Pairing dynamics in strongly correlated superconductivity : the sticky question.

André-Marie Tremblay

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KITP 21 juillet 2009

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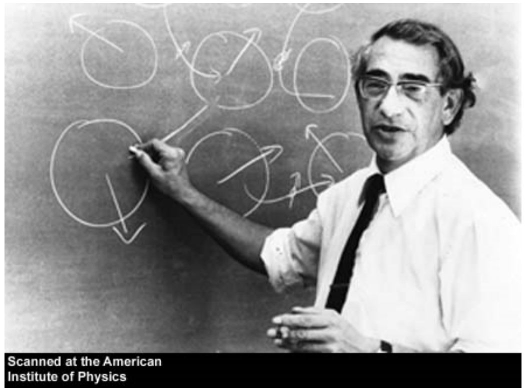
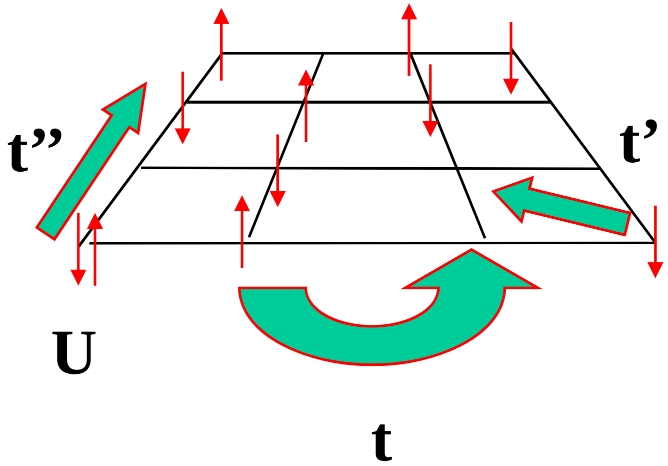
The model

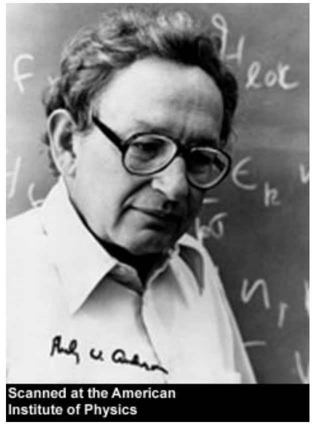
Hubbard model

Simplest microscopic model for *Cu O*$_2$ planes.



μ



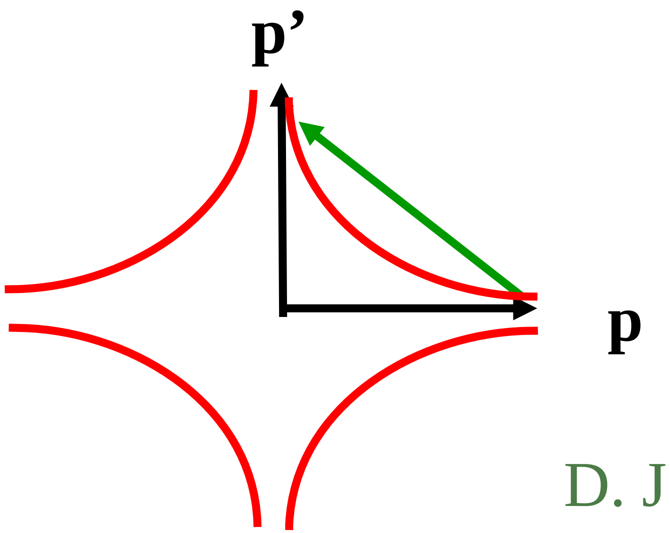


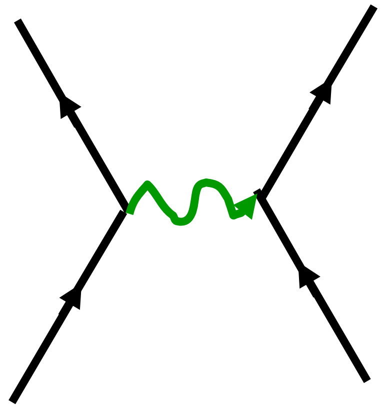
$$H = -\sum_{<ij>\sigma} t_{i,j} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

No mean-field factorization for d-wave superconductivity

Cartoon « BCS » weak-coupling picture

$$\Delta_{\mathbf{p}} = -\frac{1}{2V}\sum_{\mathbf{p}'} U(\mathbf{p}-\mathbf{p}')\frac{\Delta_{\mathbf{p}'}}{E_{\mathbf{p}'}}\left(1-2n\left(E_{\mathbf{p}'}\right)\right)$$





Exchange of spin waves?
Kohn-Luttinger
T_c with pressure

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

P.W. Anderson Science 317, 1705 (2007)

A cartoon strong coupling picture

P.W. Anderson Science 317, 1705 (2007)

$$J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = J \sum_{\langle i,j \rangle} \left(\frac{1}{2} c_i^\dagger \vec{\sigma} c_i \right) \cdot \left(\frac{1}{2} c_j^\dagger \vec{\sigma} c_j \right)$$

$$d = \langle \hat{d} \rangle = 1/N \sum_{\vec{k}} (\cos k_x - \cos k_y) \langle c_{\vec{k},\uparrow} c_{-\vec{k},\downarrow} \rangle$$

$$H_{MF} = \sum_{\vec{k},\sigma} \varepsilon(\vec{k}) c_{\vec{k},\sigma}^\dagger c_{\vec{k},\sigma} - 4Jm\hat{m} - Jd(\hat{d} + \hat{d}^\dagger) + F_0$$

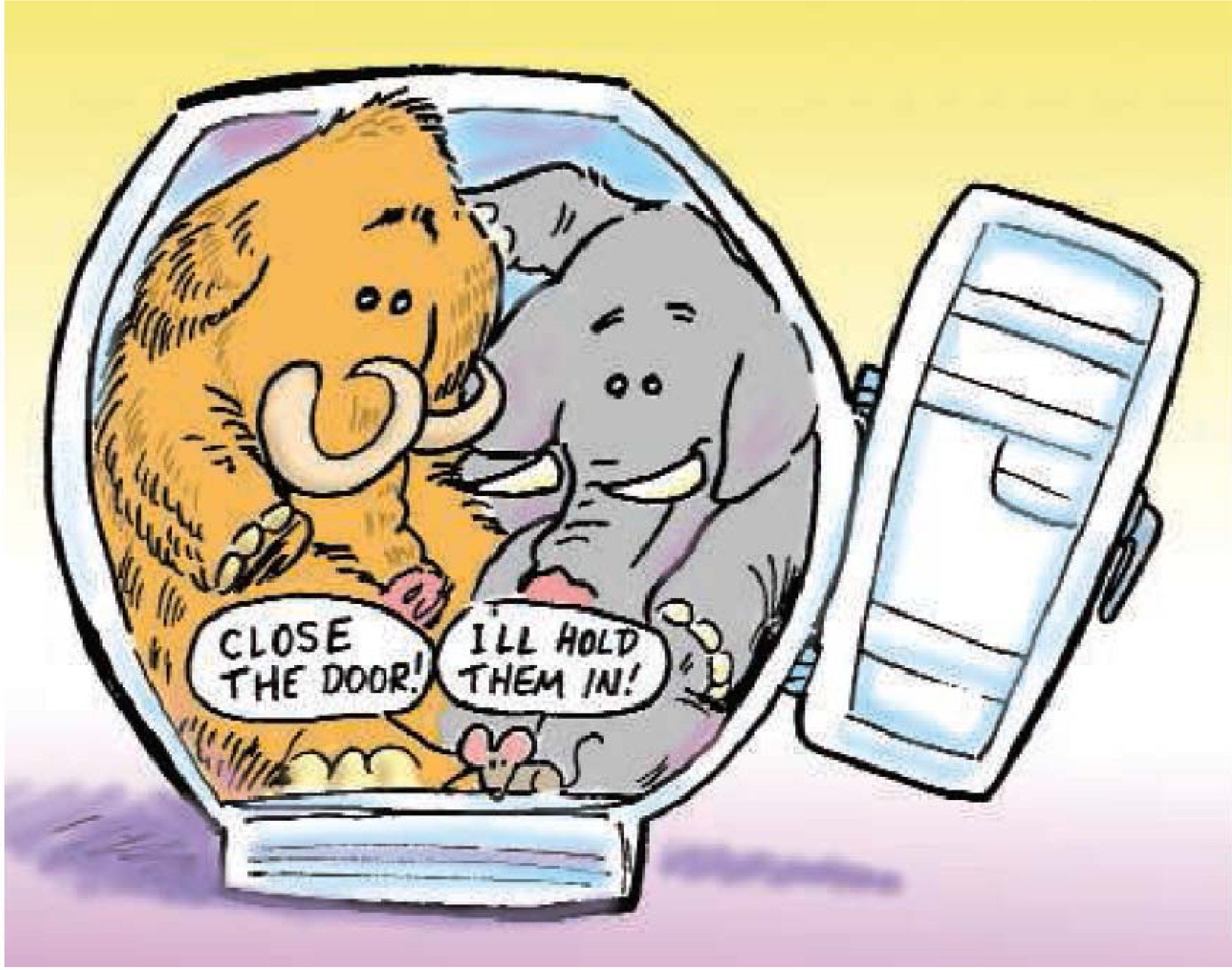
Pitaevskii Brückner:

Pair state orthogonal to repulsive core of Coulomb interaction

Miyake, Schmitt–Rink, and Varma
P.R. B **34**, 6554-6556 (1986)

What is the glue?

P.W. Anderson Science 317, 1705 (2007)

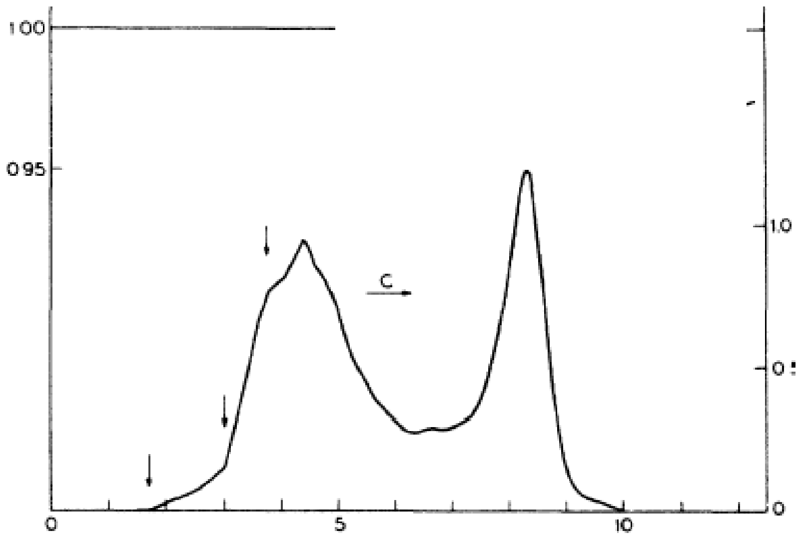


"We have a mammoth and an elephant in our refrigerator—do we care much if there is also a mouse?"

In « conventional superconductors »

$$\langle c_{i\uparrow}(t) c_{j\downarrow}(0) \rangle$$

$\alpha^2 F(\omega)$

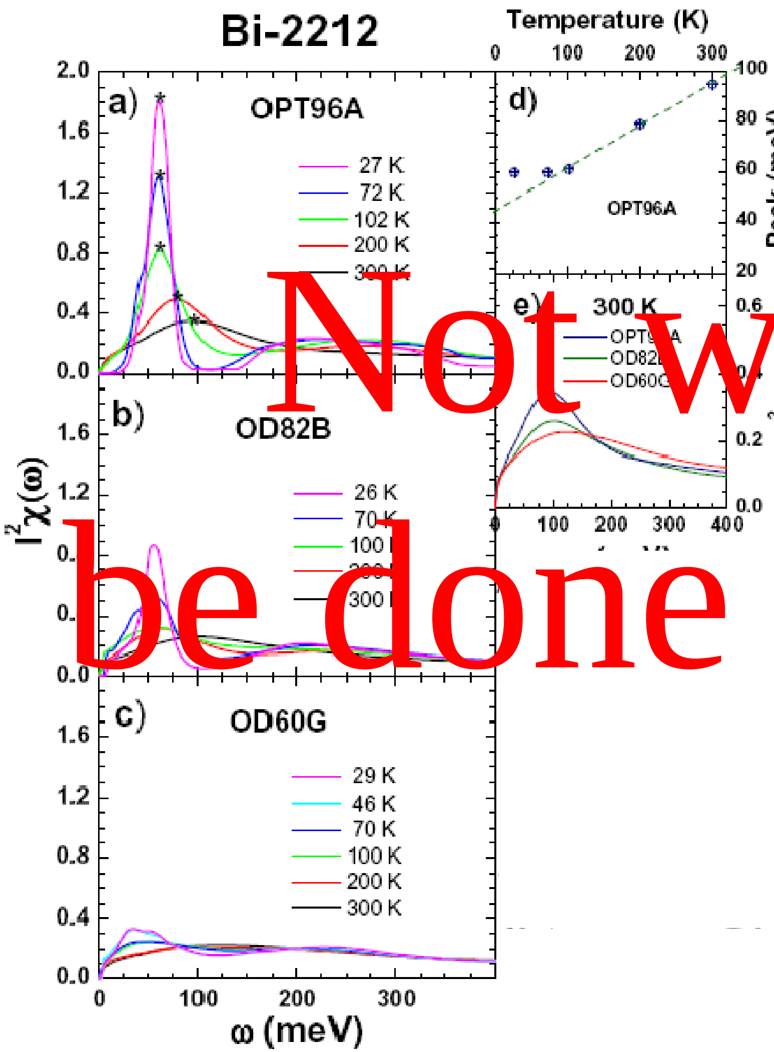


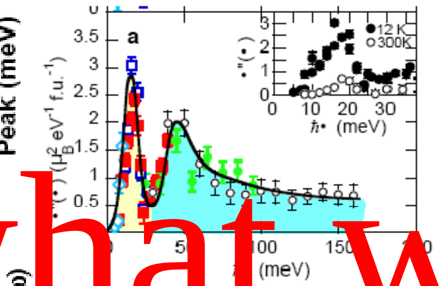
ω

Scalapino, Schrieffer, Wilkins PR (1966)
McMillan Rowell PRL (1965)
Rowell, Anderson, Thomas PRL (1963)

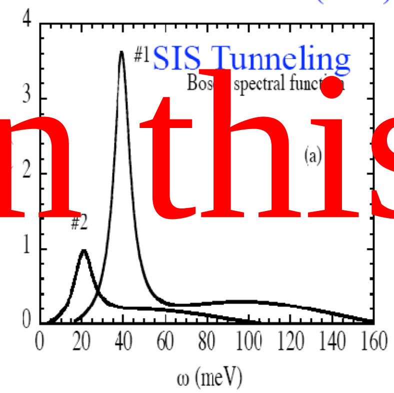
Migdal-Eliashberg approach in High T_c

Vignolle, Nature (2007)





Zasadzinski *et al.* (2005)



Not what will be done in this talk

Hwang, Timusk, Carbotte PRB (2007)
PRL (2008), Nature (1999)

Courtesy, T. Timusk

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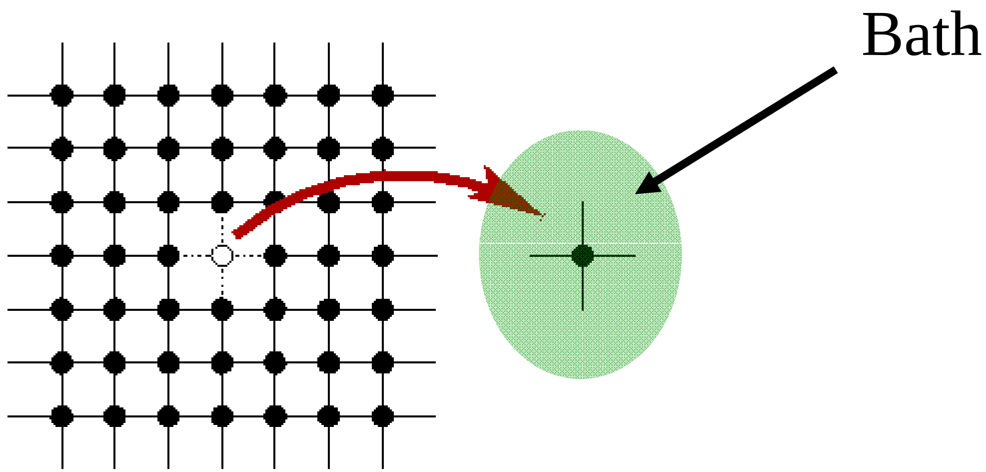
The method

Strong coupling: Quantum cluster methods. The beginnings in infinite dimension



W. Metzner and D. Vollhardt, PRL (1989)

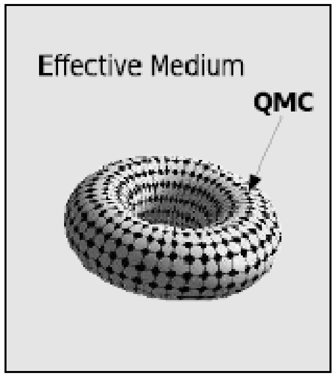
A. Georges and G. Kotliar, PRB (1992)

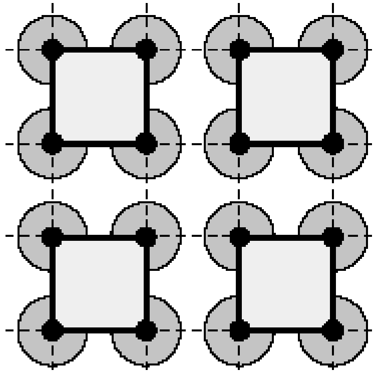
M. Jarrell PRB (1992)

DMFT, (d = 3)

Quantum clusters

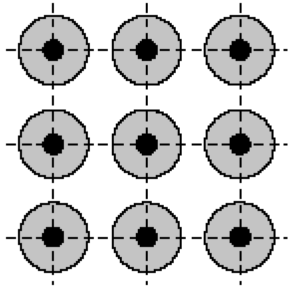
C-DMFT





DCA

DMFT



Hettler …Jarrell…Krishnamurty PRB **58** (1998)
Kotliar et al. PRL **87** (2001)
M. Potthoff *et al.* PRL **91,** 206402 (2003).
Maier, Jarrell et al., Rev. Mod. Phys. **77**, 1027 (2005)

SFT : Self-energy Functional Theory

Grand potential, and $F[\Sigma]$ Legendre transform of Luttinger-Ward funct.

