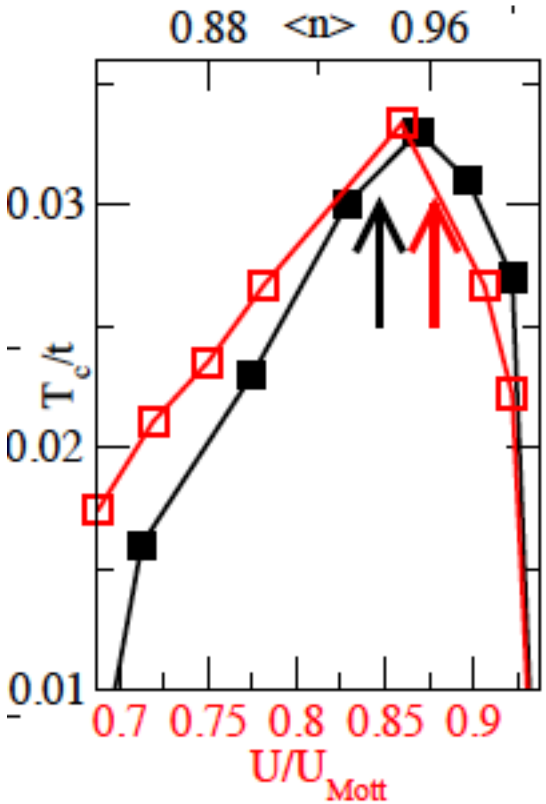
Transition temperature and gap



t~0.3eV=>T_c^{max}~170K

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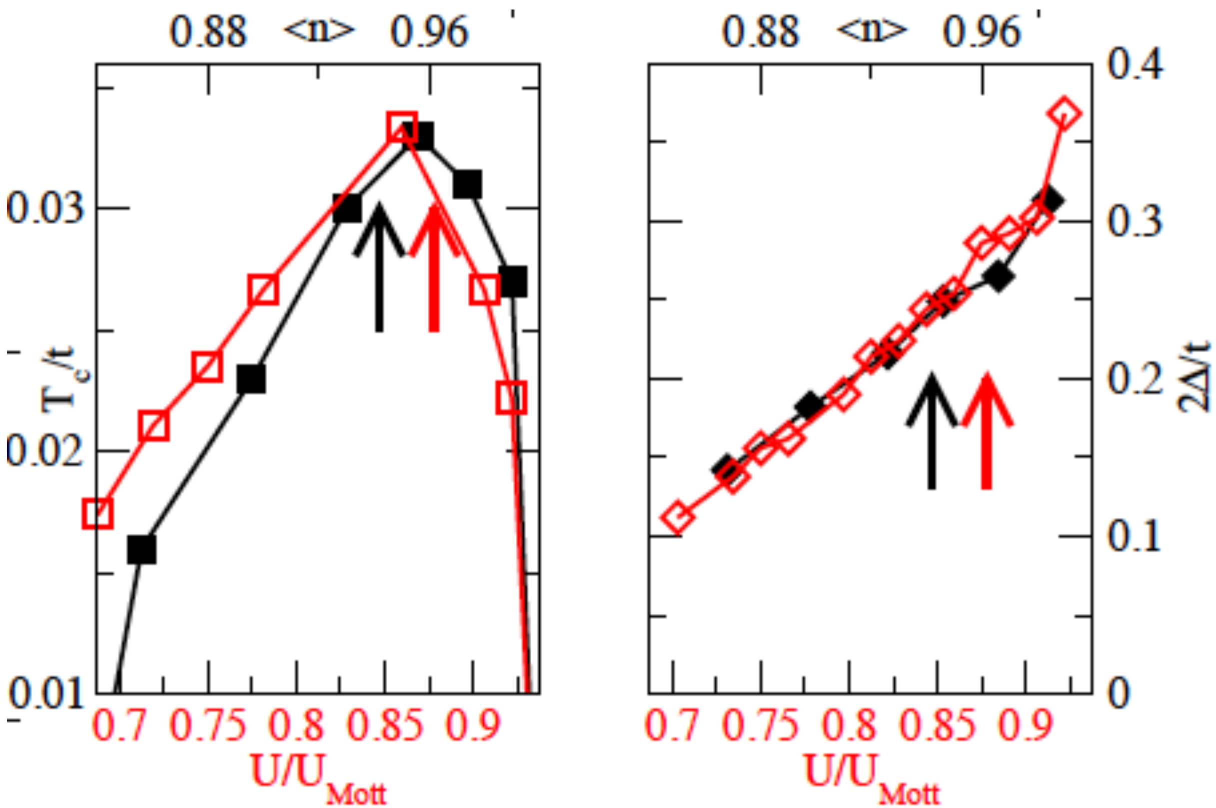

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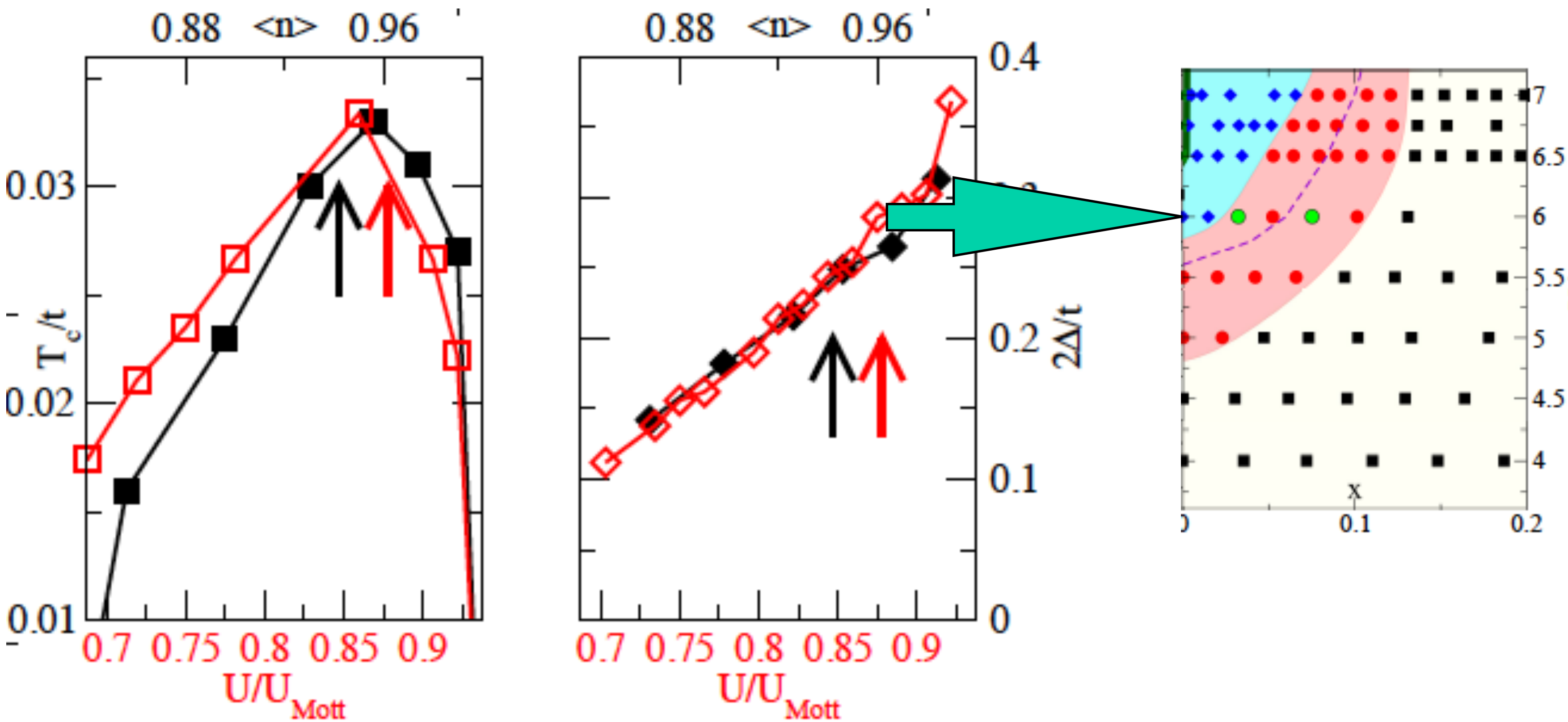

Superconductivity cut off by pseudogap.
Transition is strongly first order

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Some other physical properties

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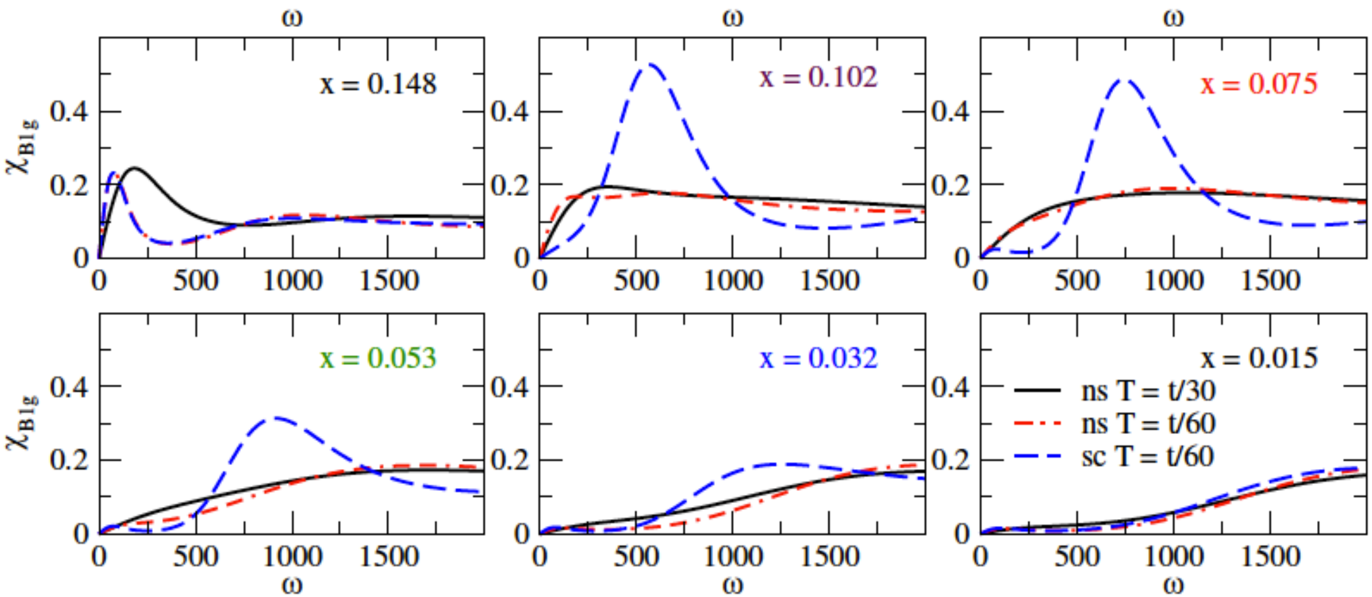
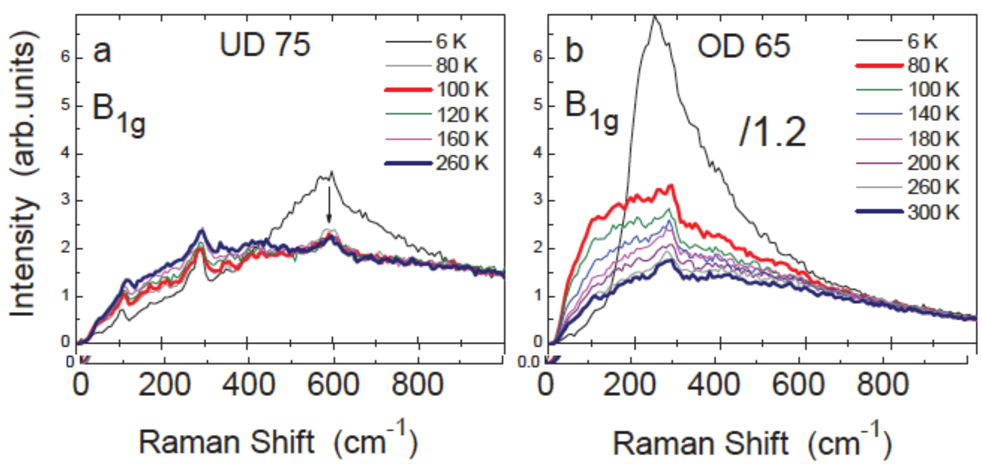
Raman scattering