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

is stationary with respect to Σ.

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 $F[\Sigma]$.

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

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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Advantages

- Can be solved by unbiased methods (QMC, exact diagonalization…)
- Takes short range correlations into account essentially exactly
- Mean-field symmetry-breaking terms for phase transitions are in the bath

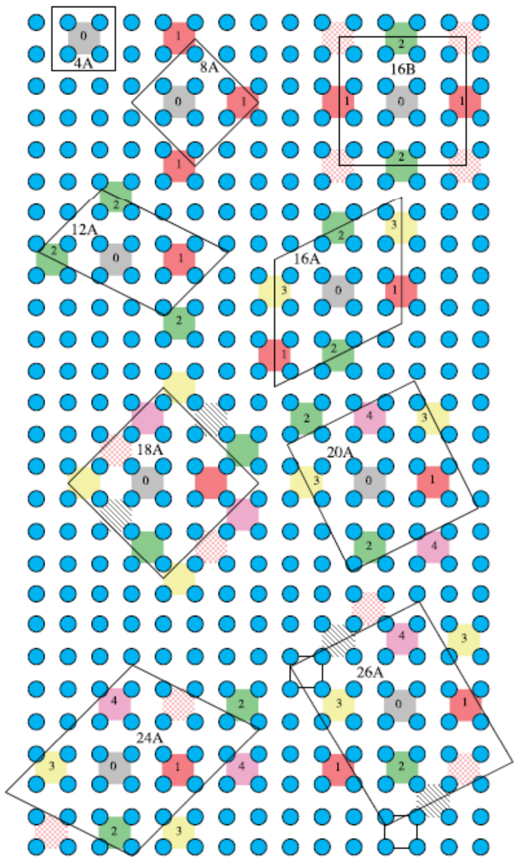
Warnings

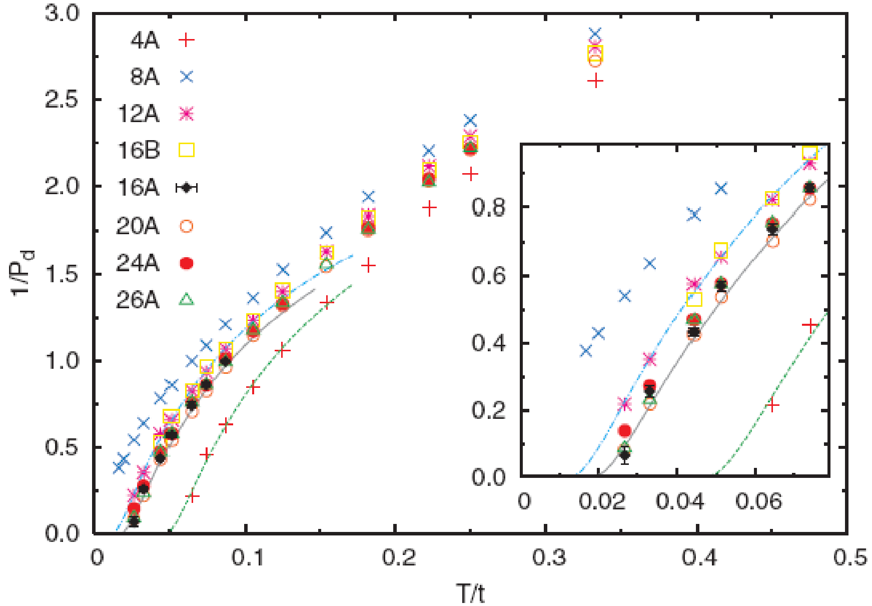
- Rate of convergence to the thermodynamic limit (depends on the method and observable that is considered)
- Periodization

D-wave in the Hubbard model?

DCA

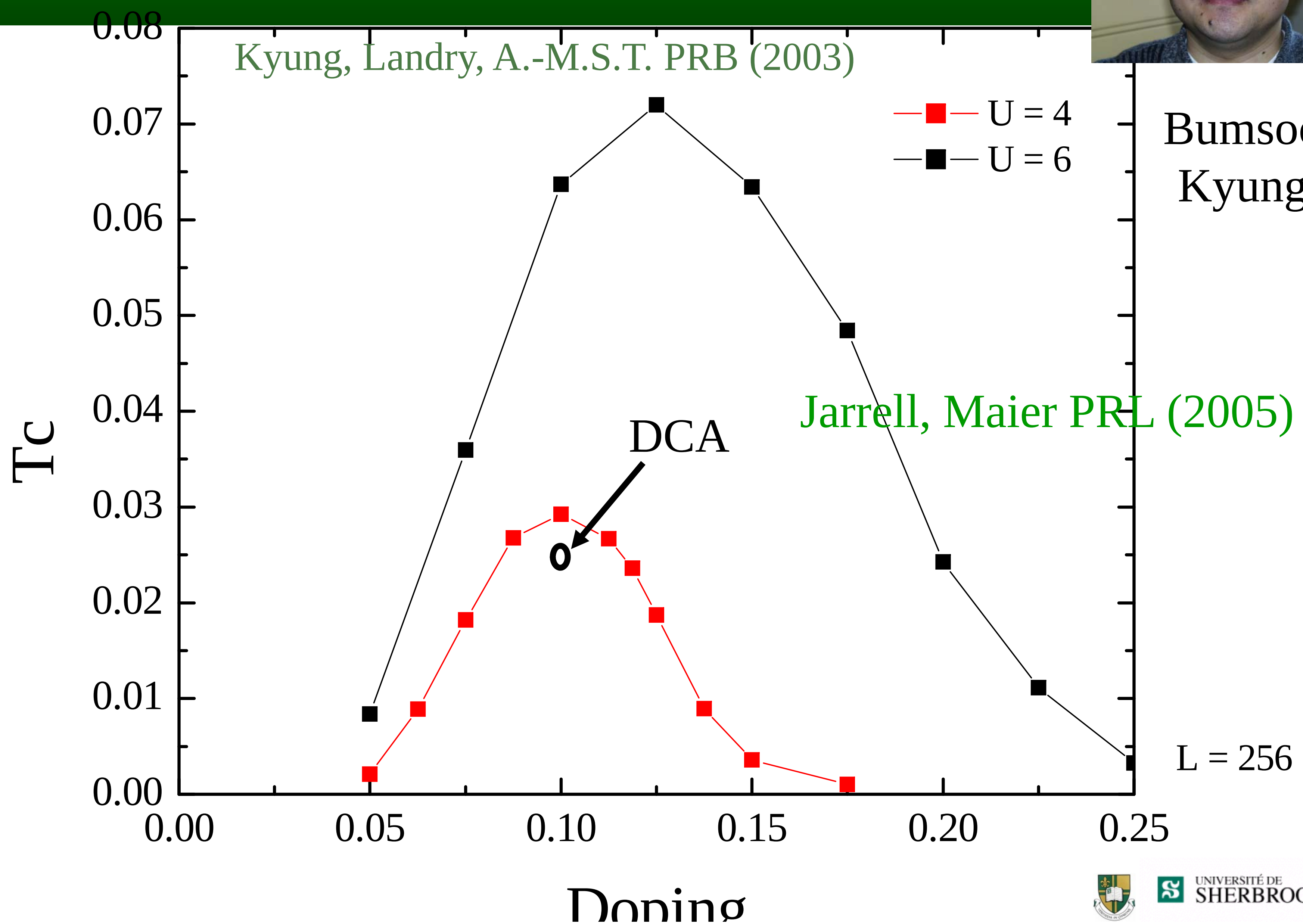
Maier Jarrell et al., PRL (2005)

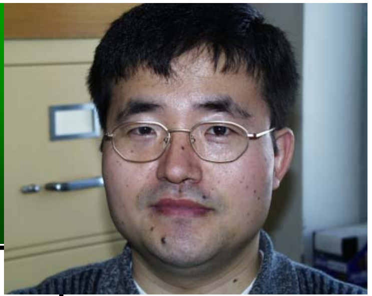




T_c=0.023t,
10% doping

Phase diagram, TPSC





Bumsoo Kyung

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Numerical evidence: d-wave superconductivity in Hubbard model

- K. Haule, and G. Kotliar PRB **76**, 104509 (2007)
- S. Kancharla, B. Kyung, D. Sénéchal, M. Civelli, M. Capone, G. Kotliar, and A.-M. S. Tremblay, PRB **77**, 184516 (2008)
- Review: Th. Maier, M. Jarrell, Th. Pruschke, M.H. Hettler, RMP (2005)
- Th. Maier, M. Jarrell, Th. Pruschke, and J. Keller PRL **85**, 1524 (2000)
- A. Paramekanti, Mohit Randeria, and Nandini Trivedi, PRL **87,** 217002 (2001).
- S. Sorella, G. B. Martins, F. Becca, C. Gazza, L. Capriotti, A. Parola, and E. Dagotto PRL **88**, 117002 (2002)
- D. Poilblanc and D.J. Scalapino Phys. Rev. B **66**, 052513 (2002) (2002)
- D. Sénéchal, P.-L. Lavertu, M.-A. Marois and A.-M.S. Tremblay, PRL **94**, 156404 (2005)
- T.A. Maier, M. Jarrell, T.C. Schulthess, P. R. C. Kent, and J.B. White, Phys. Rev. Lett. **95**, 237001 (2005)

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But…

Gaussian Basis QMC: no

Aimi and Imada, J. Phys. Soc. Japan **76,** 113708, (2007).

Refined variational approach: no

Aimi and Imada, J. Phys. Soc. Jpn (2007)

Phenomenology of cuprates and others from quantum clusters: Some previous results

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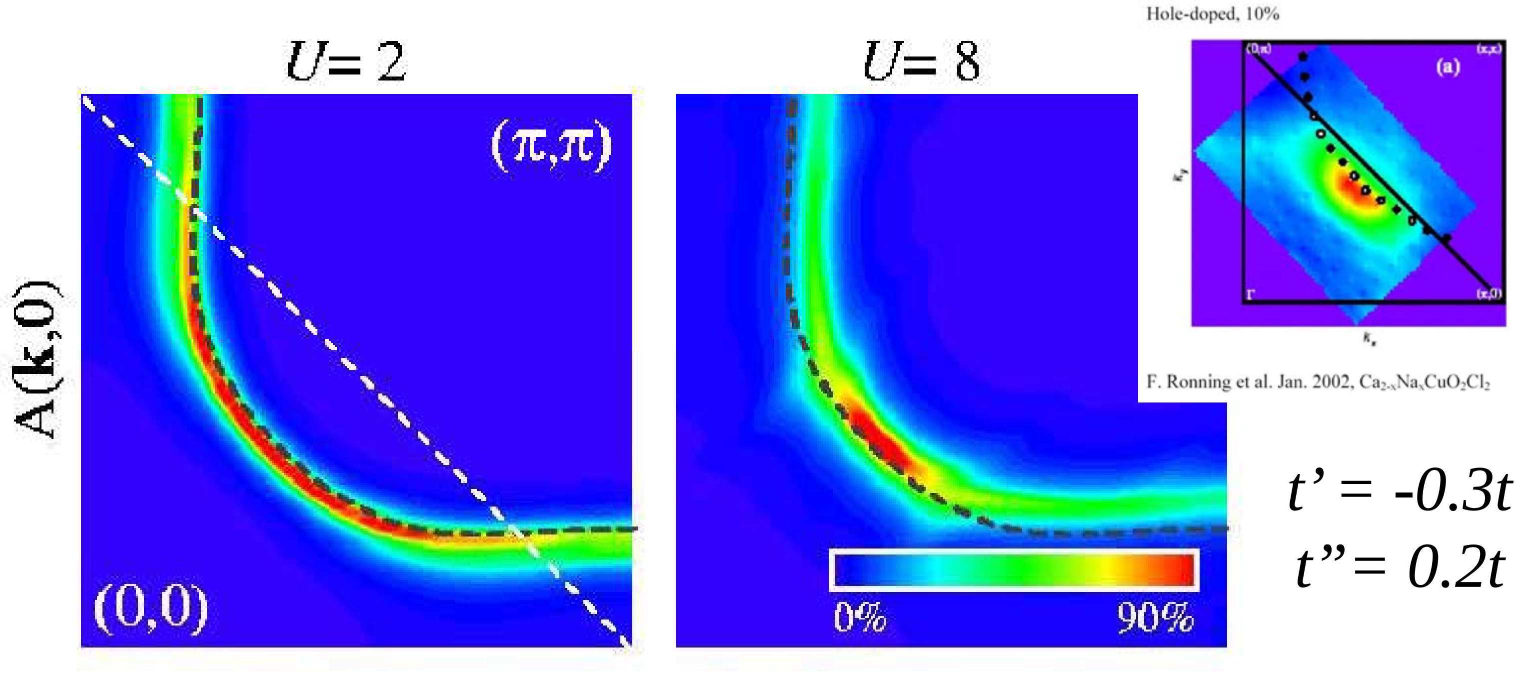
Hole-doped (17%)

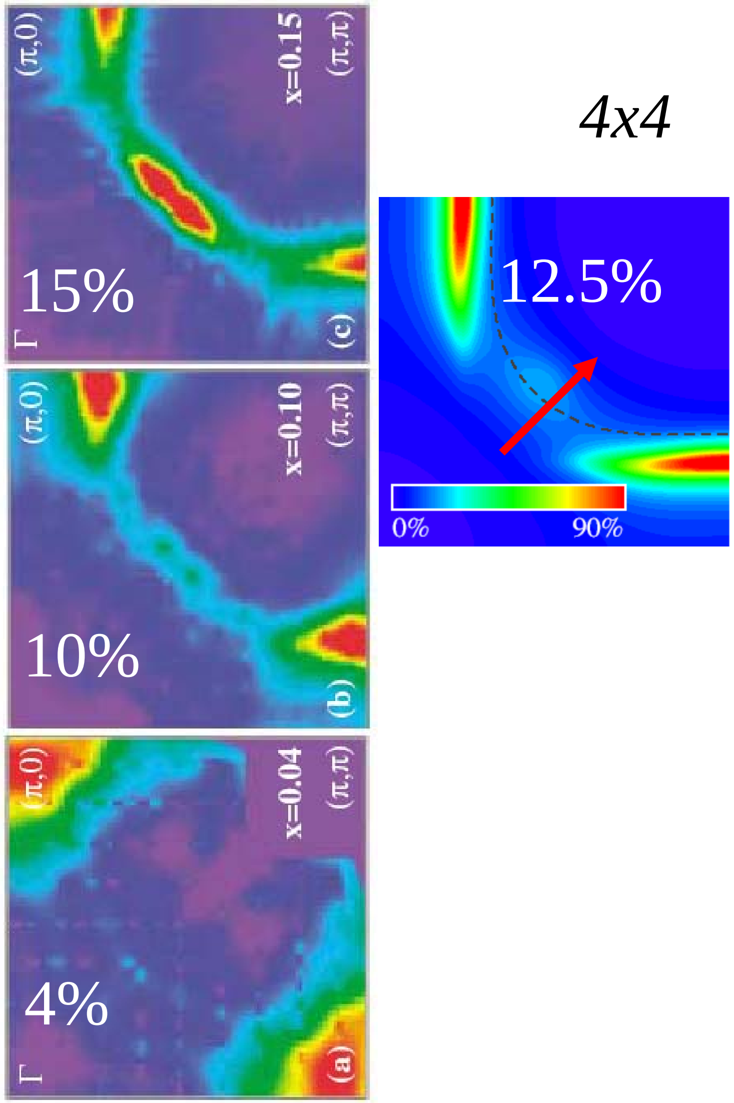


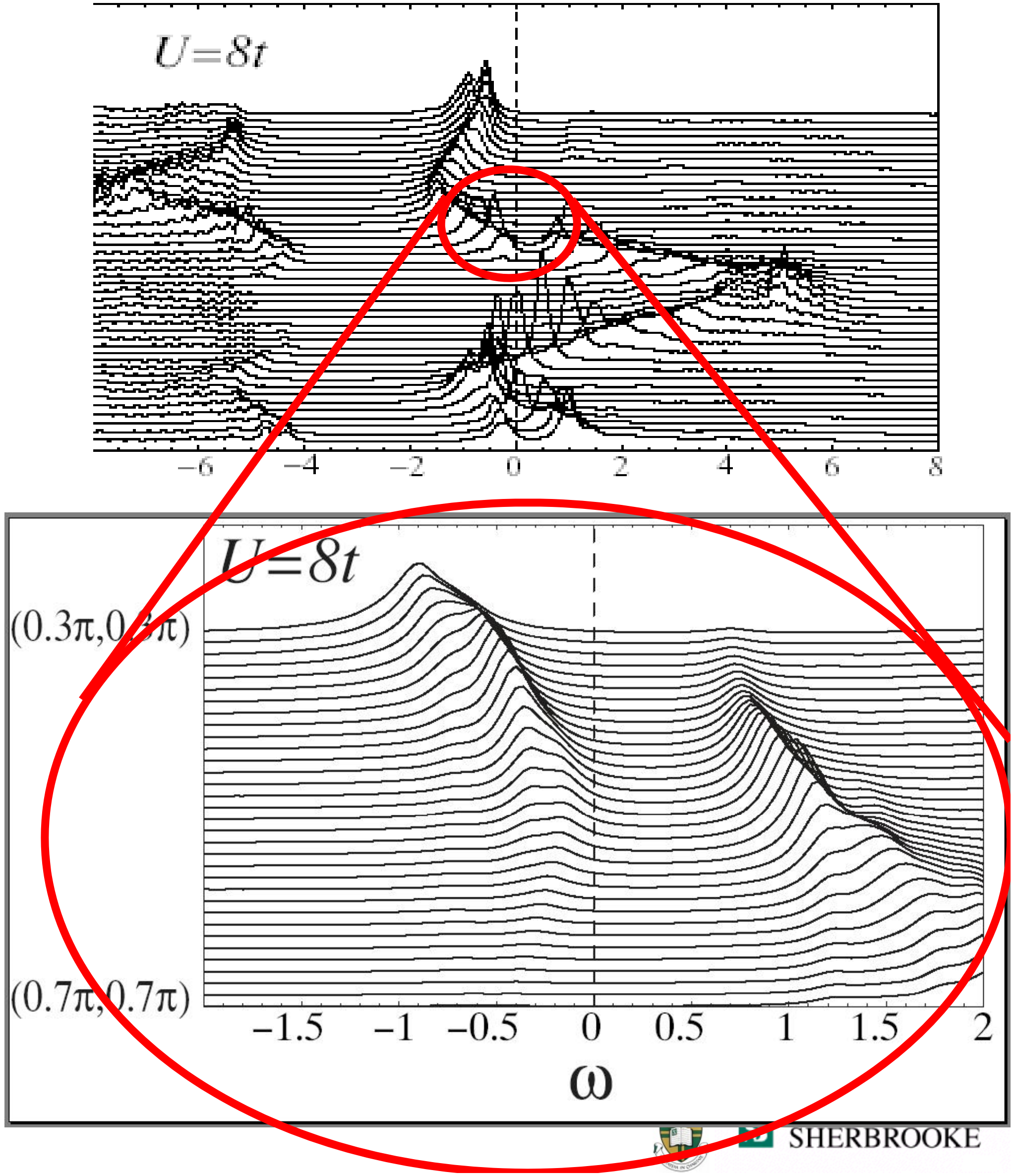
t’ = -0.3t
t” = 0.2t

η = *0.12t*
η = *0.4t*

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

Electron-doped 12.5%, *U=8t*





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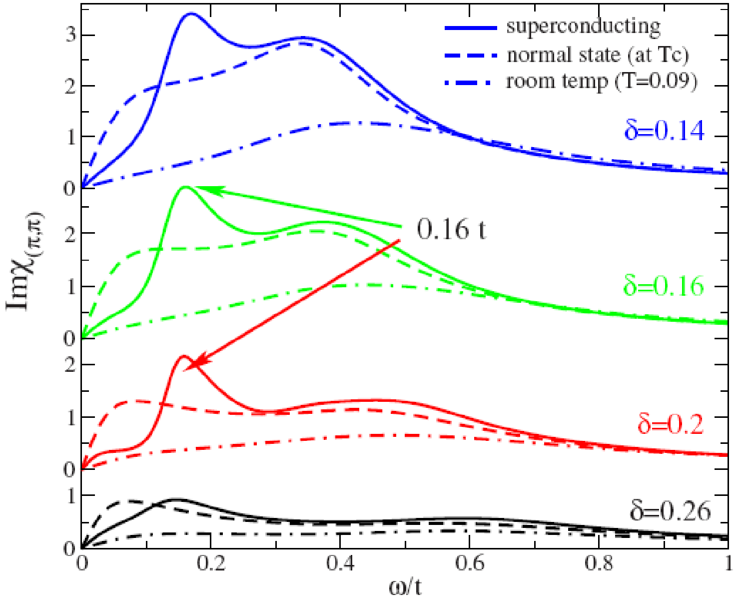
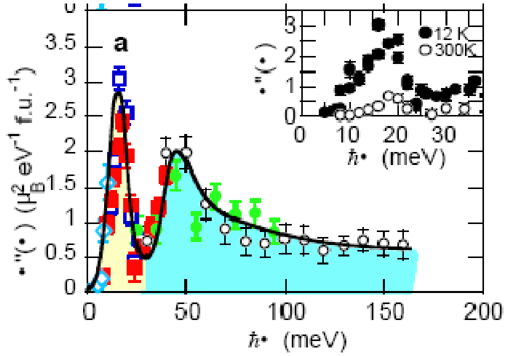
Spectral function for spin fluctuations

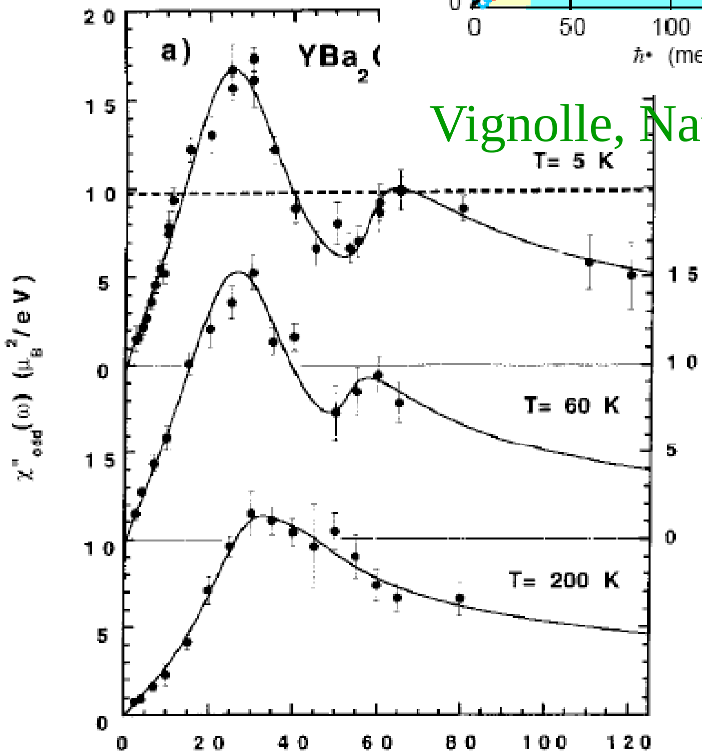
Haule Kotliar, PRB (2007)



LSCO

Underdoped Y





Vignolle, Nature (2007)

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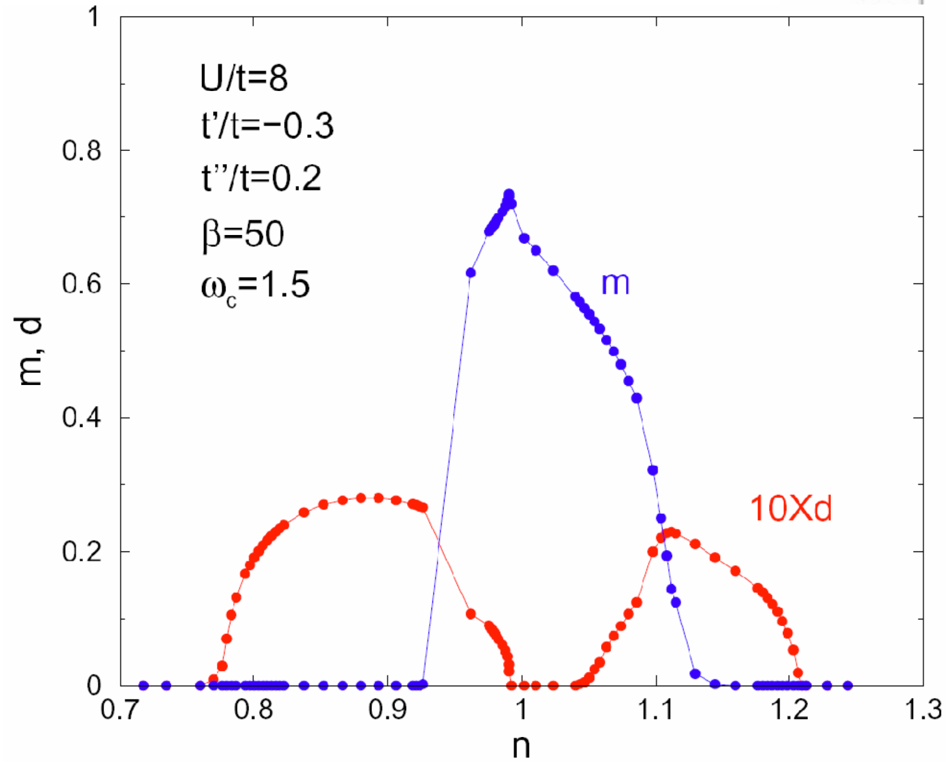
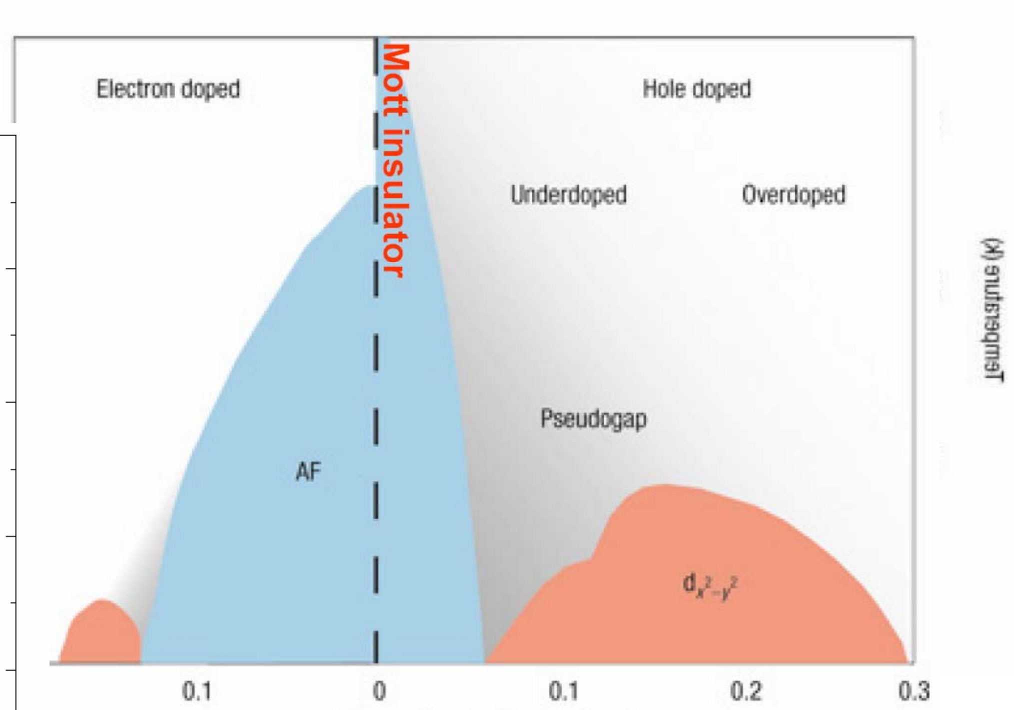
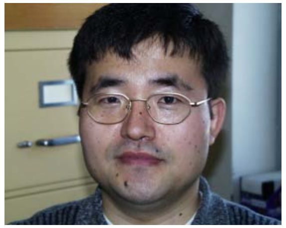
Overall phase diagram with CDMFT





Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST Phys. Rev. B (2008)