Calculation



Data
Sacuto et al

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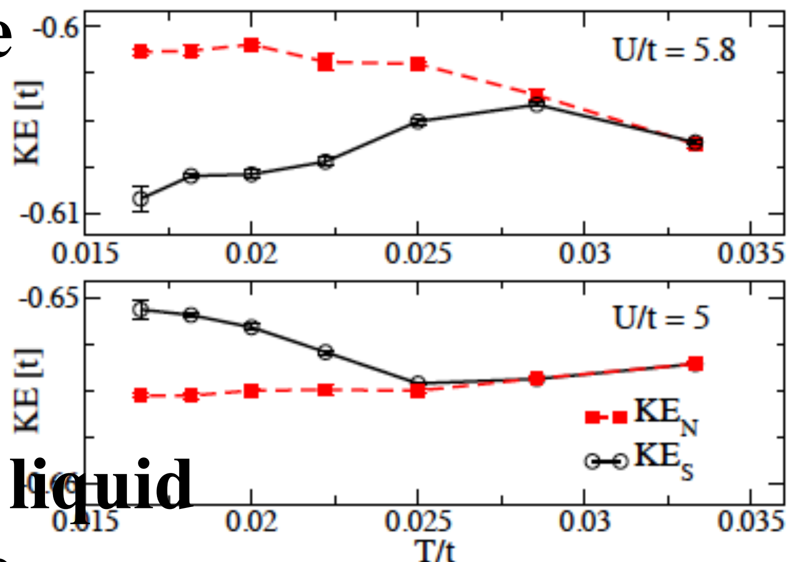
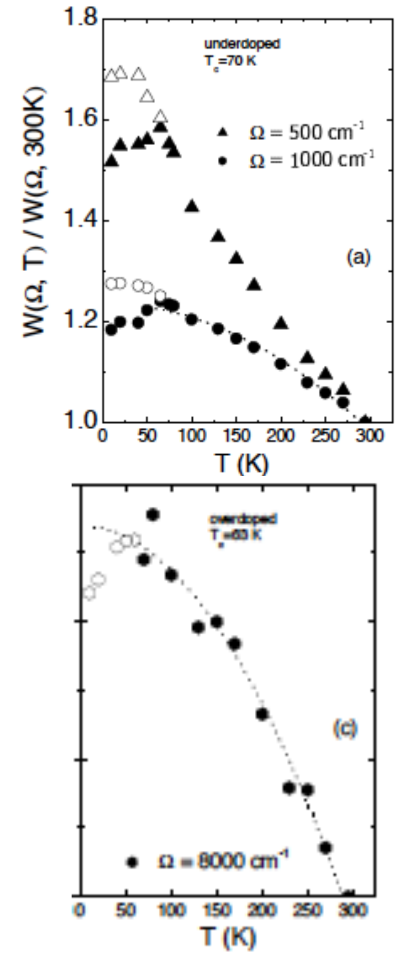
Temperature dependence of kinetic energy

Pseudogapped regime

Fermi liquid regime





This trend in KE change is observed in optics: Santander-Syro, Lobo, Bontemps arXiv:0404.2901

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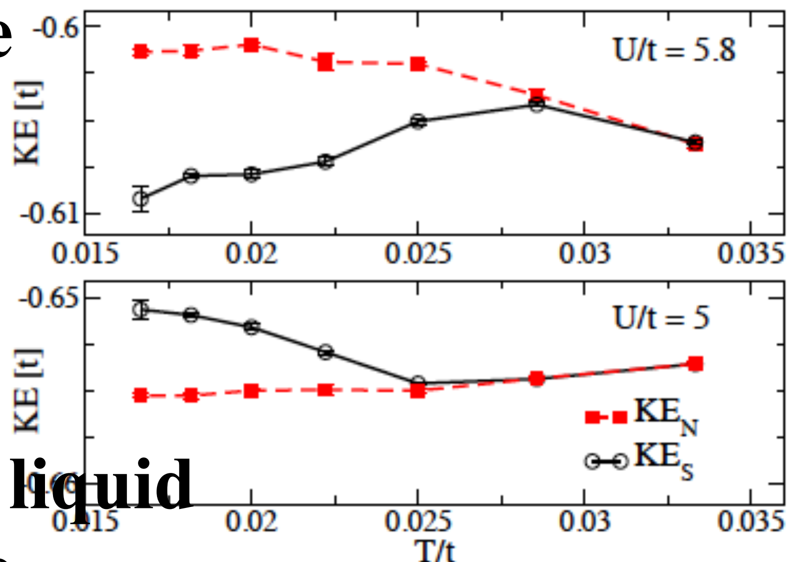
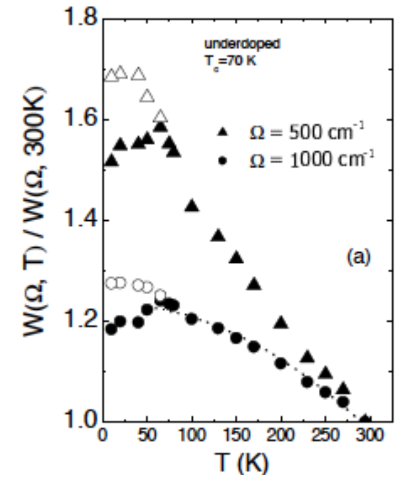
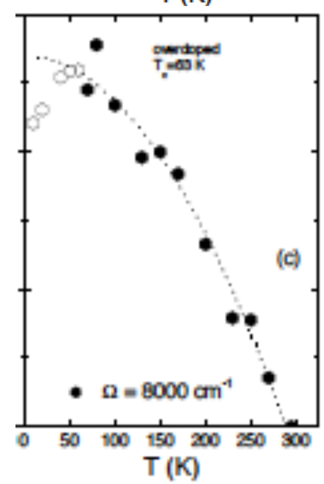
Temperature dependence of kinetic energy

Pseudogapped regime



Fermi liquid regime





SC and PG are competing ``phases”. PG reduces kinetic energy: SC weaks PG, allows KE magnitude to rise

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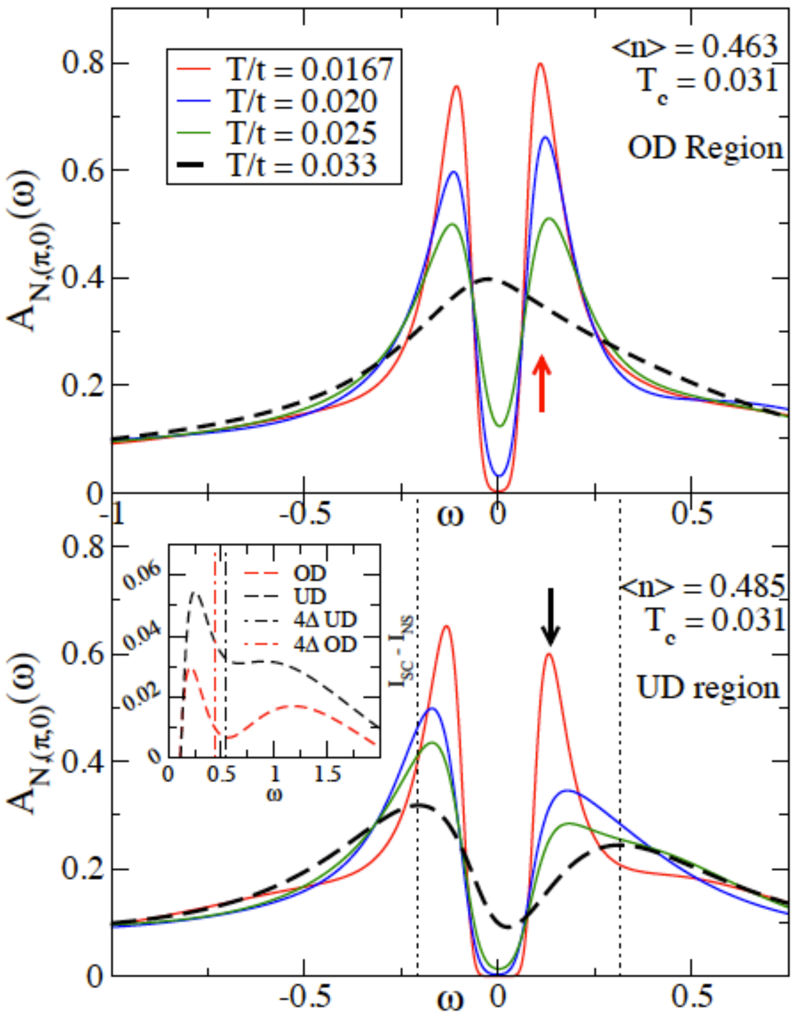
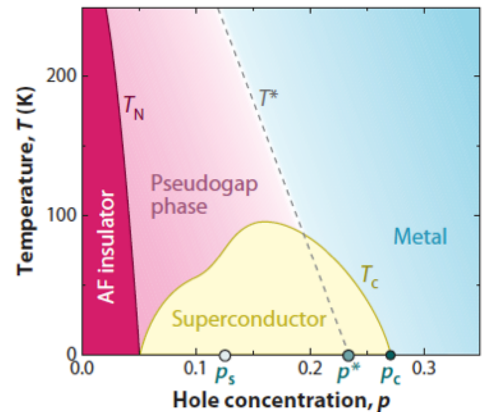
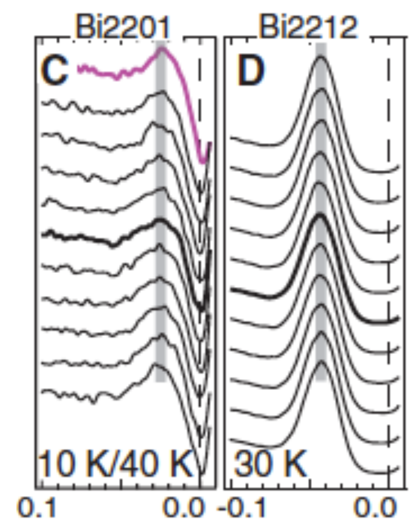
Superconductivity and the pseudogap







SC Gap smaller than PG

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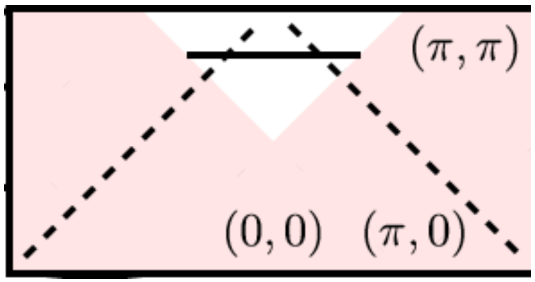
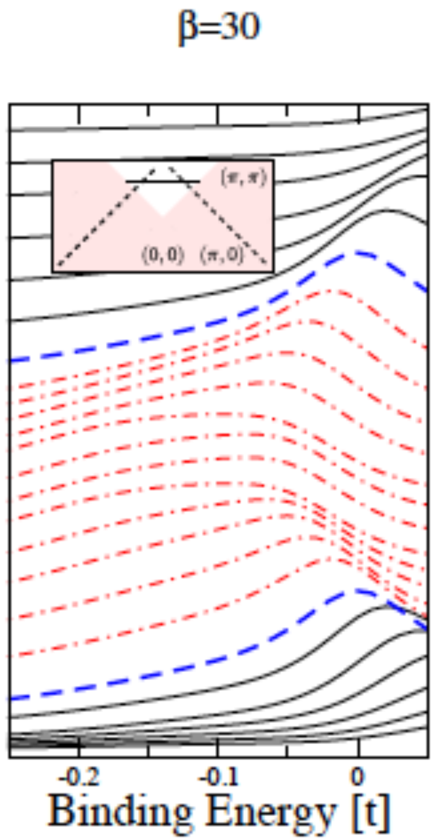
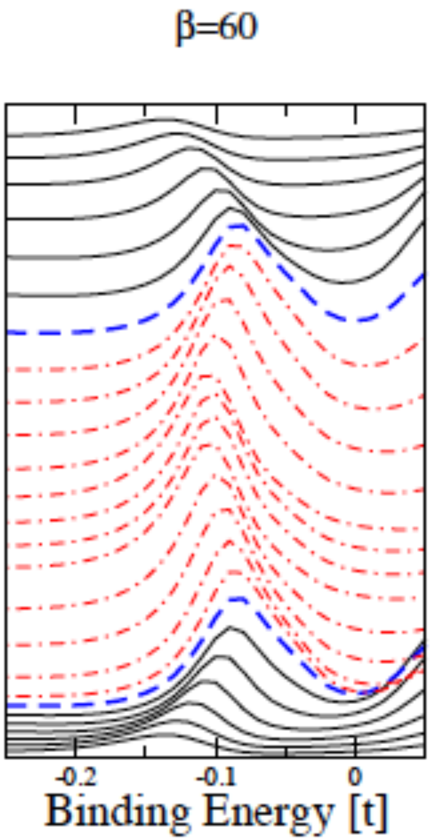
Simulated ARPES Spectra
Fermi Liquid (no pseudogap)







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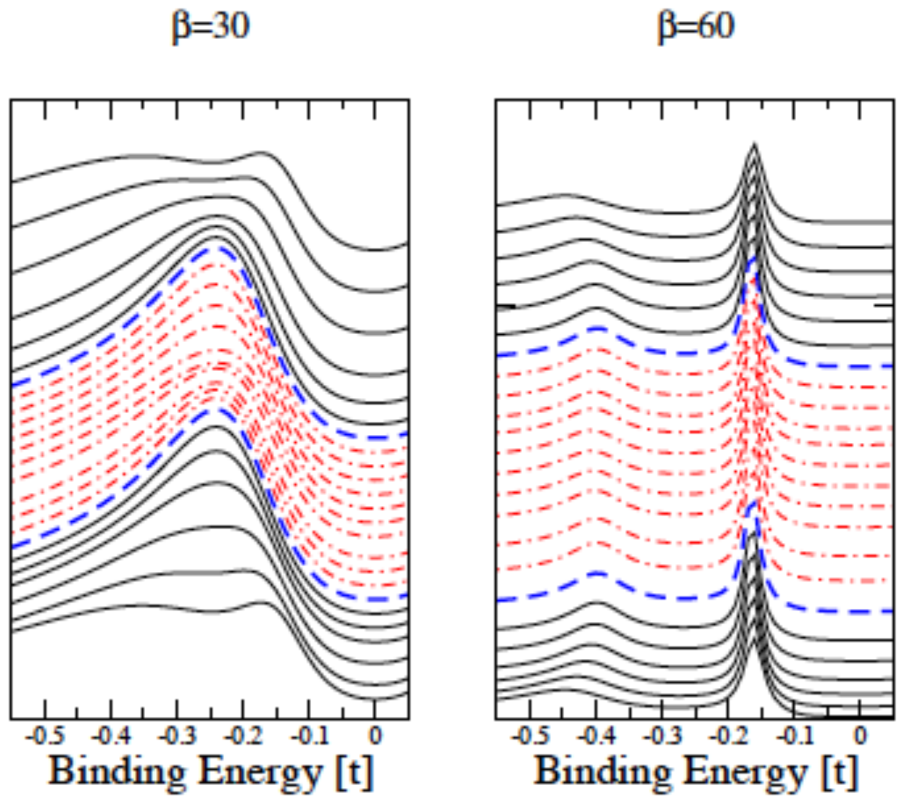
Simulated ARPES Spectra
PG regime

New states created inside gap. Existing peak moved up in energy



Note: ‘peak-dip-hump’ structure

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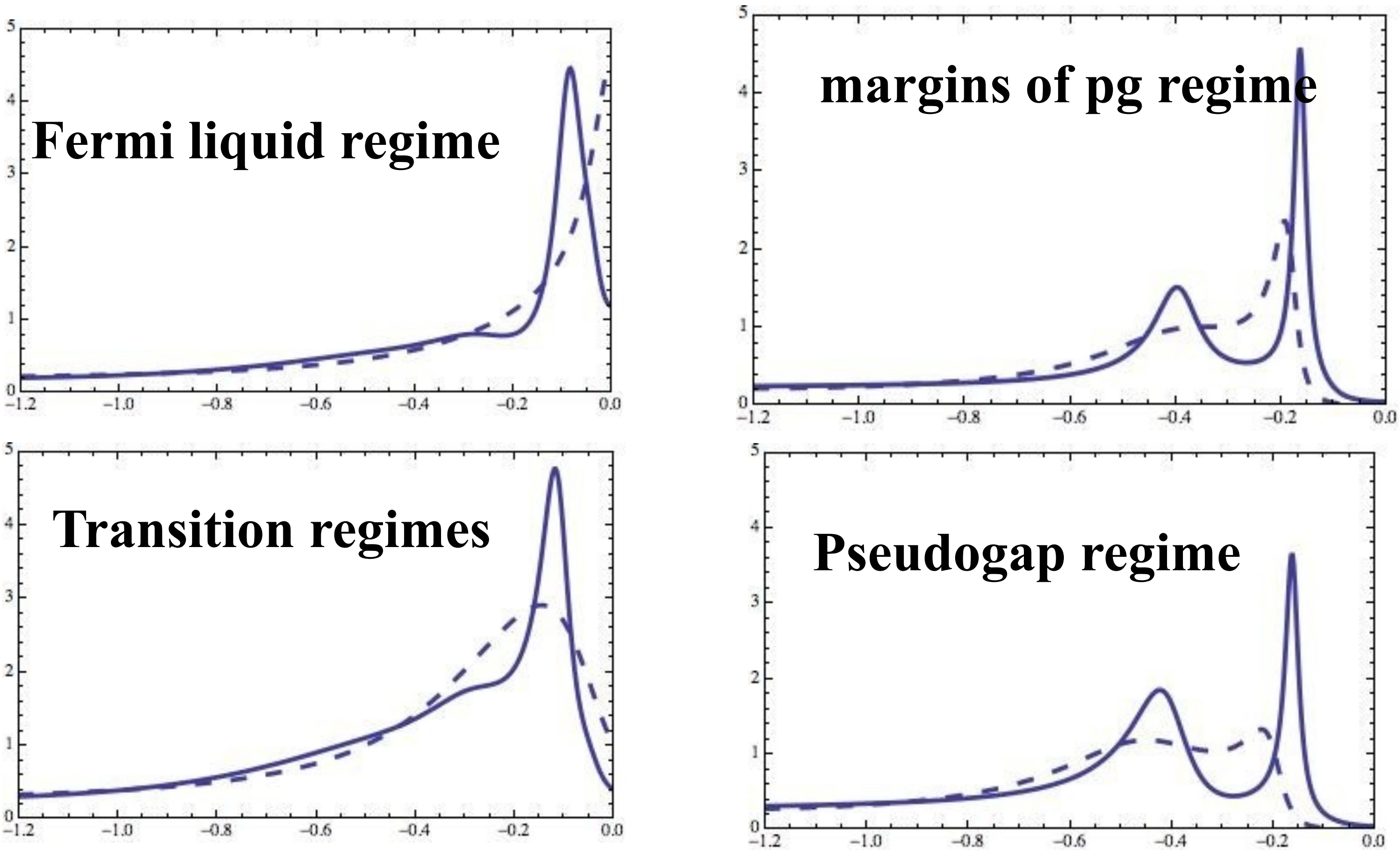
Evolution of photoemission Spectra