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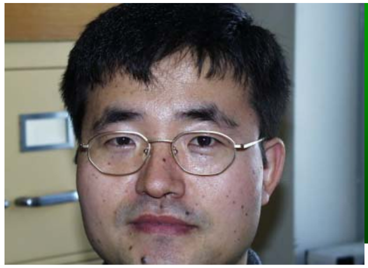
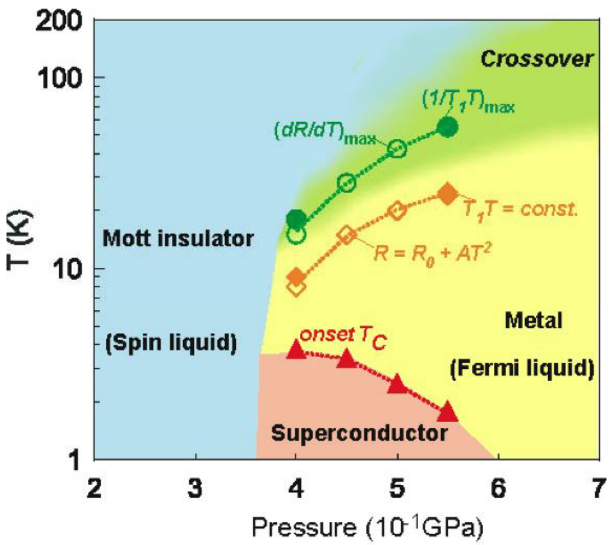
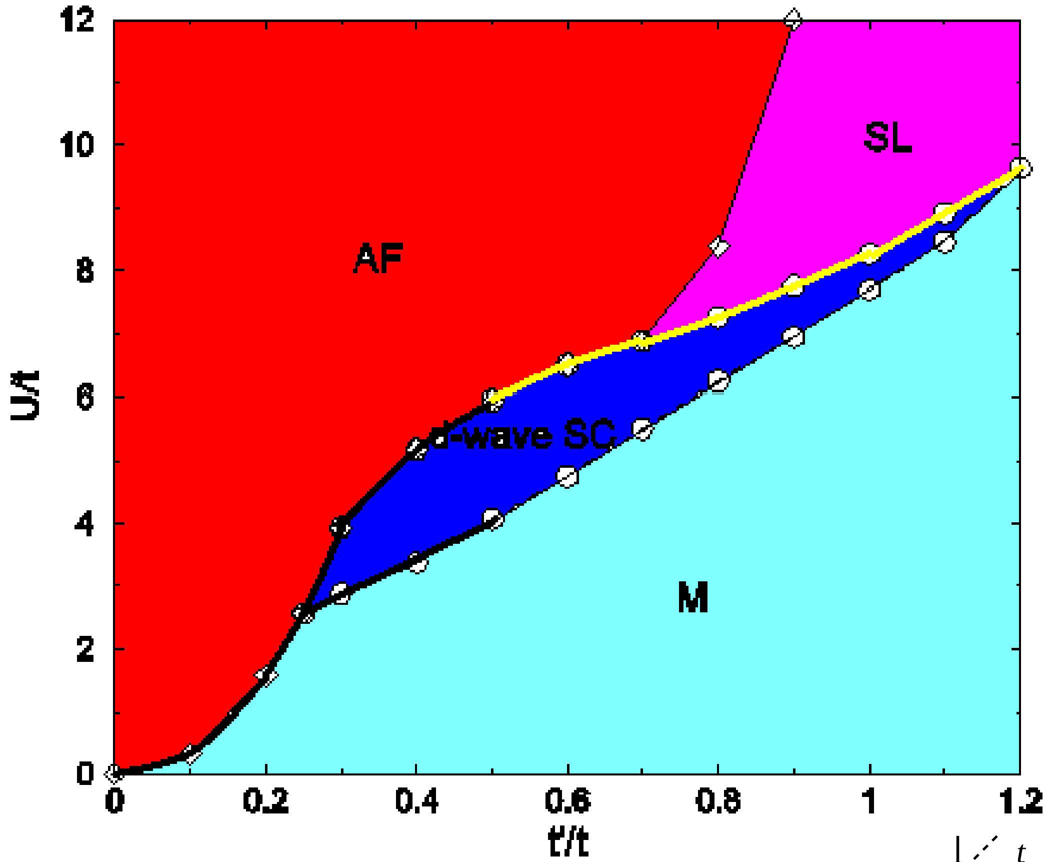


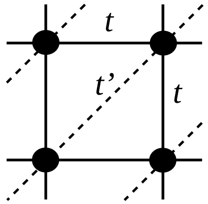
Theoretical phase diagram BEDT

X= $Cu_2(CN)_3$ (t'~ t)



Y. Kurisaki, et al.



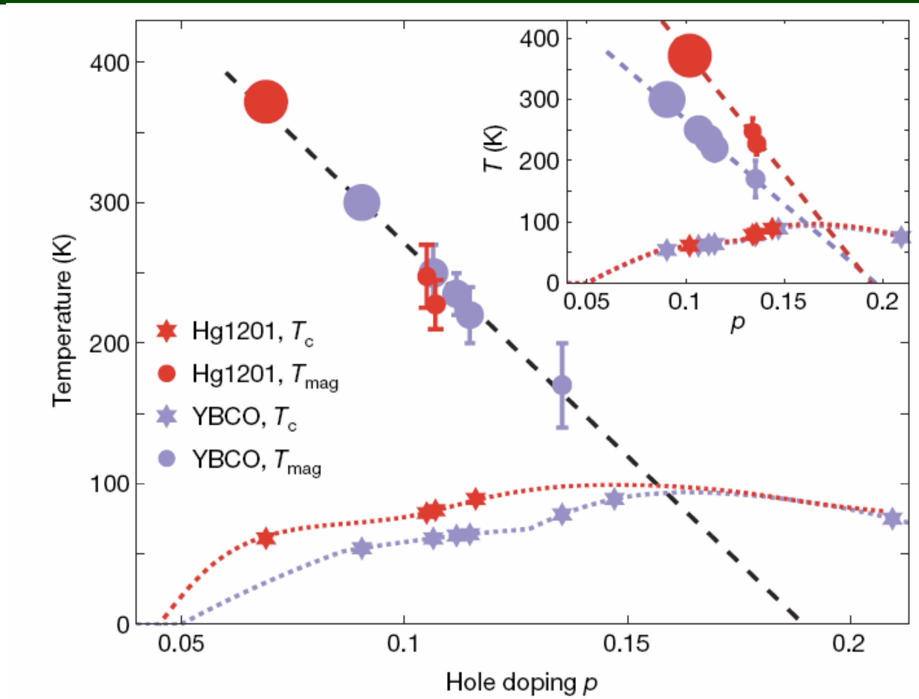


Kyung, A.-M.S.T. PRL 97, 046402 (2006)

Phys. Rev. Lett. **95**, 177001(2005)   Y. Shimizu, et al. Phys. Rev. Lett. **91**, (2003)

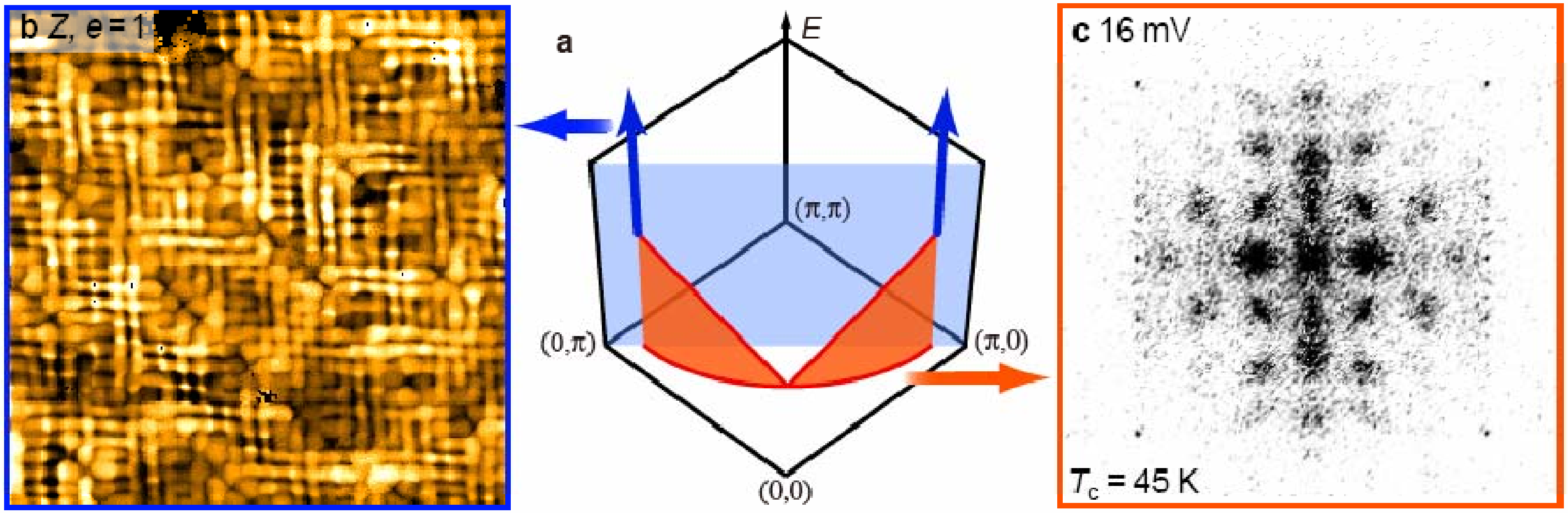
What it does not explain (yet)

Order and pseudogap



Li, Baledent, … Greven, Nature (2008)
Xia… Kapitulnik (2008)
Mook …, PRB (2004)
Borisenko … PRL (2004)
Kaminski … Nature (2002)
Sidis … (2001)
Sonier … Science (2001)

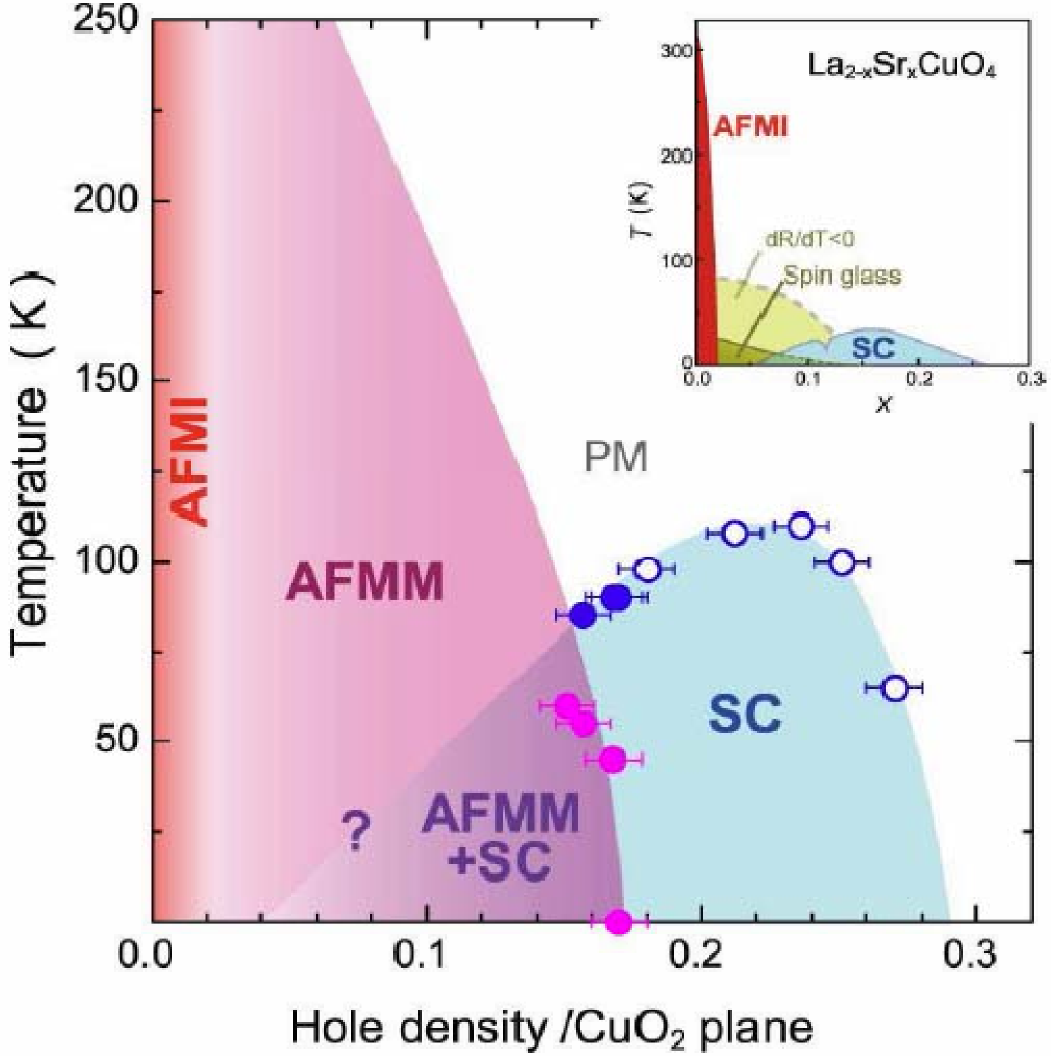
Charge order in the pseudogap

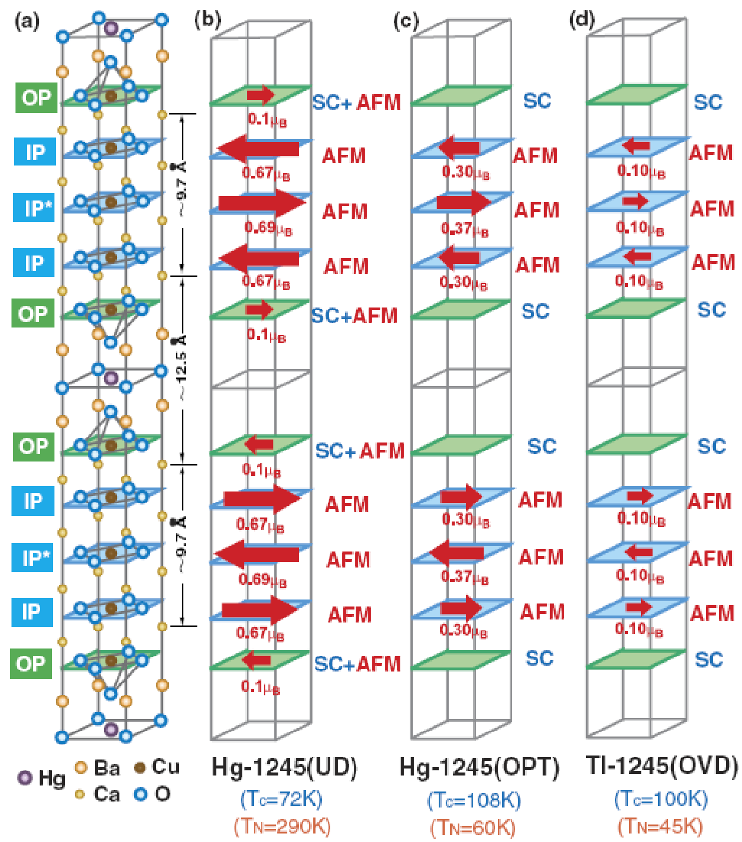


Kohsaka, Taylor .. Davis, Science (2007)
Wise, Boyer … Hudson, Nature Phys. (2008)
Hanaguri, Lupien … Nature (2004)
Howald, Fournier, Kapitulnik (2001)

Another possibility

H. Mukuda, Y. Yamaguchi, S. Shimizu, … A. Iyo arXiv:0810.0880





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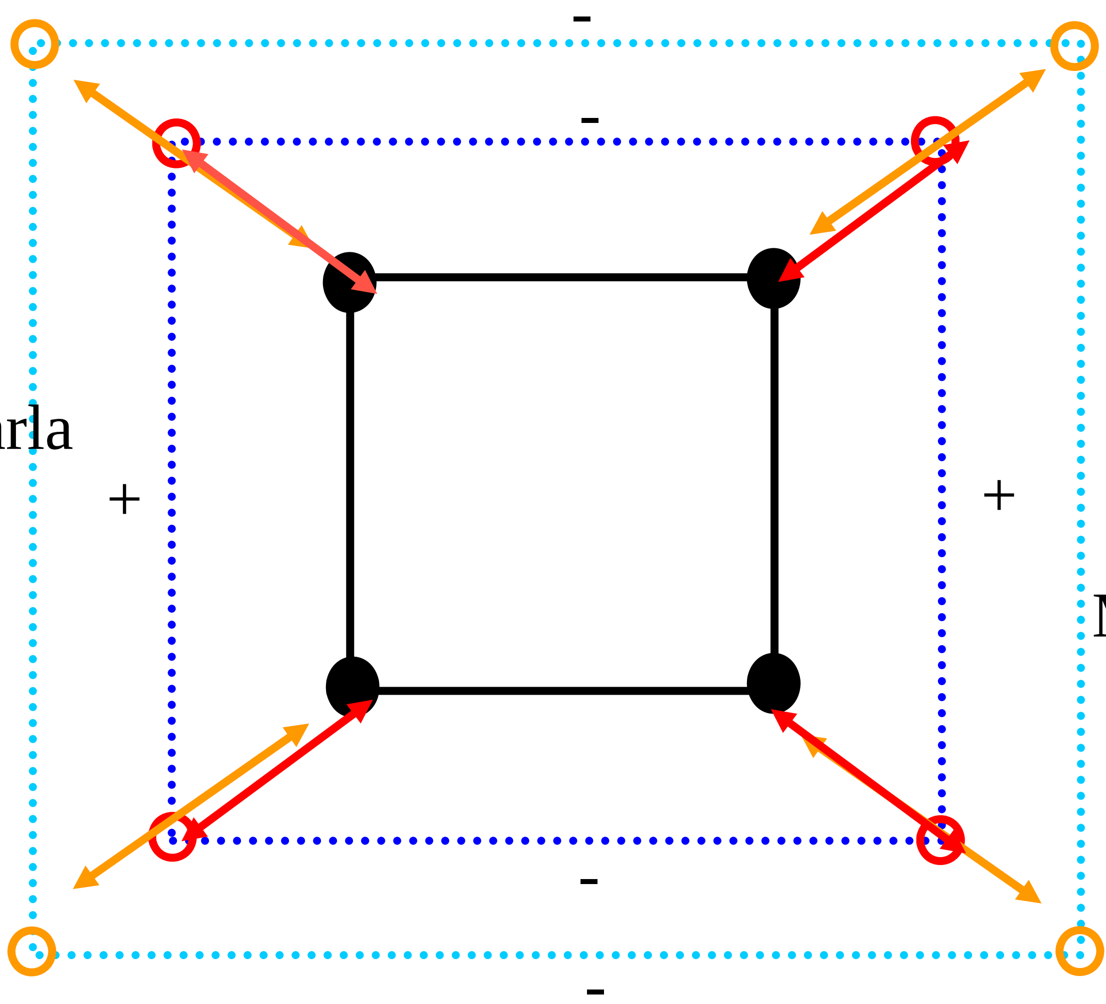
Method : CDMFT+ED

Finite bath

CDMFT + ED

Sarma Kancharla



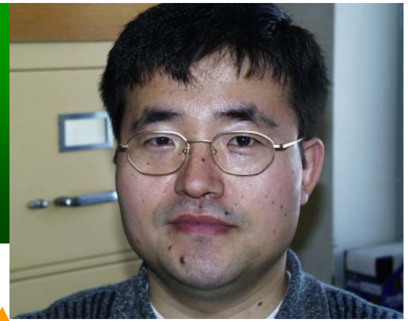
Marcello Civelli

Caffarel and Krauth, PRL (1994)

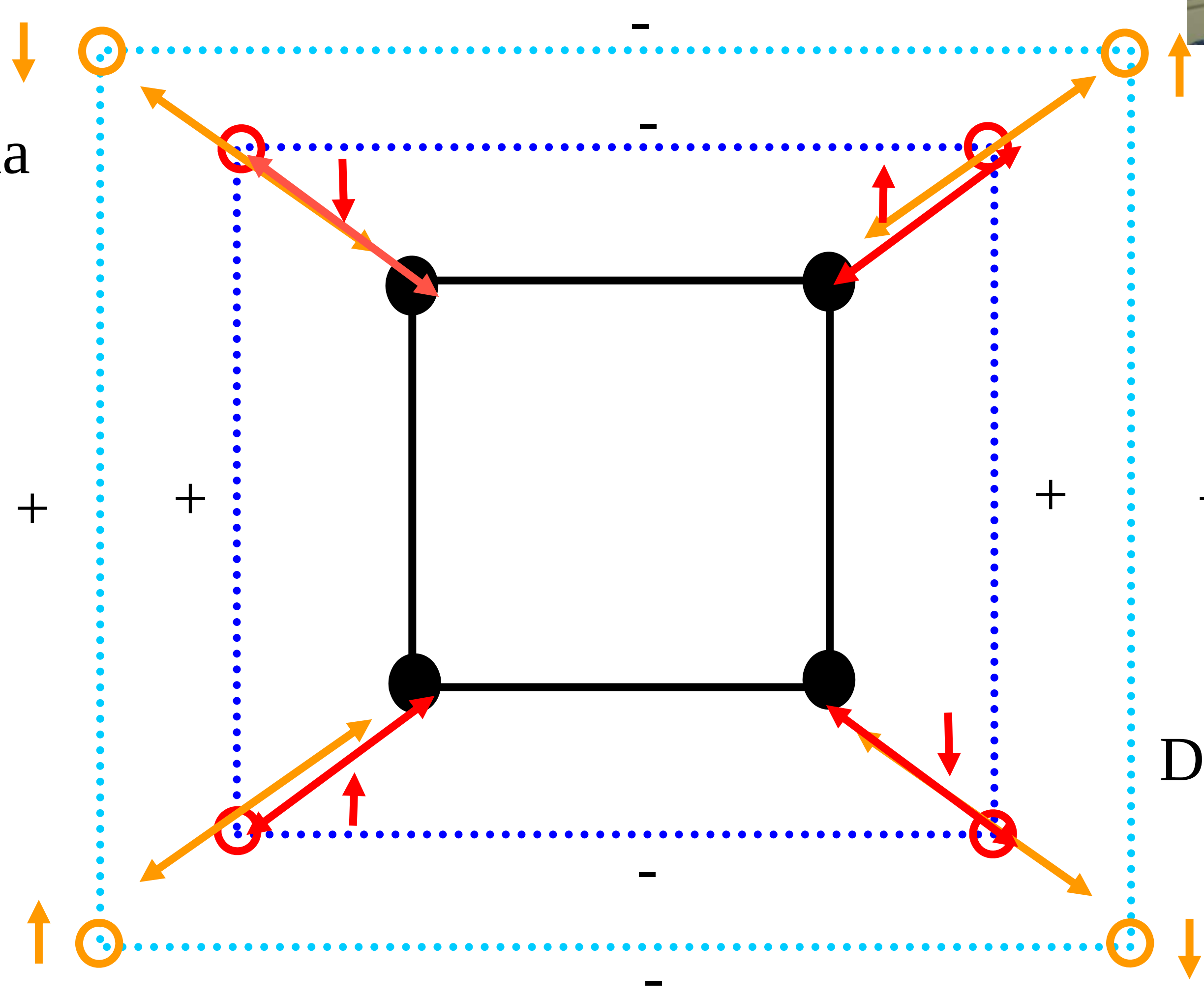
No Weiss field on the cluster!

Competition AFM-dSC

S. Kancharla



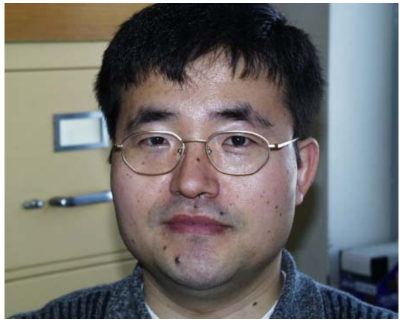
B. Kyung



David Sénéchal

See also, Capone and Kotliar, Phys. Rev. B 74, 054513 (2006),
Macridin, Maier, Jarrell, Sawatzky, Phys. Rev. B 71, 134527 (2005)

Pairing Glue in the Hubbard Model



Bumsoo Kyung

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David Sénéchal

C-DMFT with ED

David Sénéchal

arXiv:0812.1228

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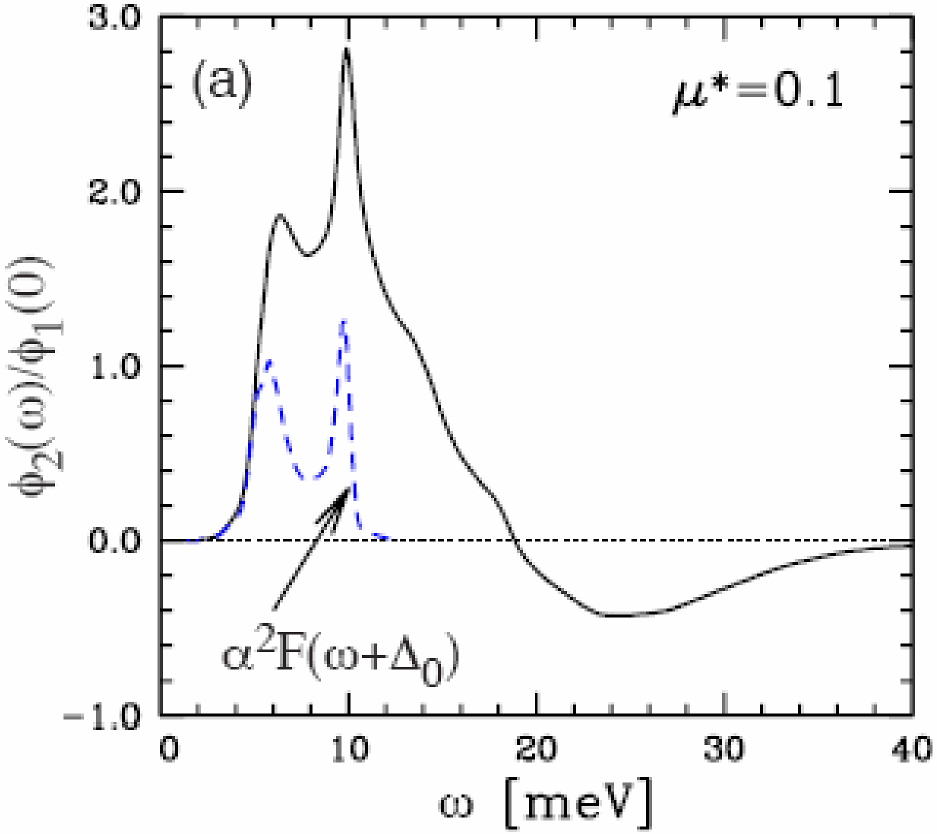
Gap Function and Electron-Phonon Interaction in Lead

Maier, Poilblanc, Scalapino, PRL (2008)

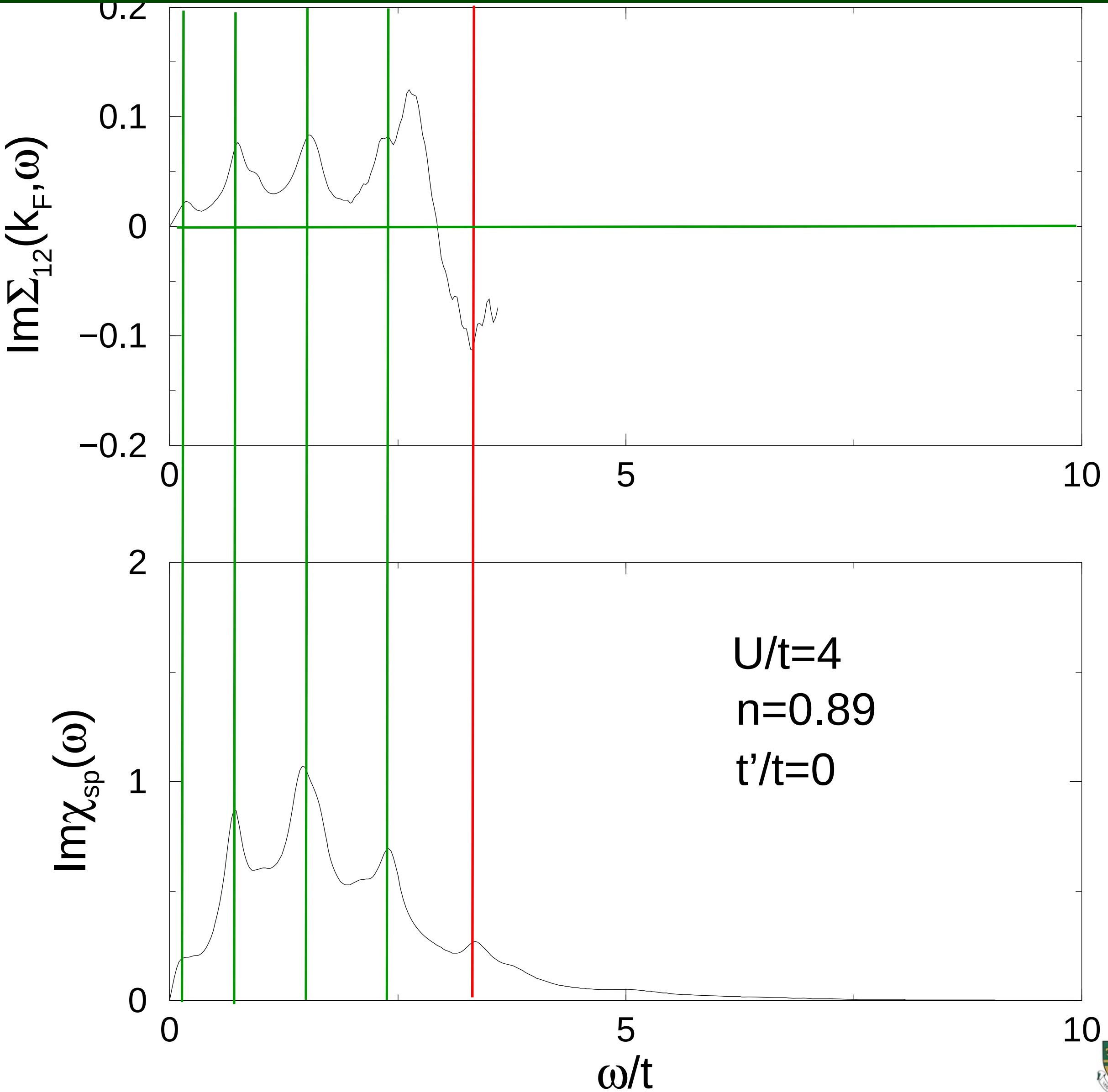


Im off diagonal vs local spin

Effect of *U*

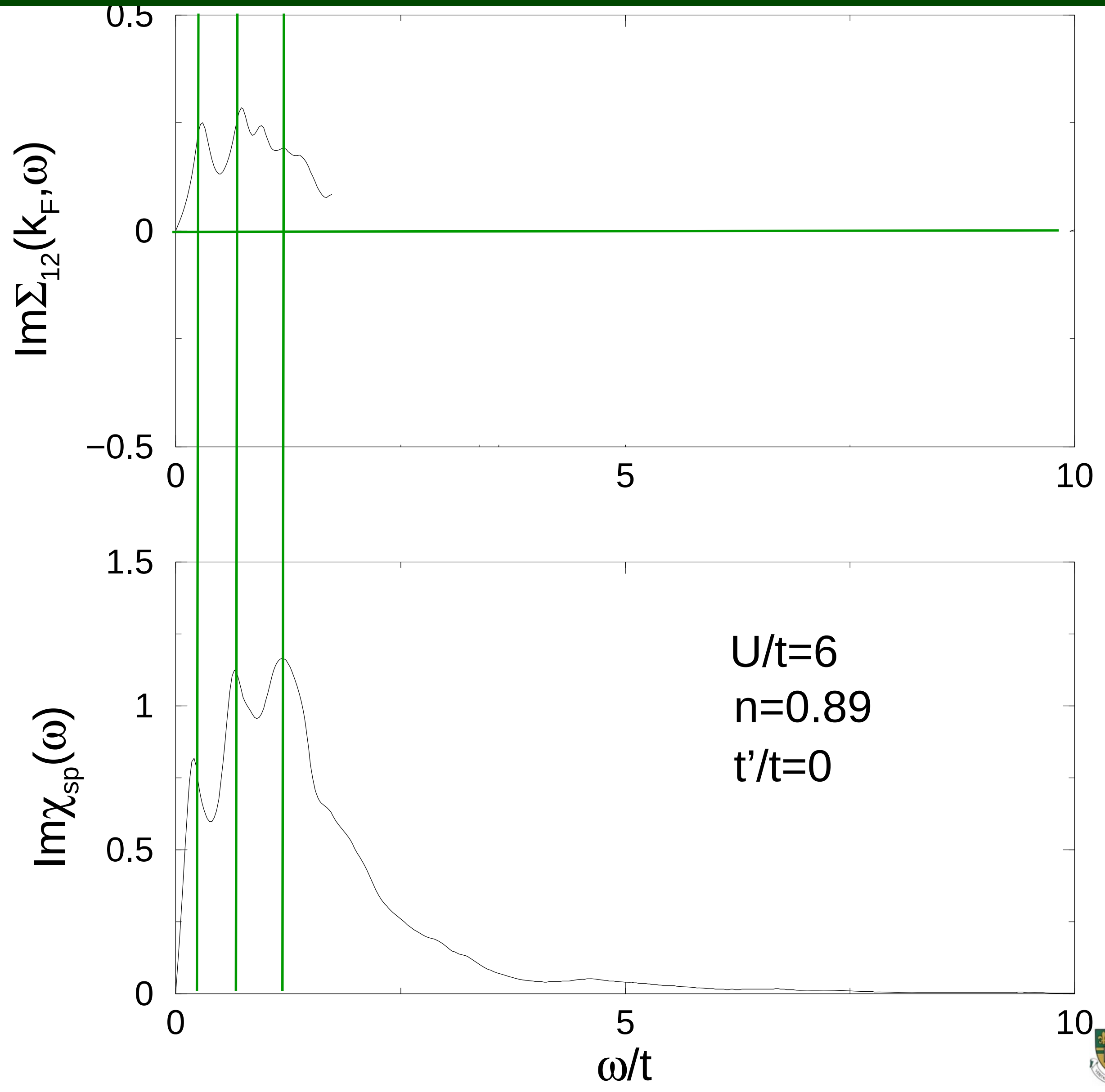
$t' = t'' = 0$

U=4 δ=0.11



0.2
0.1
0
−0.1
−0.2
$\mathrm{Im}\Sigma_{12}(k_F,\omega)$
0
5
10
2
1
0
$\mathrm{Im}\chi_{sp}(\omega)$
U/t=4
n=0.89
t'/t=0
0
5
10
ω/t