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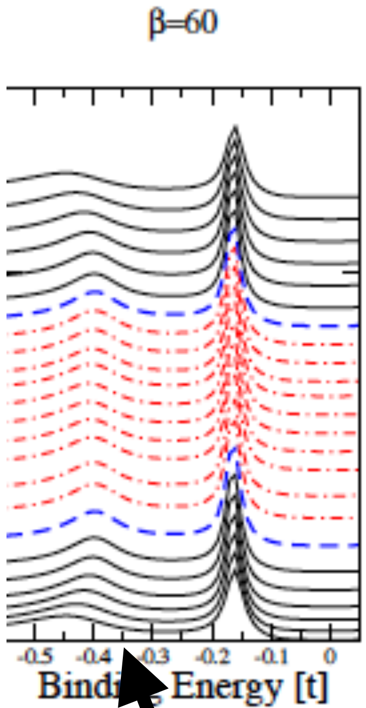
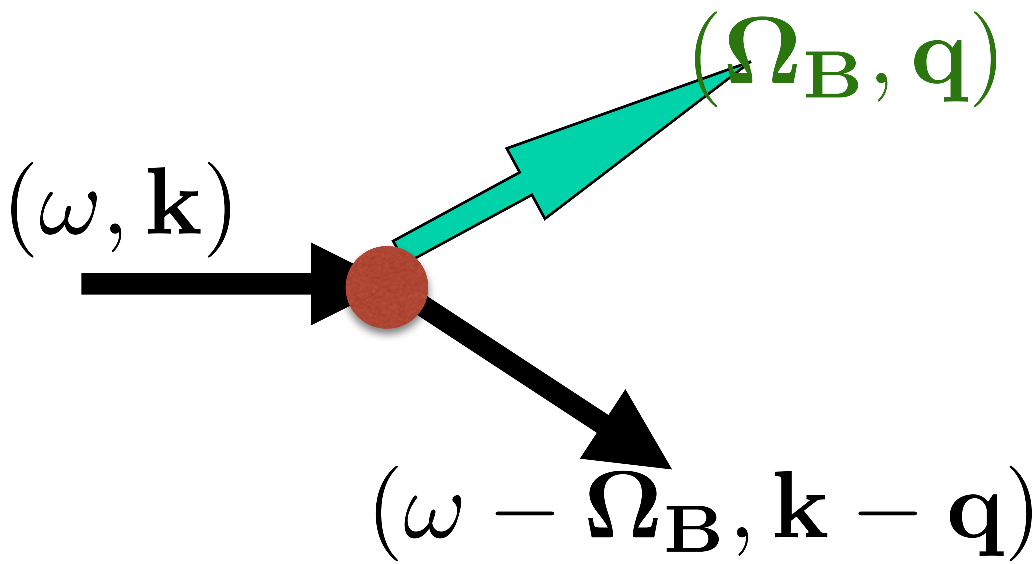
Physics of the ``hump”



Standard interpretation: ``shakeoff”



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

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Mathematically

$$\mathbf{A}(\mathbf{k},\omega) = \mathbf{Im}\left[\mathbf{G}(\mathbf{k},\omega)\right] = \frac{\boldsymbol{\Sigma}^{(2)}(\omega)}{\left(\omega - \varepsilon_{\mathbf{k}} - \boldsymbol{\Sigma}^{(1)}(\omega)\right)^{2} + \left(\boldsymbol{\Sigma}^{(2)}(\omega)\right)^{2}}$$

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

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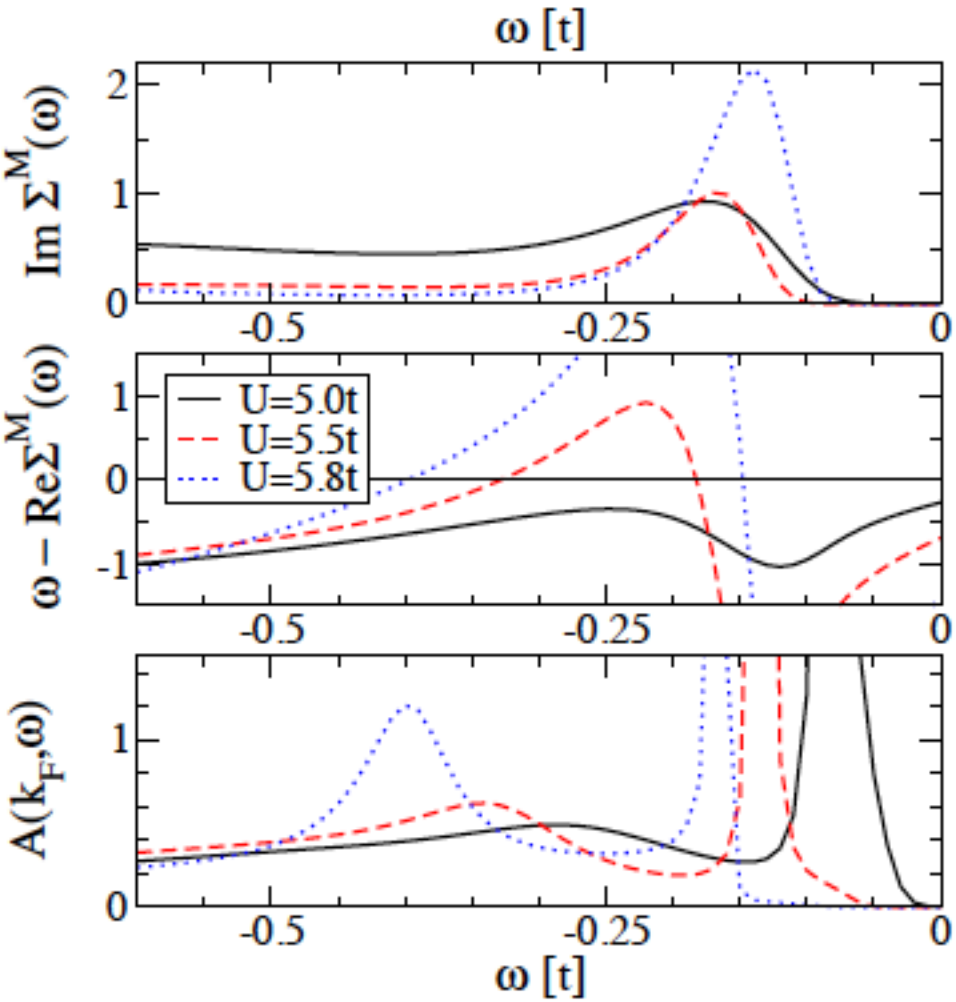
We find: 'hump' is a resonance coming from a zero crossing of the real part of the self



$$\frac{\mathbf{\Sigma}^{(2)}(\omega)}{\left(\omega - \varepsilon_{\mathbf{k}} - \mathbf{\Sigma}^{(1)}(\omega)\right)^2 + \left(\mathbf{\Sigma}^{(2)}(\omega)\right)^2}$$

'hump' when

$$\omega - \mathbf{Re\Sigma}(\omega) = \mathbf{0}$$

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Pairing mechanism

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

$$\Sigma^N_{o,e} = \frac{\Sigma^N(k,\omega_n) \mp \Sigma^N(k,-\omega_n)}{2}$$

Define gap function

$$\mathbf{\Delta(i\omega_n) = \frac{\Sigma^A(i\omega_n)}{1-\frac{\Sigma^N_o(i\omega_n)}{\omega_n}} = \int \frac{dx}{\pi}\frac{\Delta^{(2)}(x)}{i\omega_n - x}}$$

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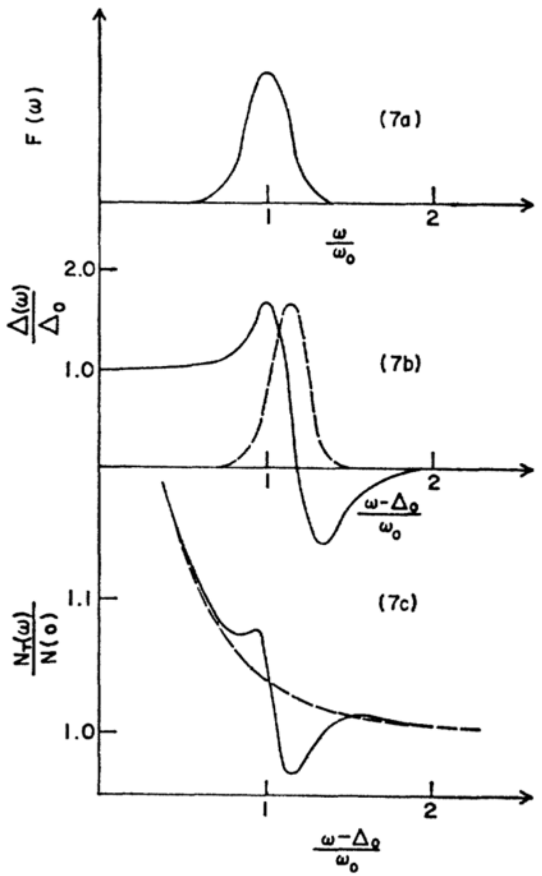
In conventional superconductors

Lead



Imaginary part of gap function peaked at frequencies of pairing phonons

Scalapino, Schreiffer, Wilkins, PBR 148 263 1966

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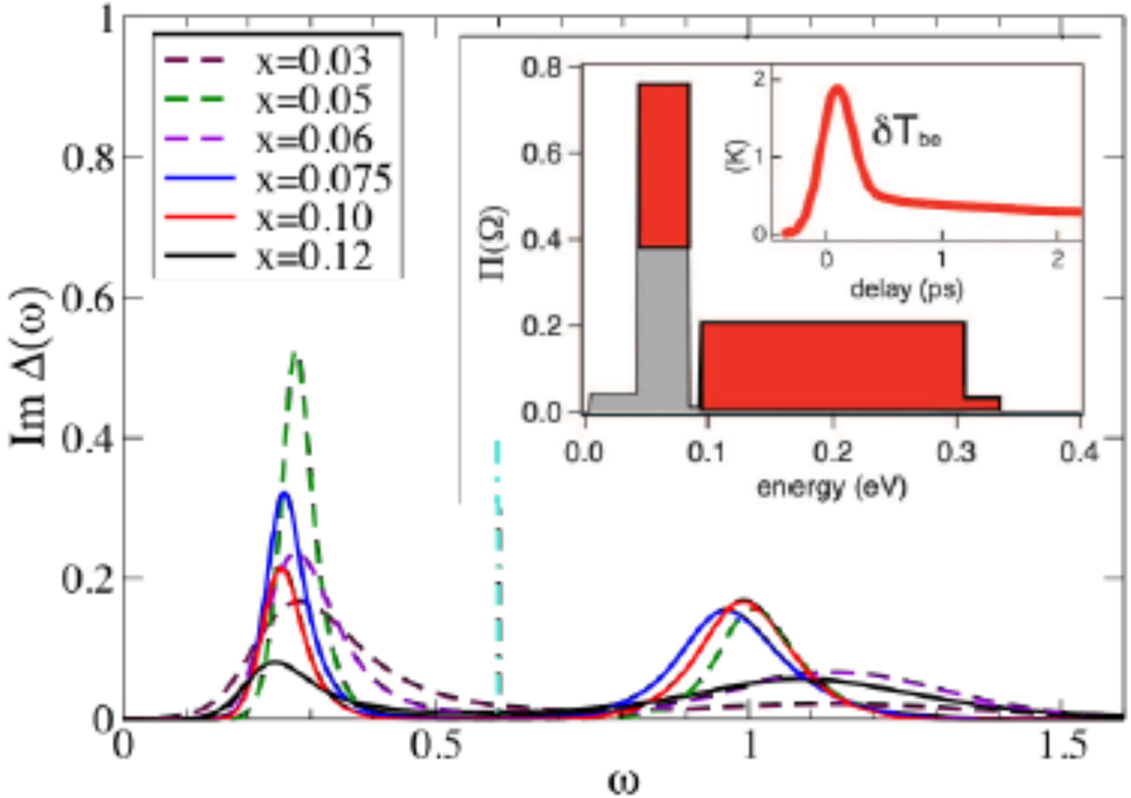
In the Hubbard model