U=6 δ=0.11



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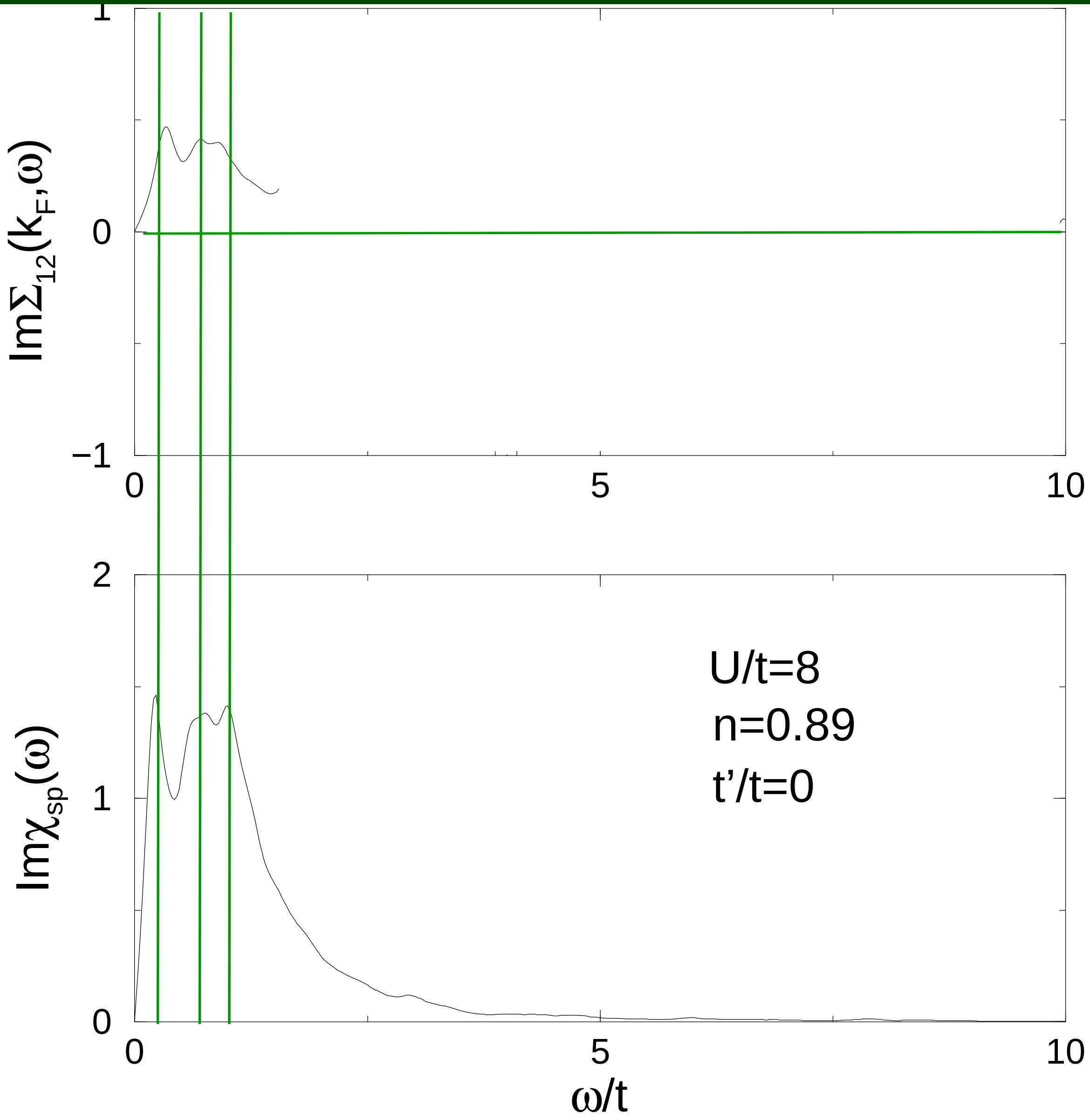
U=8 δ=0.11



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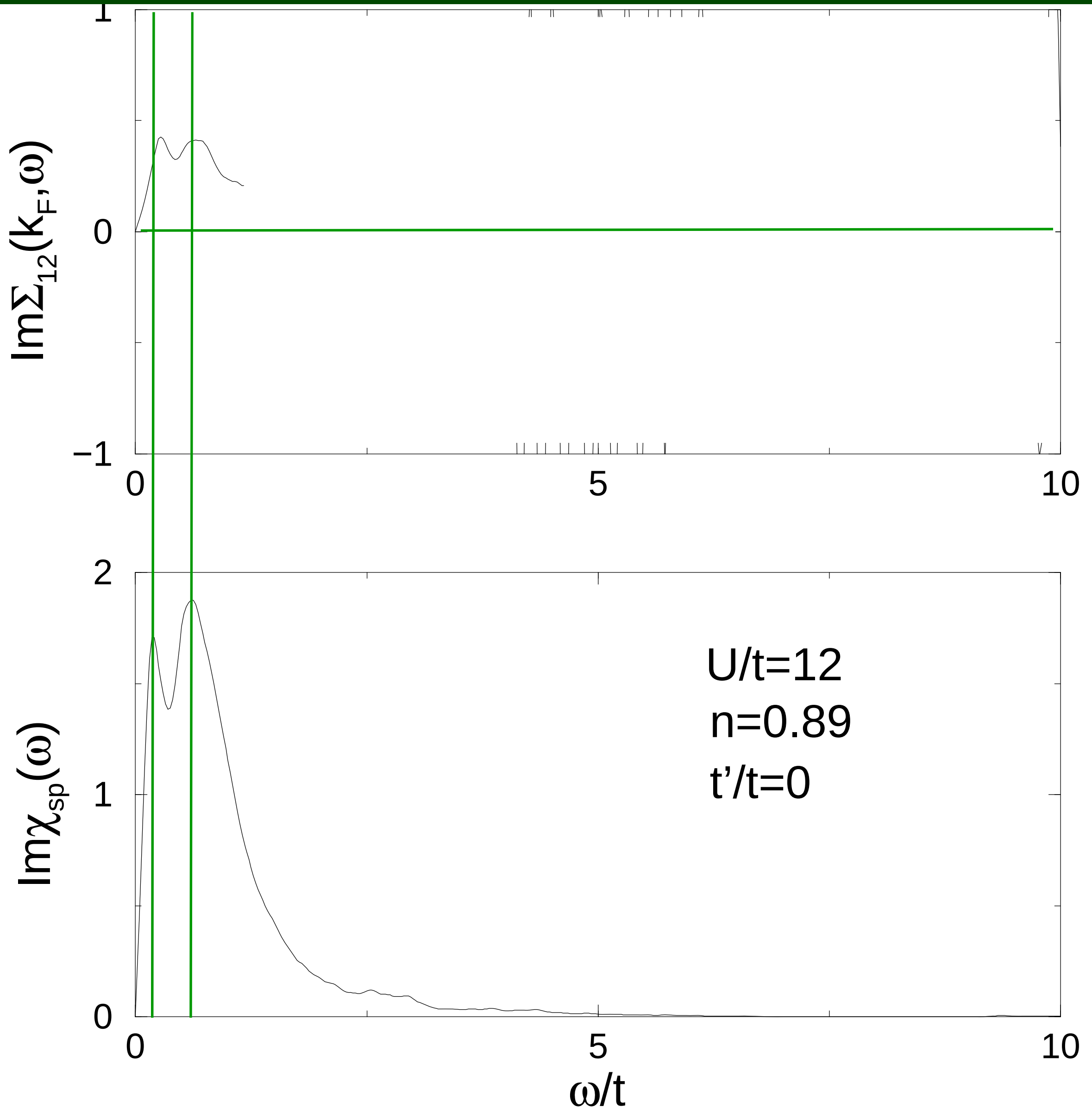
$U=12 \quad \delta=0.11$



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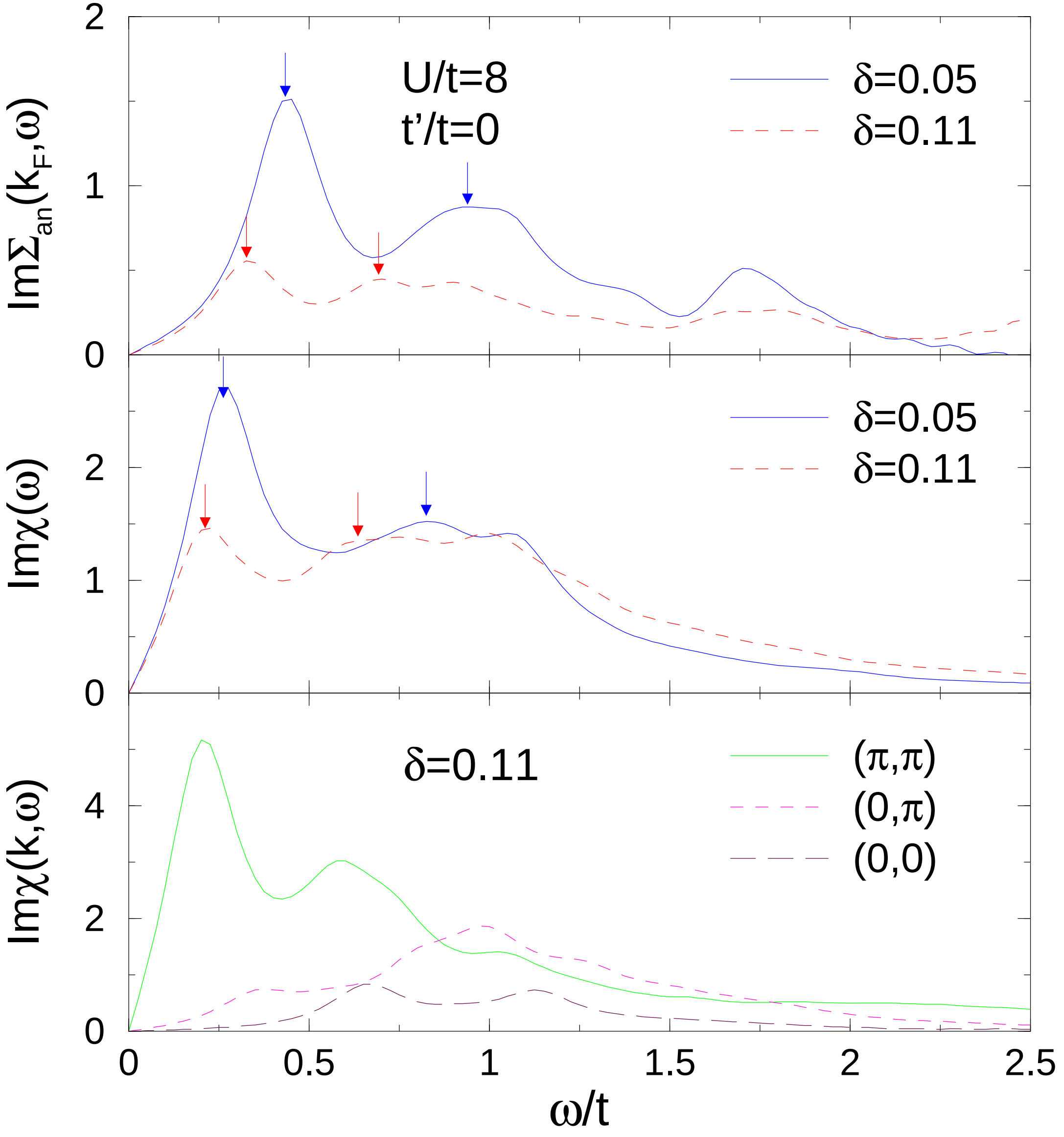
Im off diagonal vs local spin

Effect of doping

U=8 Under- and optimally doped



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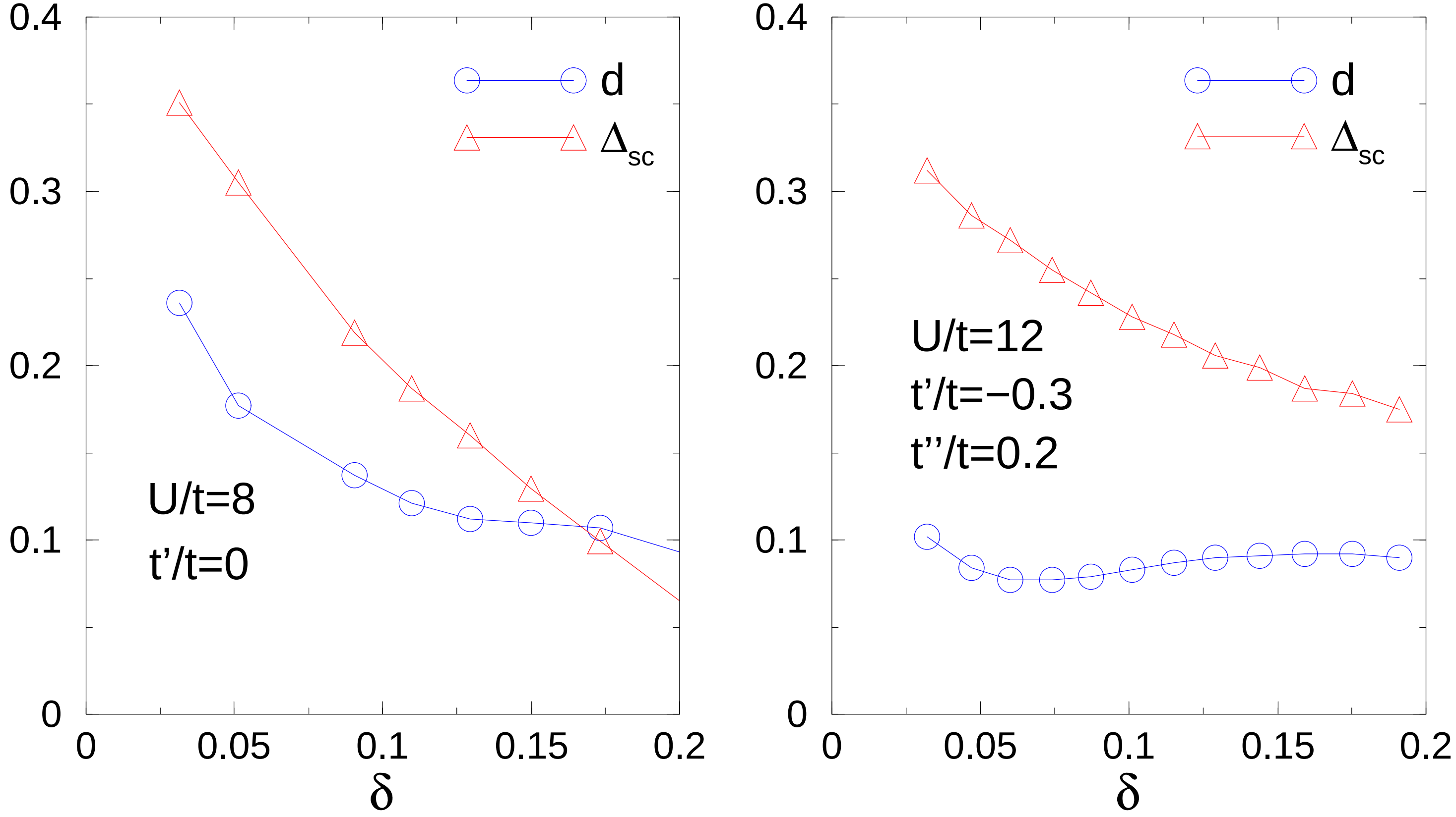
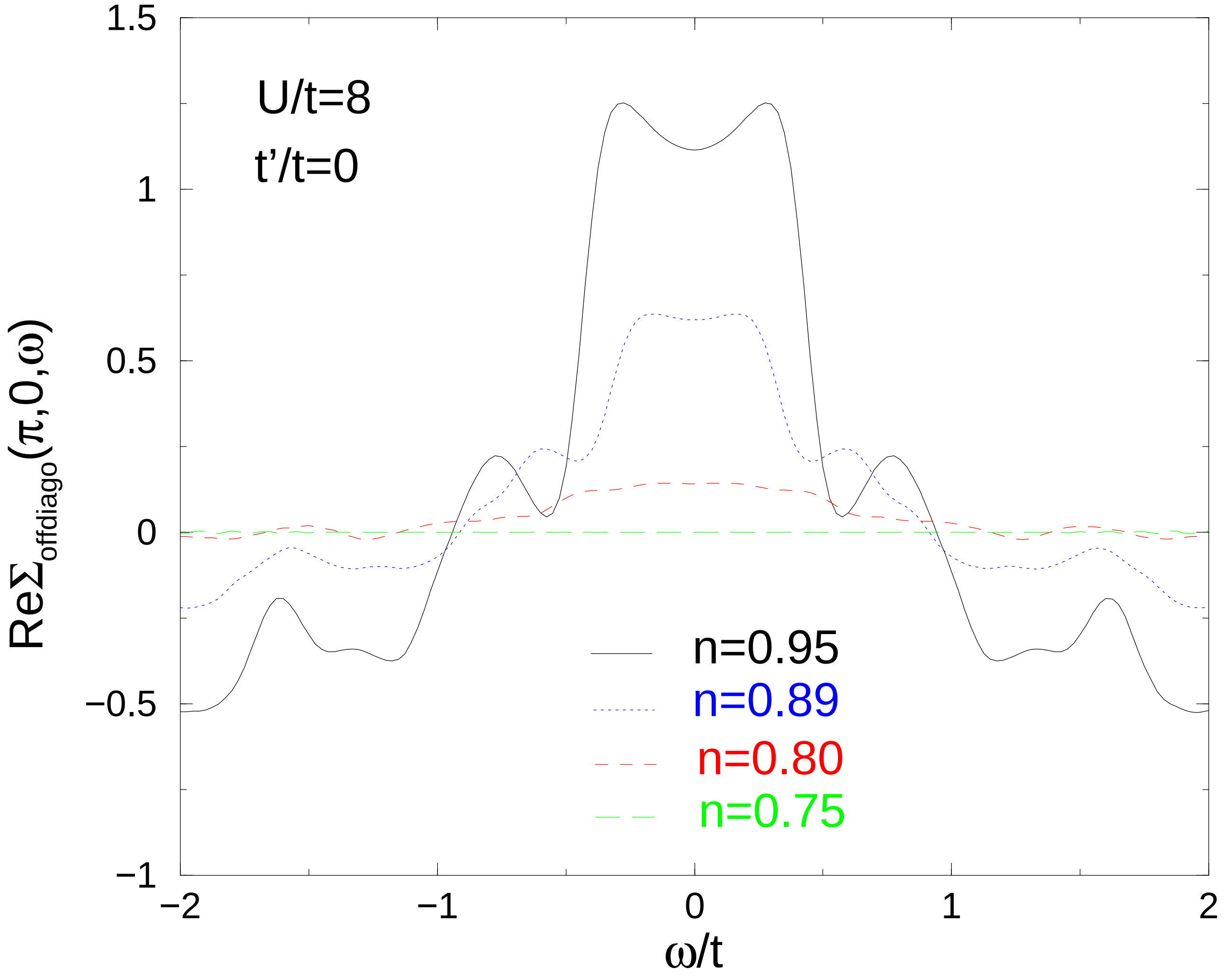
Shift in ω between Im Σ and Im χ peaks vs Δ