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



All the pairing comes from low frequencies; most from very low frequencies

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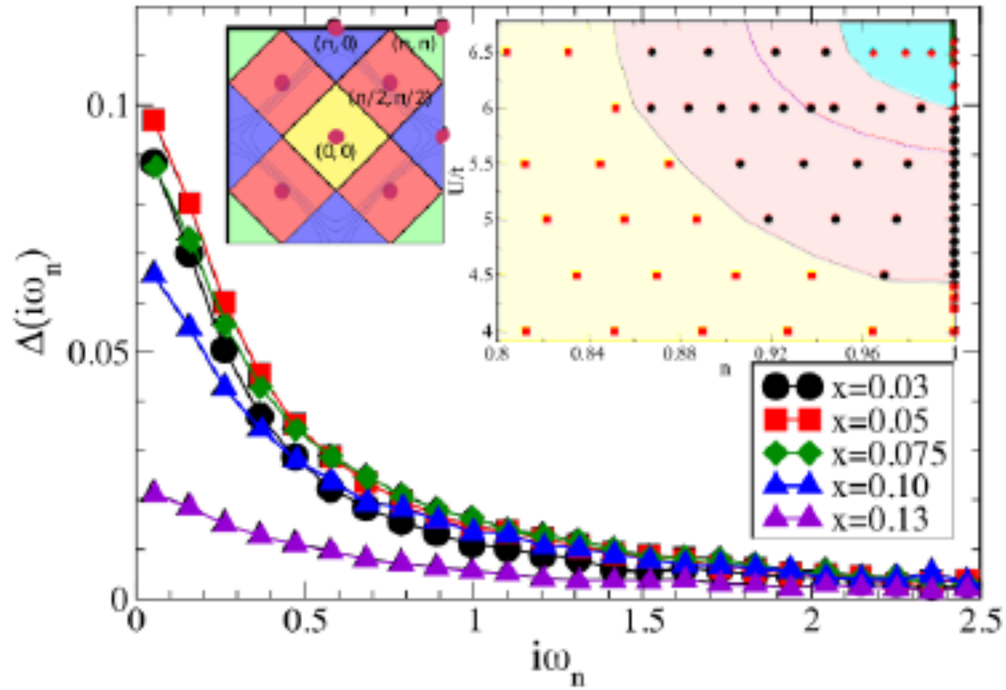
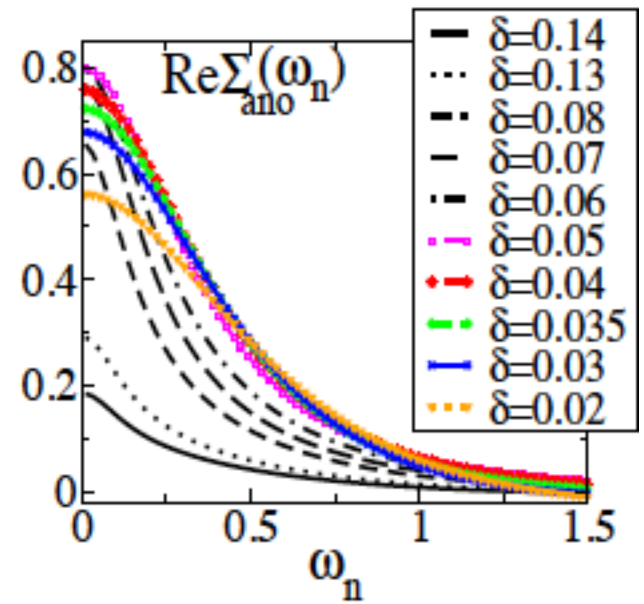
Can see this in raw data

Our results



Civelli 09 4 site CDMFT. ED solver



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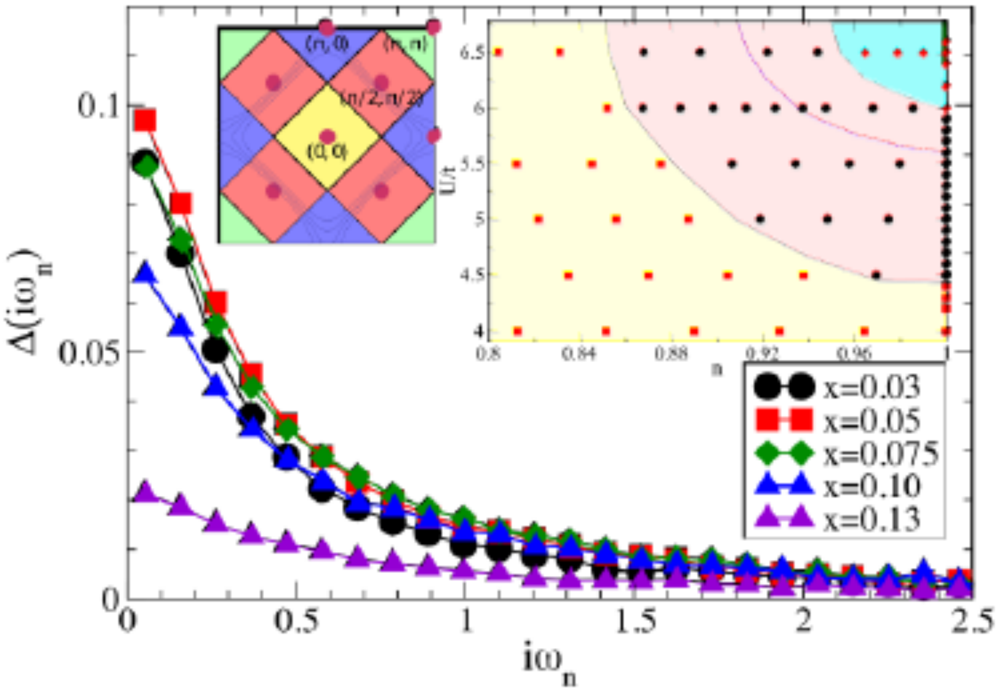
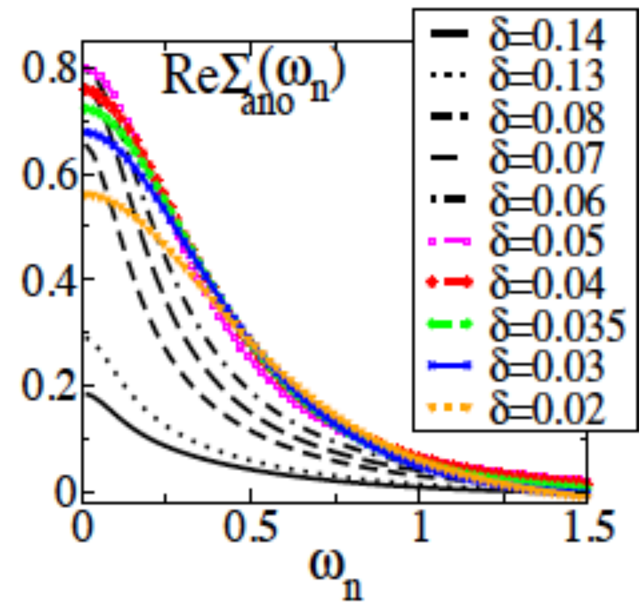
Can see this in raw data

Our results



Civelli 09 4 site CDMFT. ED solver



Note: Maier, Poilblanc, Scalapino: 20% or more of pairing comes from high frequencies ~U.

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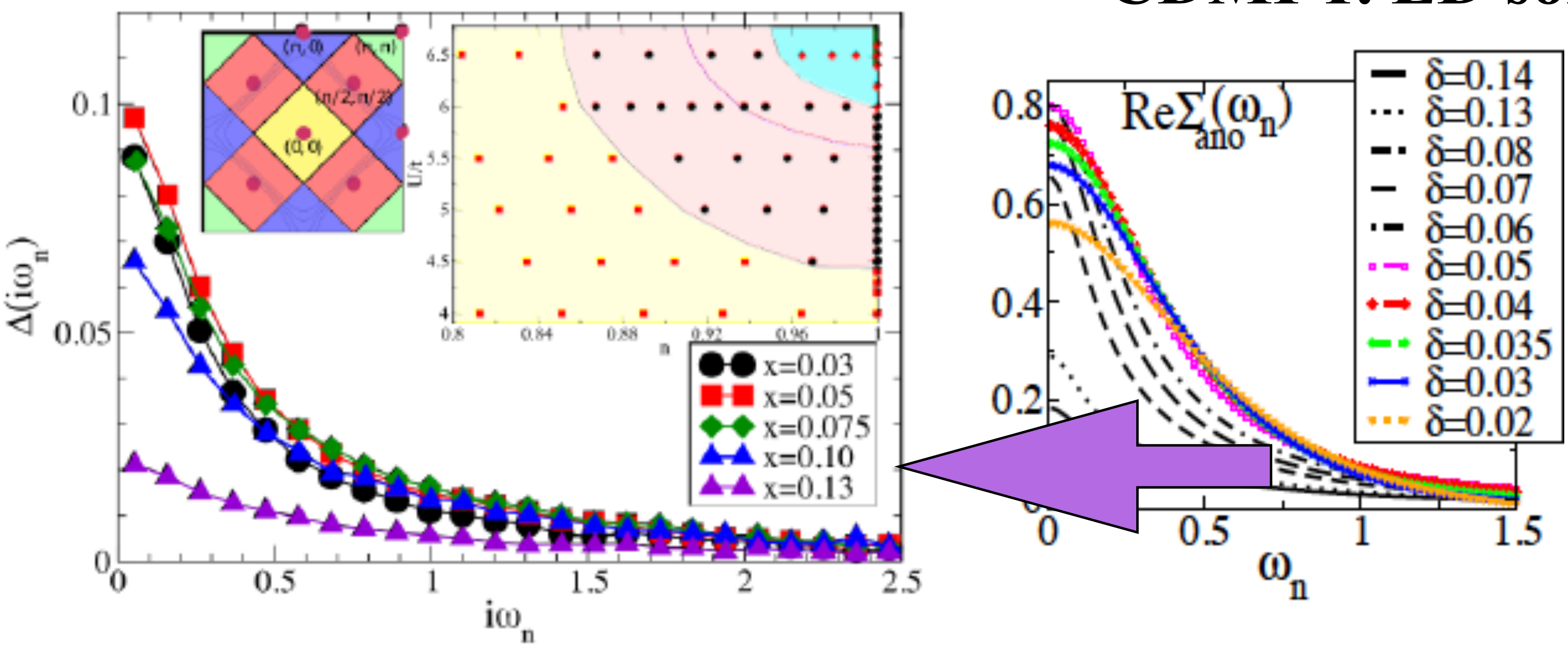
$$\Delta(i\omega_n) = \frac{\Sigma^A(i\omega_n)}{1 - \frac{\Sigma_o^N(i\omega_n)}{\omega_n}} = \int \frac{dx}{\pi} \frac{\Delta^{(2)}(x)}{i\omega_n - x}$$

Our results

Civelli 09 4 site CDMFT. ED solver



Note: Maier, Poilblanc, Scalapino: 20% or more of pairing comes from high frequencies ~U. If this were right, would see it in our raw data

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Many years ago,
D. J. Scalapino asked:

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Does the two dimensional Hubbard model have

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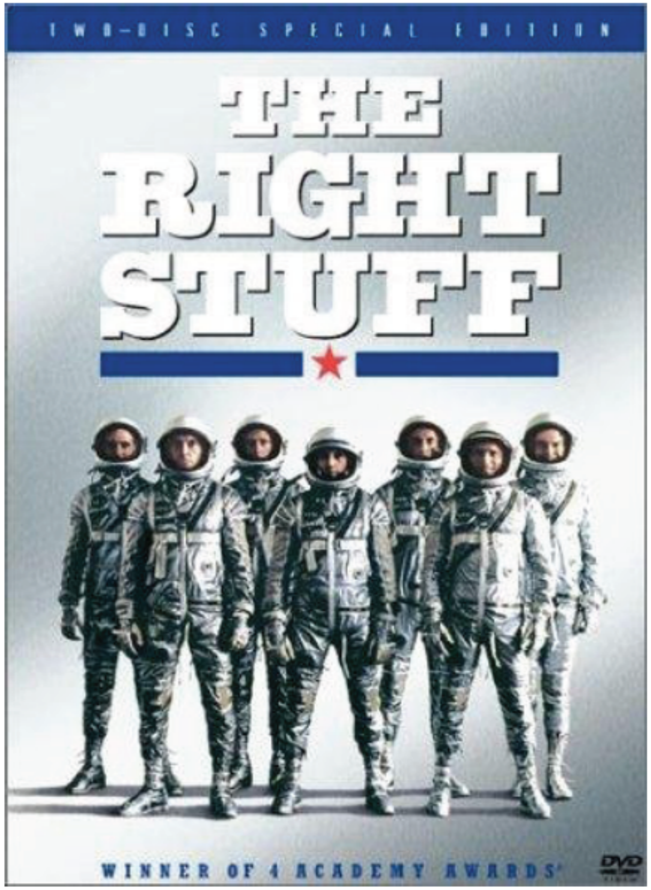

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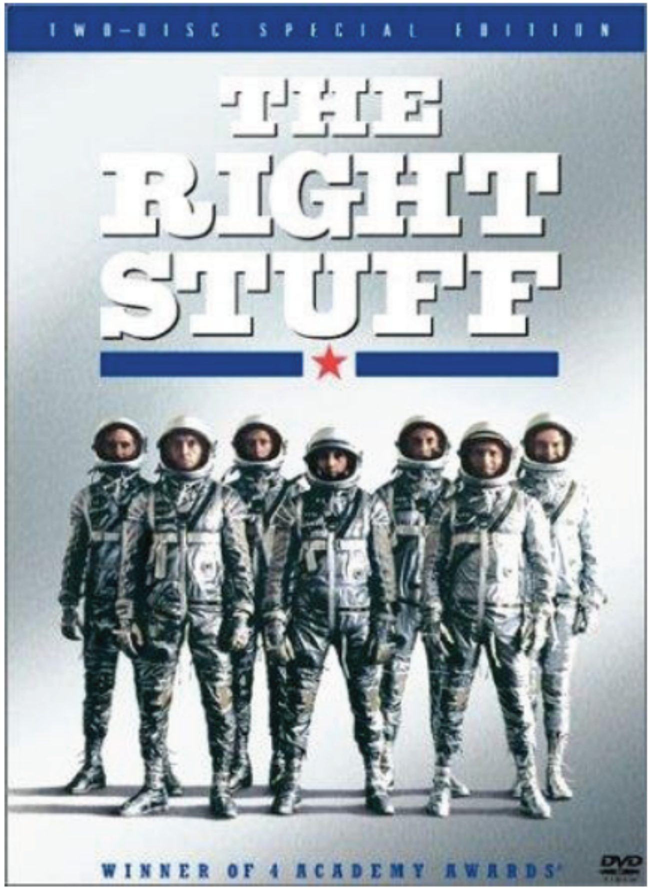
Many years ago,
D. J. Scalapino asked:

Does the two dimensional Hubbard model have



(i.e. can it account for the essential aspects of the low energy physics of the high-Tc cuprates)

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I hope that this talk has persuaded you that

The answer is YES

Implication: the pseudogap and superconductivity are basic phenomena of strong correlation physics.

Charge order, nematicity, etc are extra things ``along for the ride'

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Issues

1. We have nice numerical results—but what is the physics??
2. Limit: U~7, N ~ 16 is not as good as we would like.
   A. Stronger coupling?
   B. Larger N—are the N=8, 16 results really representative of Hubbard physics
3. Stripes and other ordered states are (presently) beyond the reach of this approach. What is their importance?

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Coda: SDW order and fluctuations in Iron Arsenide Superconductors.

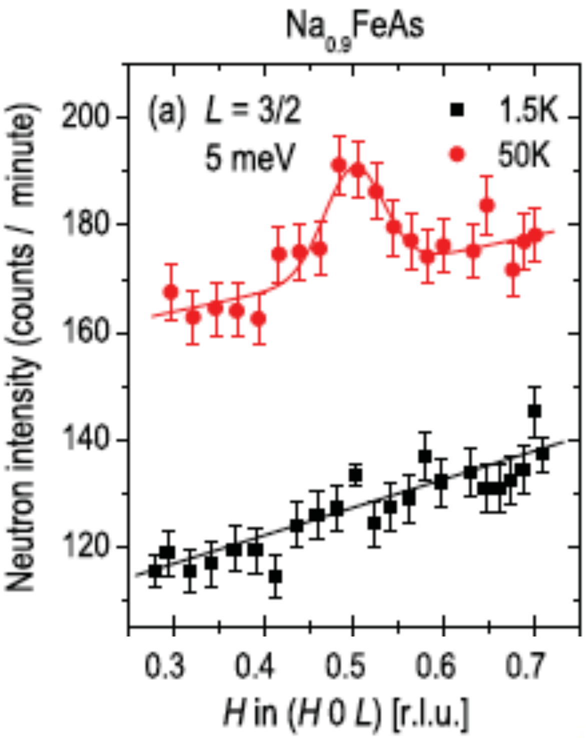
With Abhay Pasupathy & Rafael Fernandes

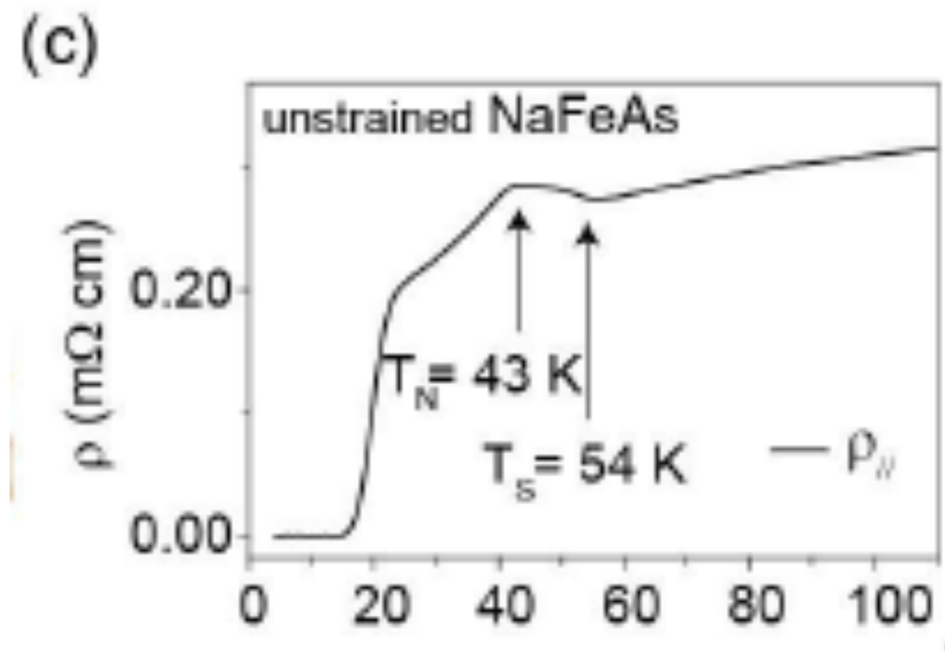
NaFeAs: `stripe' (0,Pi) order below 43K

`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
J. Wei,[2] M. Aeschlimann,[2] X. Y. Cui,[3] M. Shi,[3] J. P. Hu,[4] and D. L. Feng[1,*]





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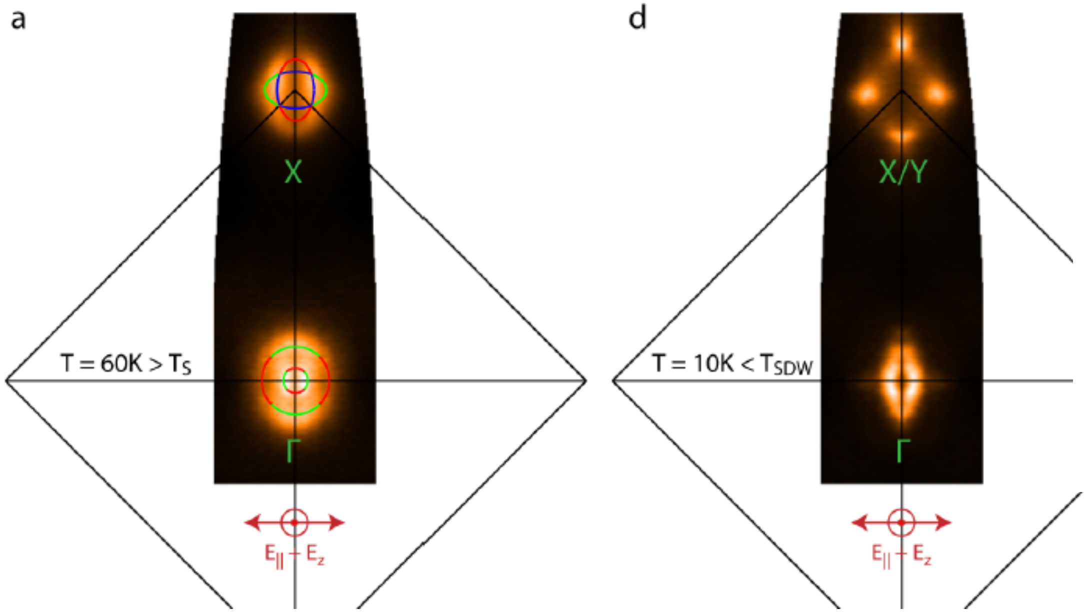
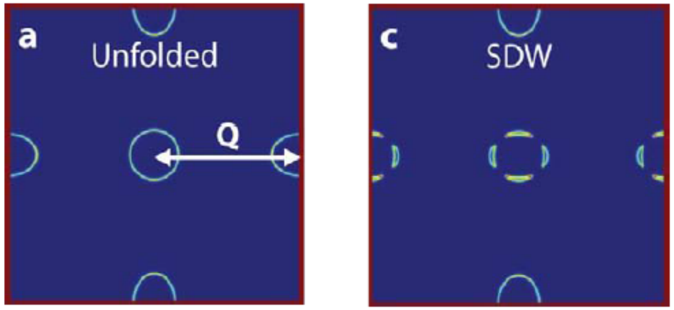
SDW rearranges the Fermi surface