What about real part of anomalous self-energy?



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What frequencies in the spin fluctuation spectrum are important?

Frequencies that contribute to the zero energy gap

$$I_\Sigma(\omega) = \frac{2\int_0^\omega \frac{d\omega'}{\pi} \frac{\mathrm{Im}\,\Sigma_{an}(\omega')}{\omega'}}{\mathrm{Re}\,\Sigma_{an}(0)}$$

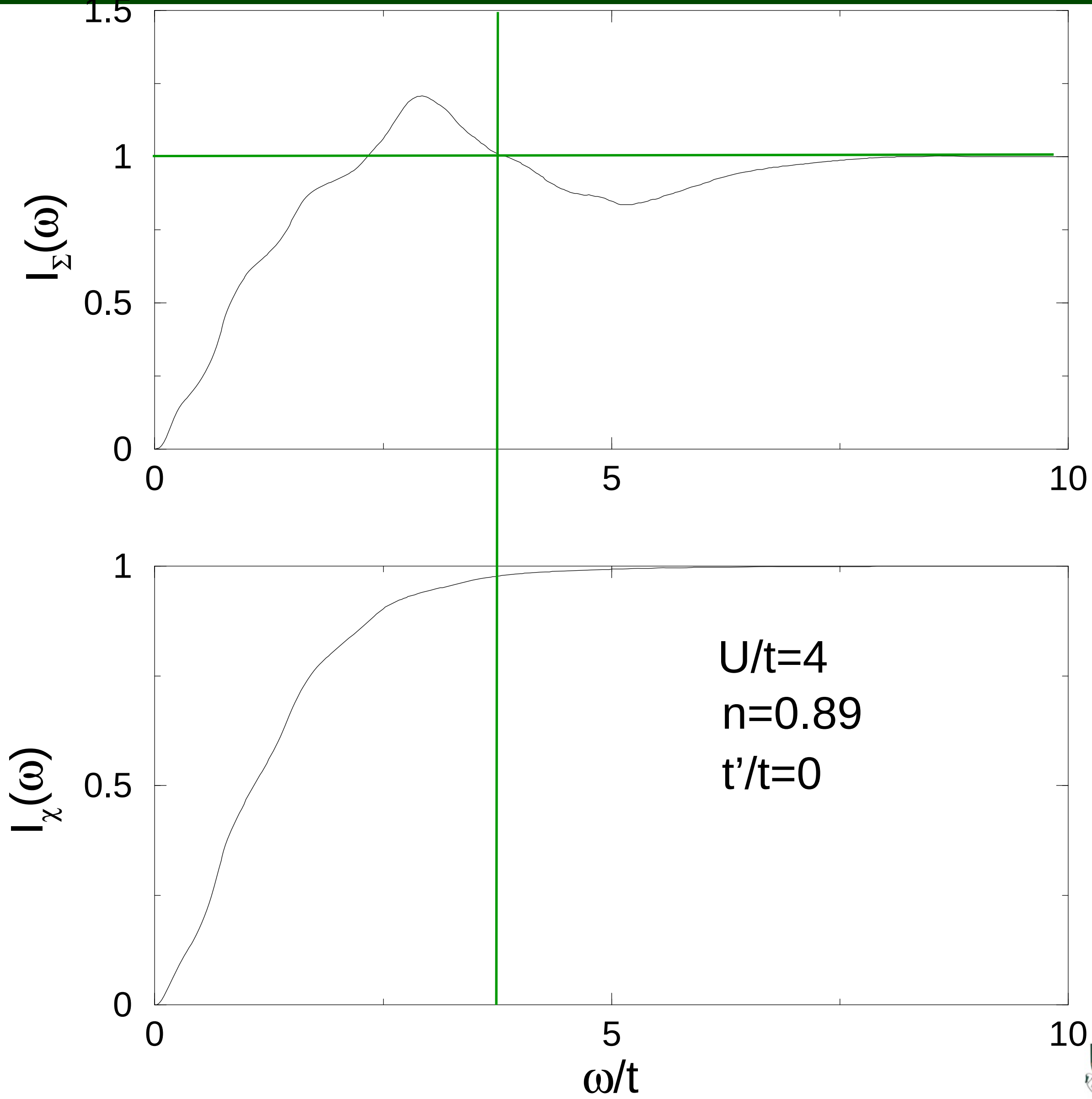
$$I_\chi(\omega) = \frac{\int_0^\omega \frac{d\omega'}{\pi} \mathrm{Im}\,\chi(\omega')}{\int_0^\infty \frac{d\omega'}{\pi} \mathrm{Im}\,\chi(\omega')}$$

Integrated self-energy vs integrated spin

Effect of U

$t' = t'' = 0$

$U = 4 \quad \delta = 0.11$



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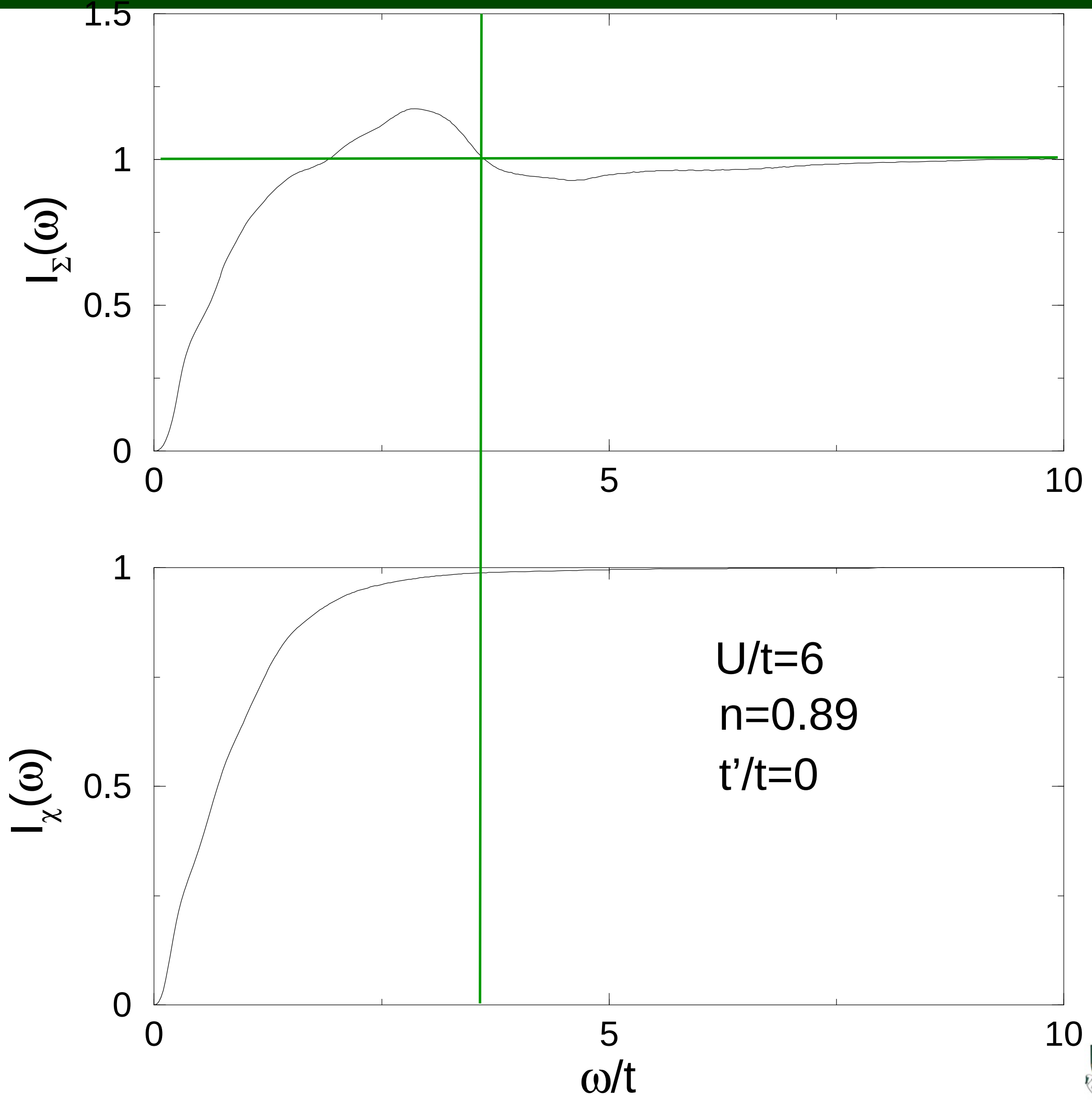
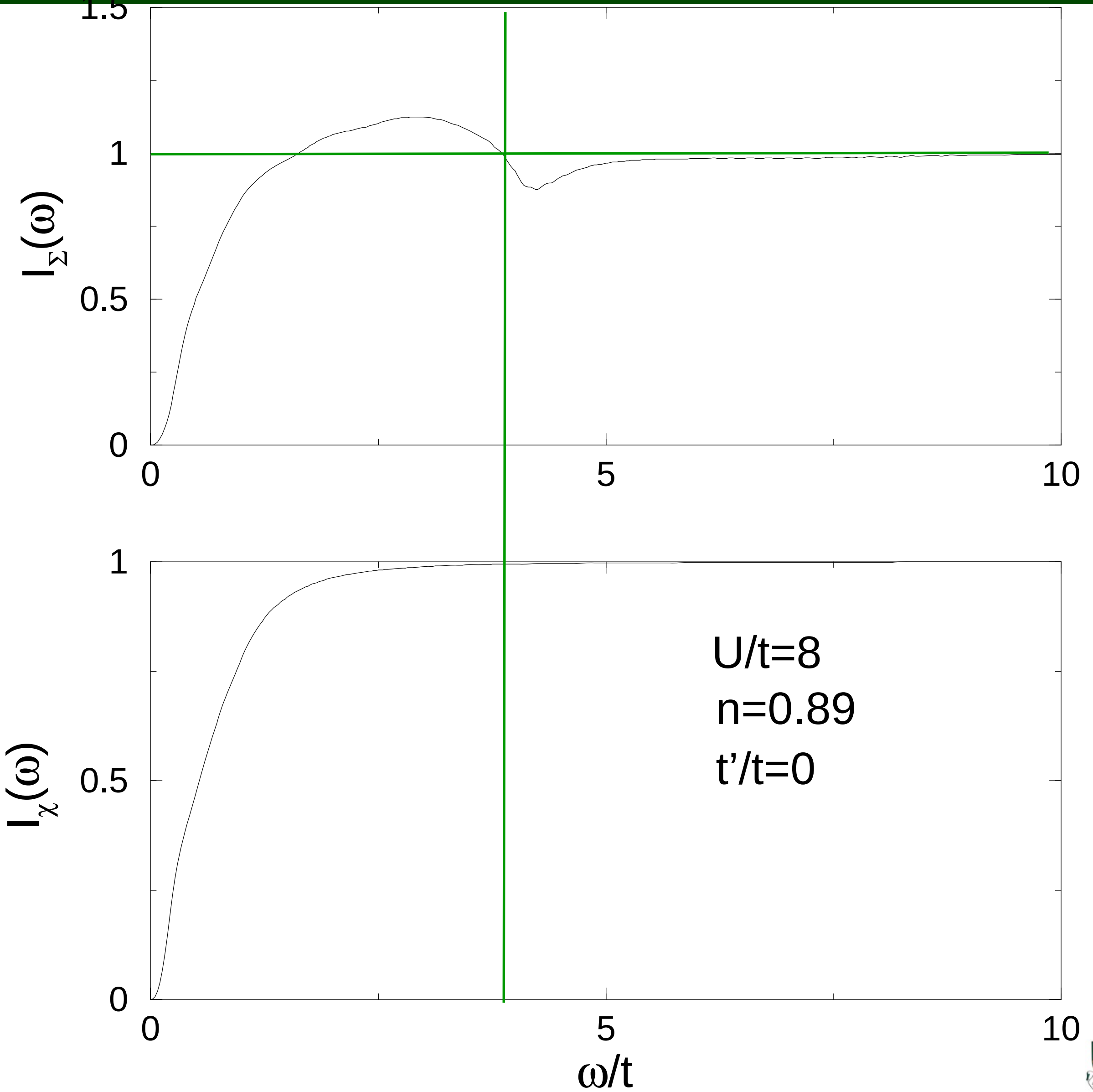
$U = 6 \quad \delta = 0.11$