Data:

M Yi[1,2], D H Lu[3], R G Moore[1], K Kihou[4,5], C-H Lee[4,5], A Iyo[4,5], H Eisaki[4,5], T Yoshida[5,6], A Fujimori[5,6], Z-X Shen[1,2]*



Calculations



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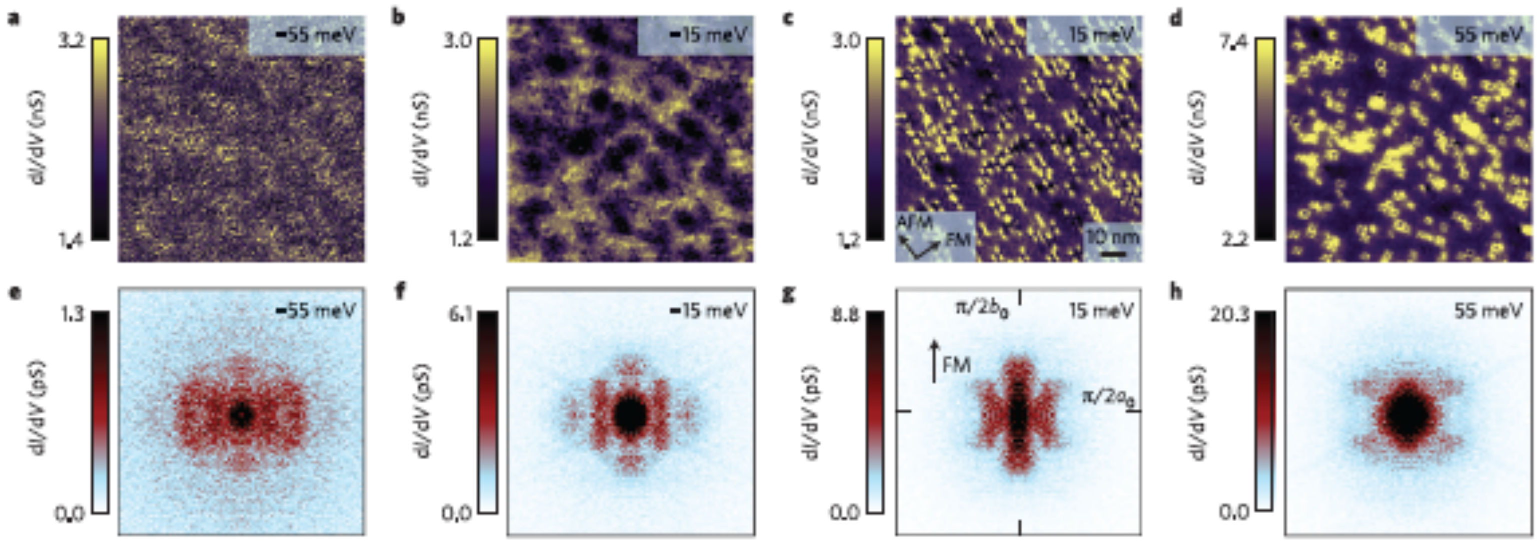
Quasiparticle Interference Reveals the Reconstruction

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

N. Phys. 10 225 (2014)



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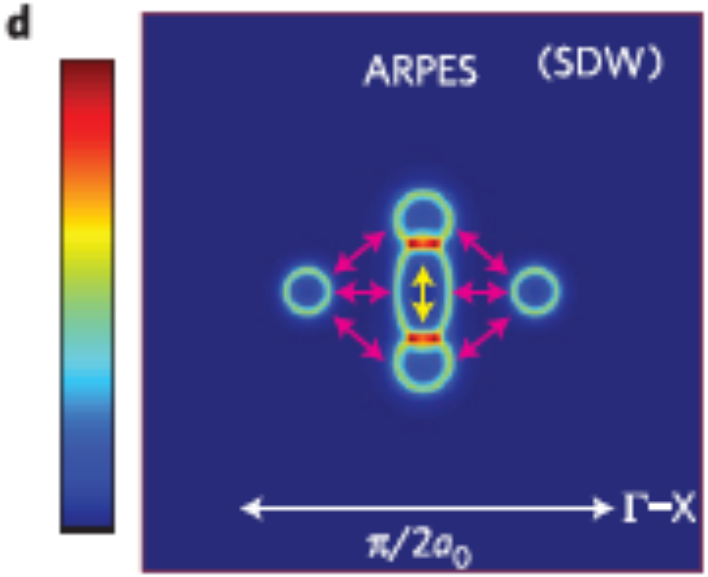
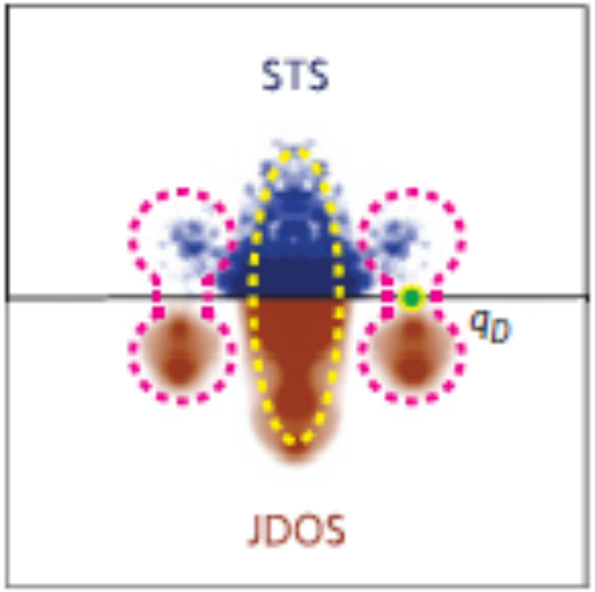
Structure in QPI reveals fermi surface





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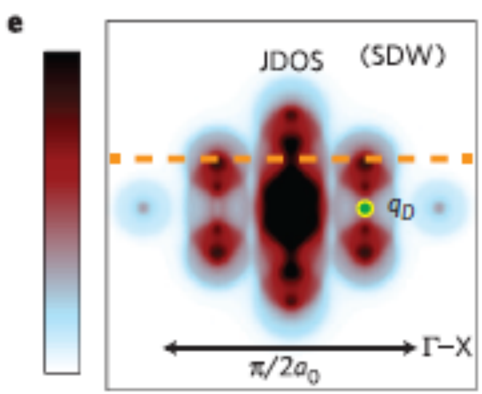
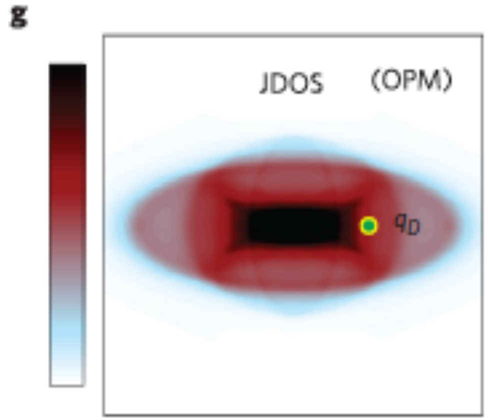
As you raise the temperature, expect the SDW-derived features to go away

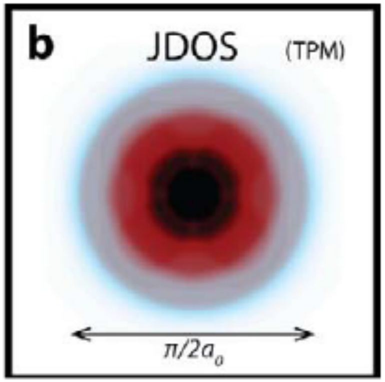
$T<T_N$~43K



$T_N<T<T_{nematic}$



$T_{nematic}<T$



Here I show you joint DOS for simplicity.
Full QPI calculations give the same physics

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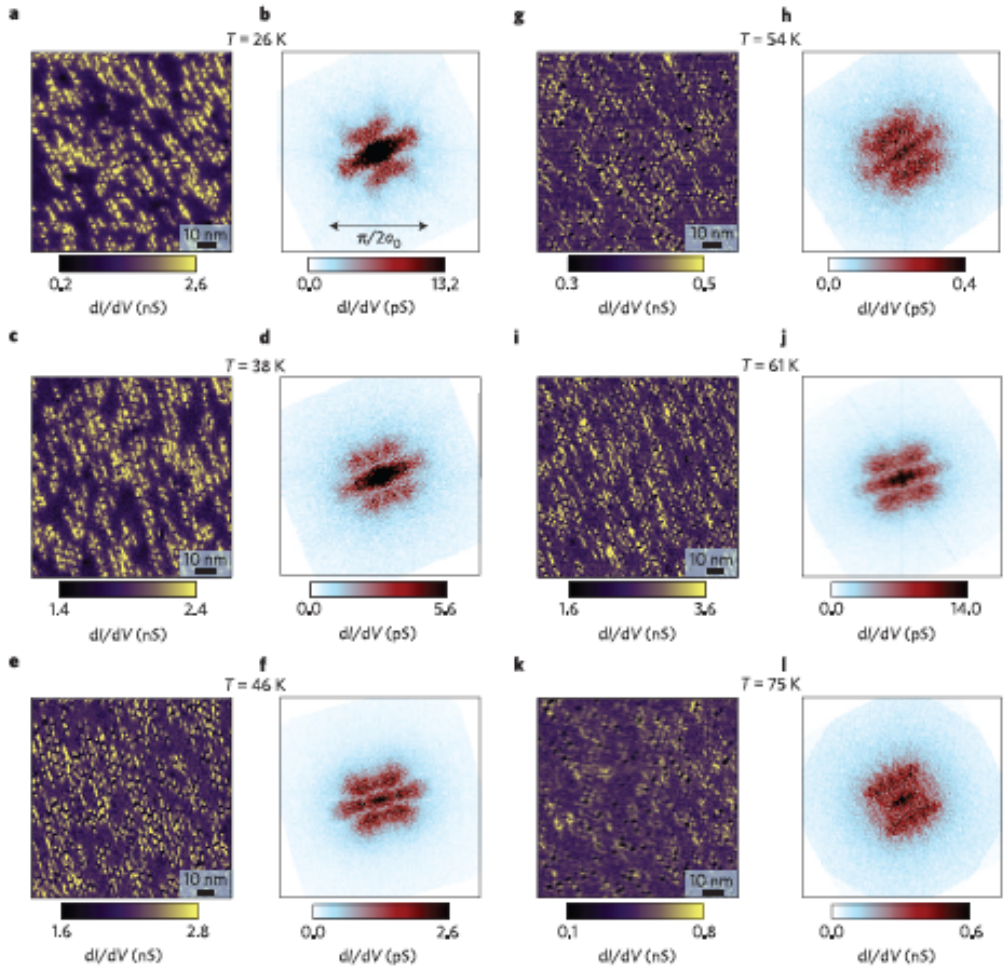
This is not what happens



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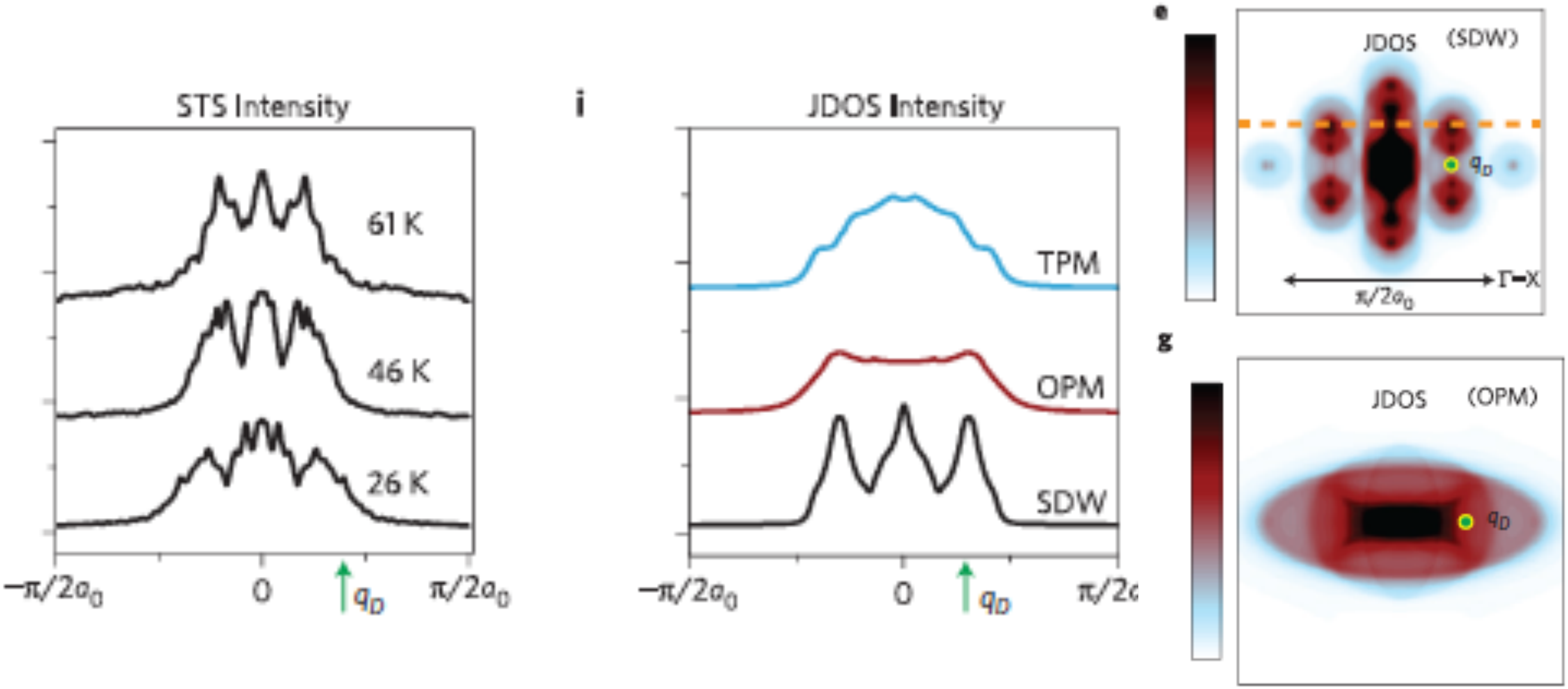
More easily visualized as a line cut



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

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Model
'Lee-Rice-Anderson' ansatz

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

This is broadened backscattering (no \`coherence factors in normal state)

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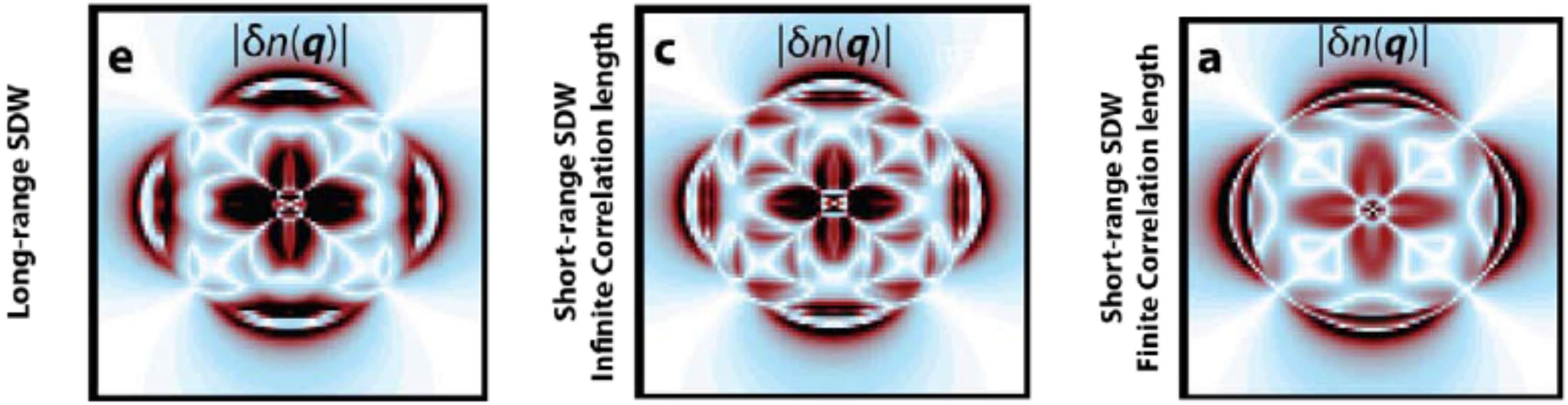
Model QPI Calculations



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

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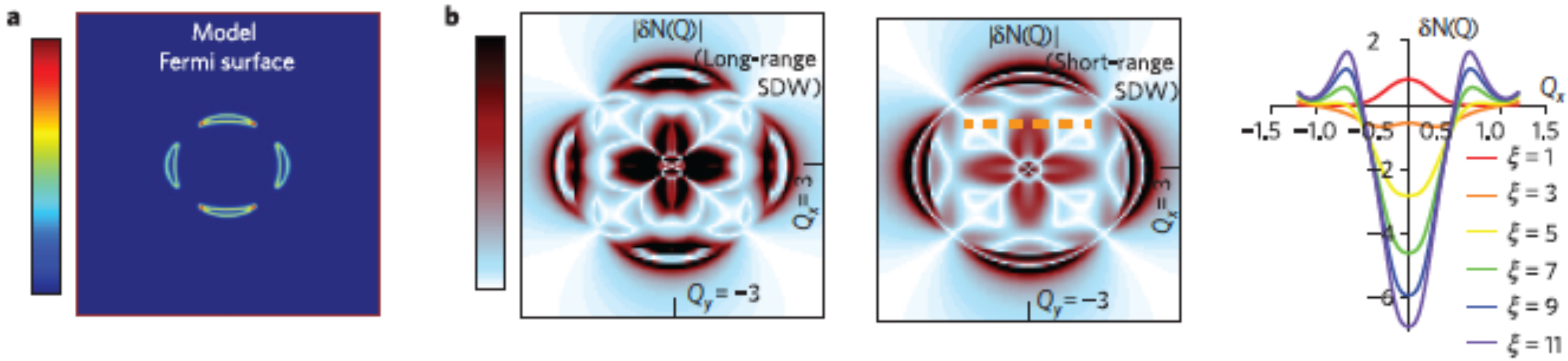
Vary correlation length



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

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

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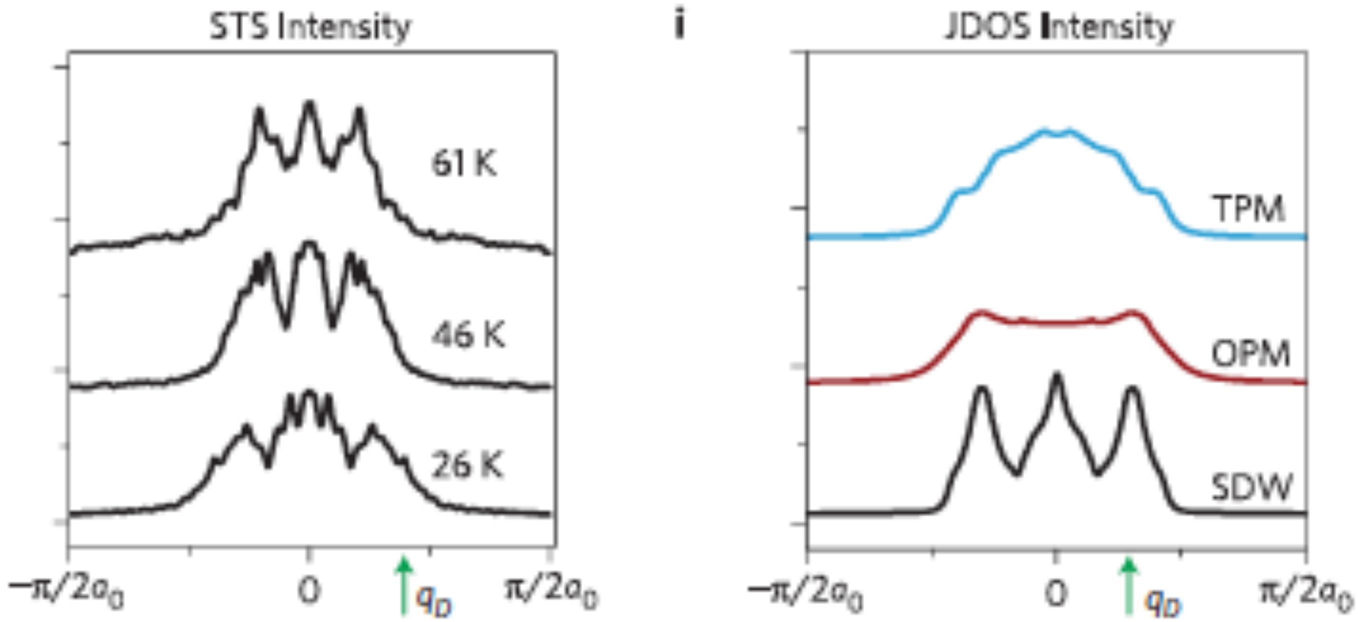
In other words

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



Paramagnetic phase has hidden structure

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Poetically

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We used to think of the fermi sea as a (relatively) placid lake with modest ripples (RPA fluctuations).

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Pasupathy's results suggest an alternative picture

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Pasupathy's results suggest an alternative picture

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Poetically

Pasupathy's results suggest an alternative picture: A stormy sea with giant amplitude, slowly moving waves.

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Poetically

Pasupathy's results suggest an alternative picture: A stormy sea with giant amplitude, slowly moving waves.

Which picture is correct. If large amplitude density wave fluctuations are present, how do we surf on them

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