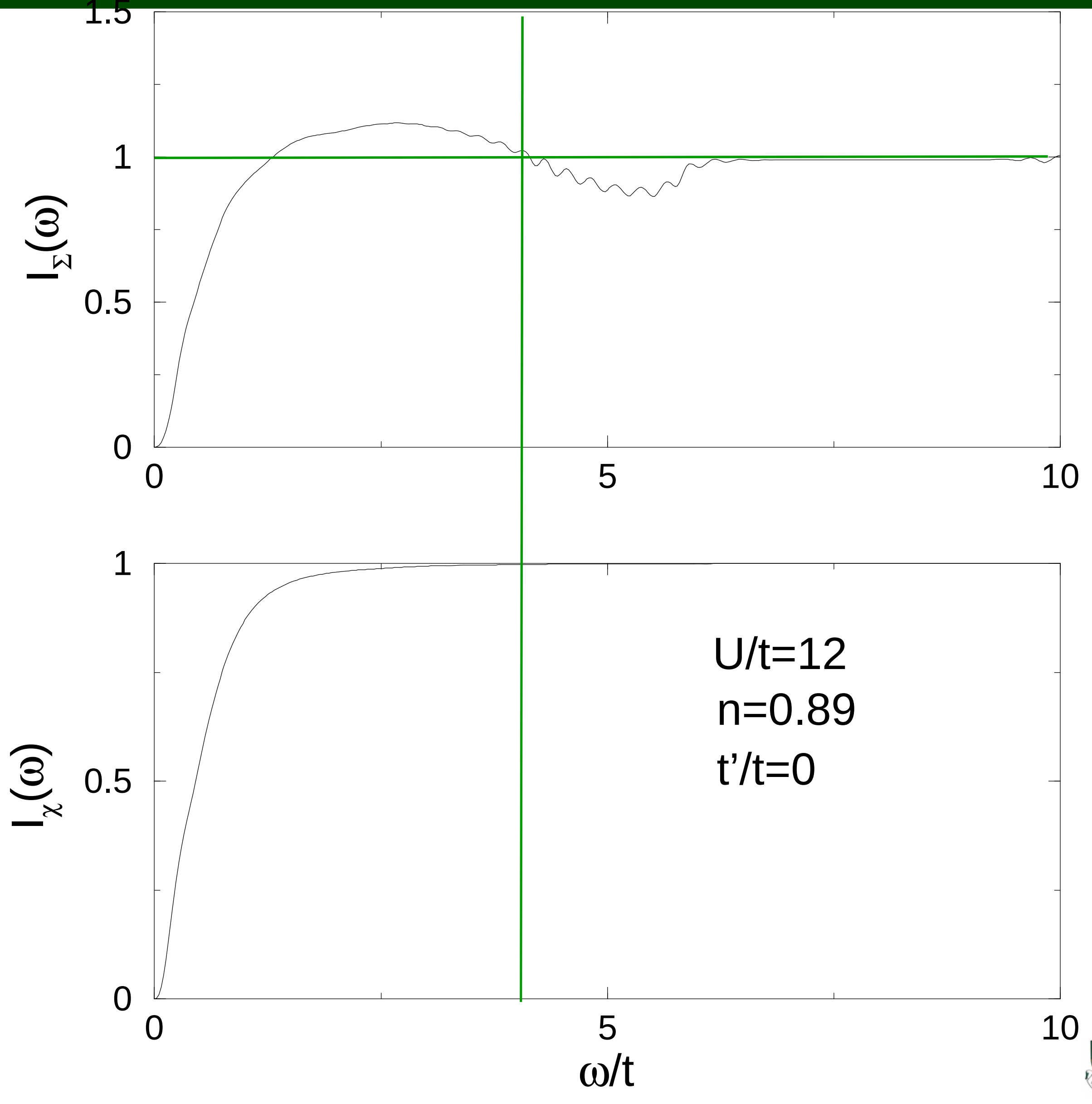


$U = 8\ \ \delta = 0.11$



1.5
1
0.5
0
$I_\Sigma(\omega)$
0
5
10
1
0.5
0
$I_\chi(\omega)$
U/t=8
n=0.89
t'/t=0
0
5
10
ω/t

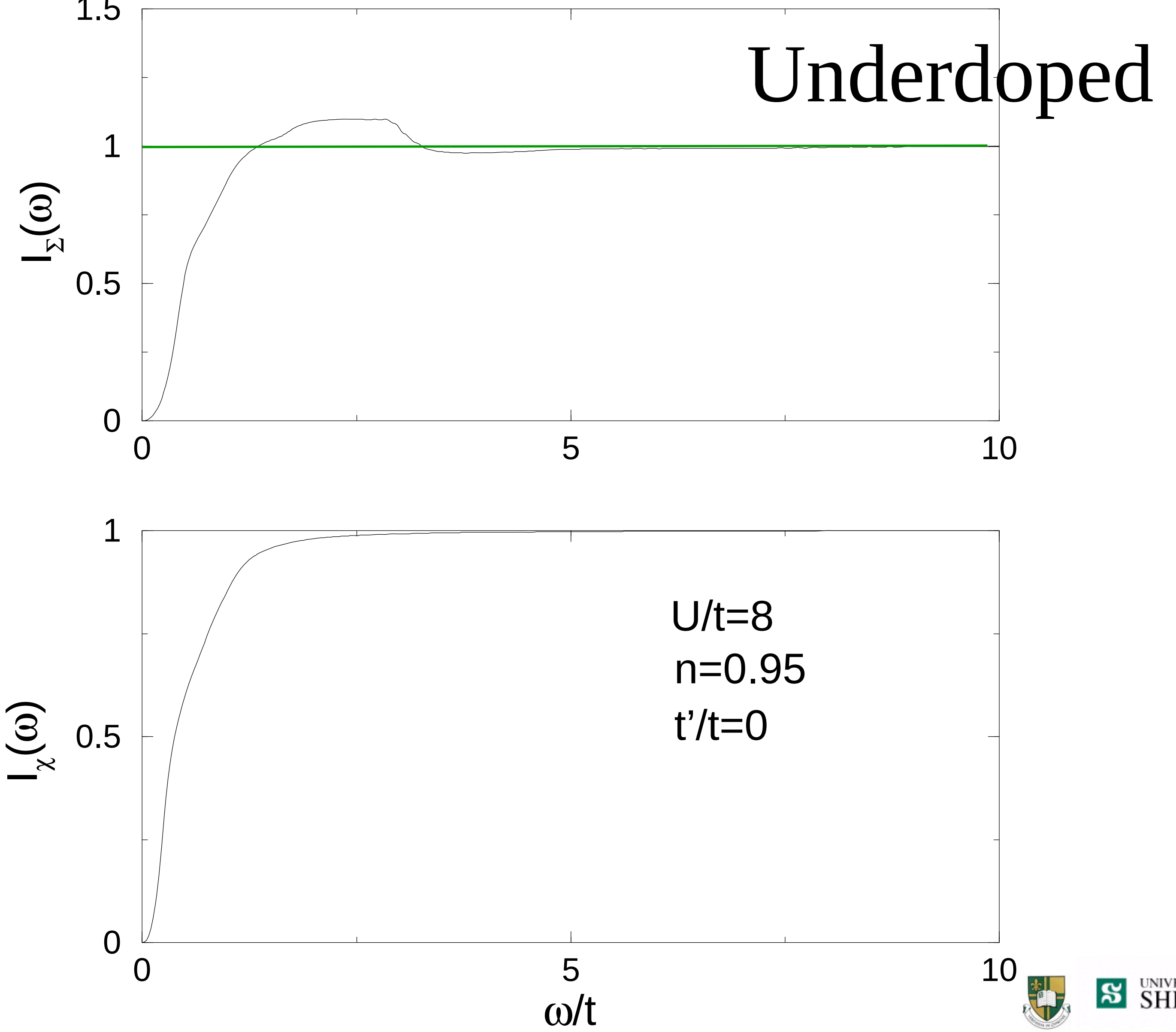
$U = 12 \quad \delta = 0.11$



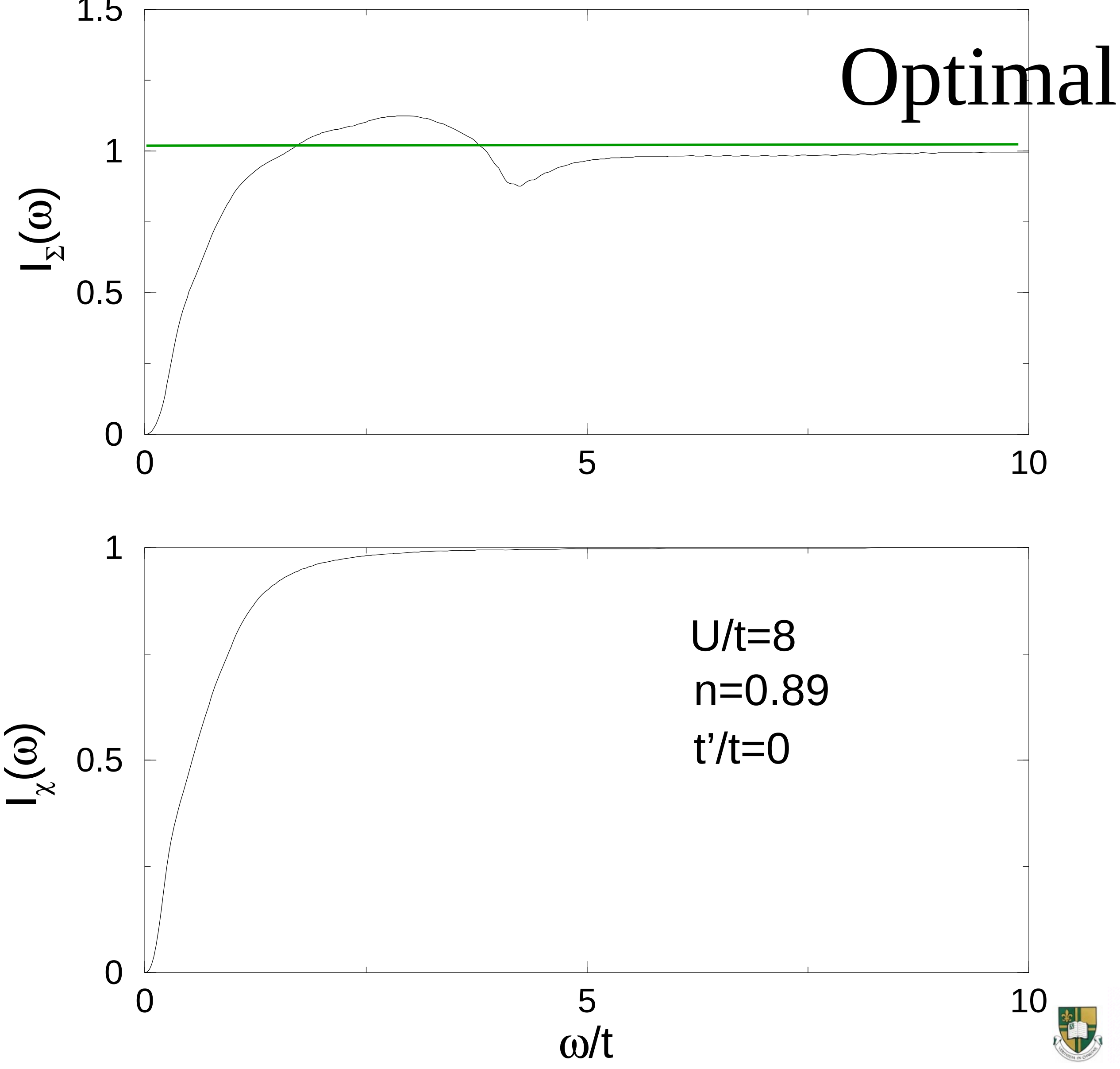
Integrated self-energy vs integrated spin

Effect of doping

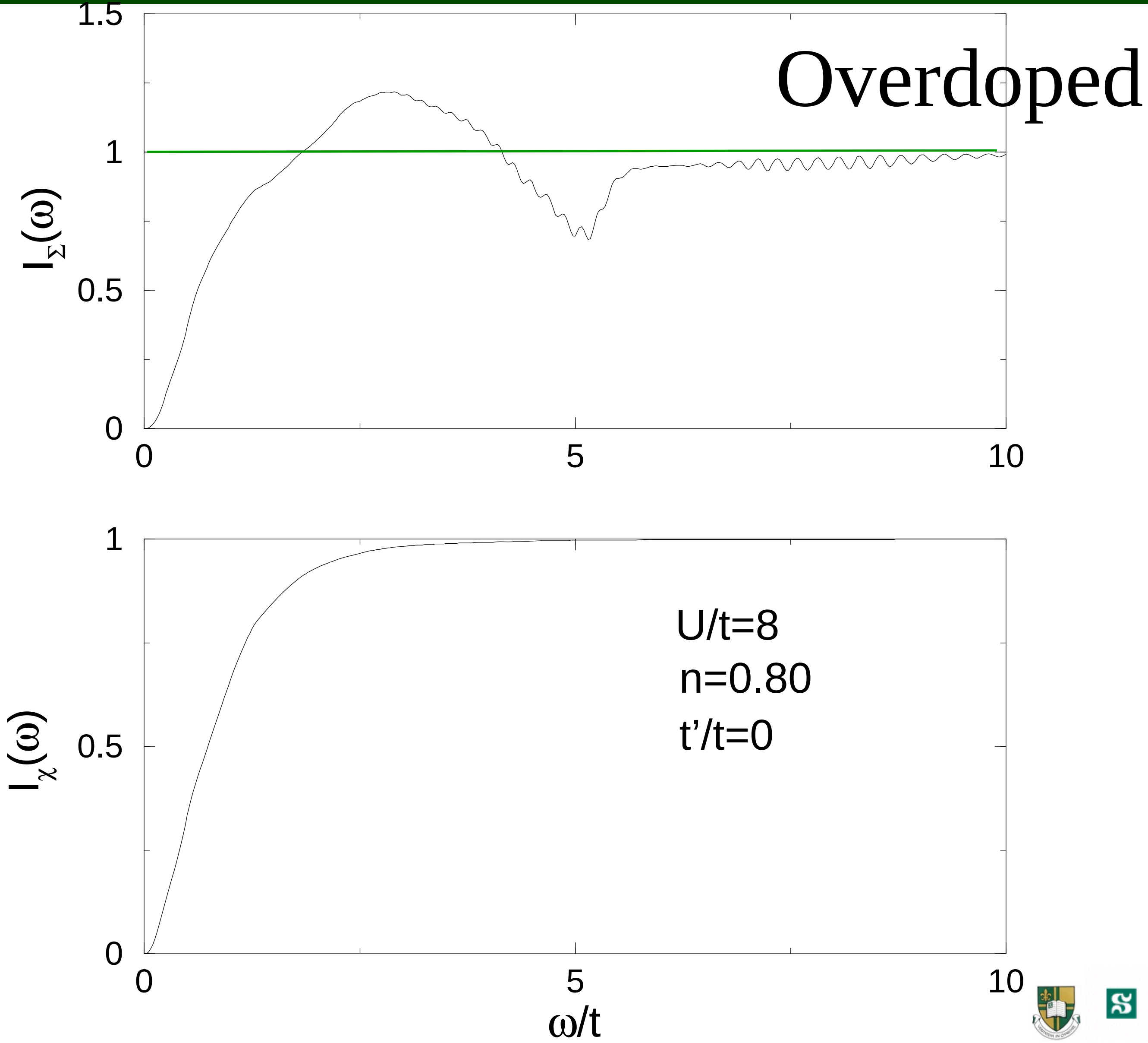
$U = 8 \quad \delta = 0.05$



$U = 8 \quad \delta = 0.11$



$U = 8 \quad \delta = 0.2$



Dynamics of the pairs and relevant frequencies for pairing

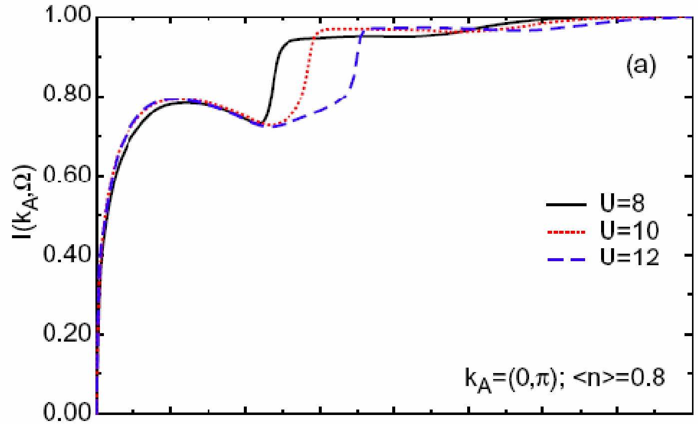
The Mammoth, the elephant

and the mouse

Instantaneous contribution ?

$$\mathrm{Re}\,\Sigma_{an}(\omega = \infty) = cst$$

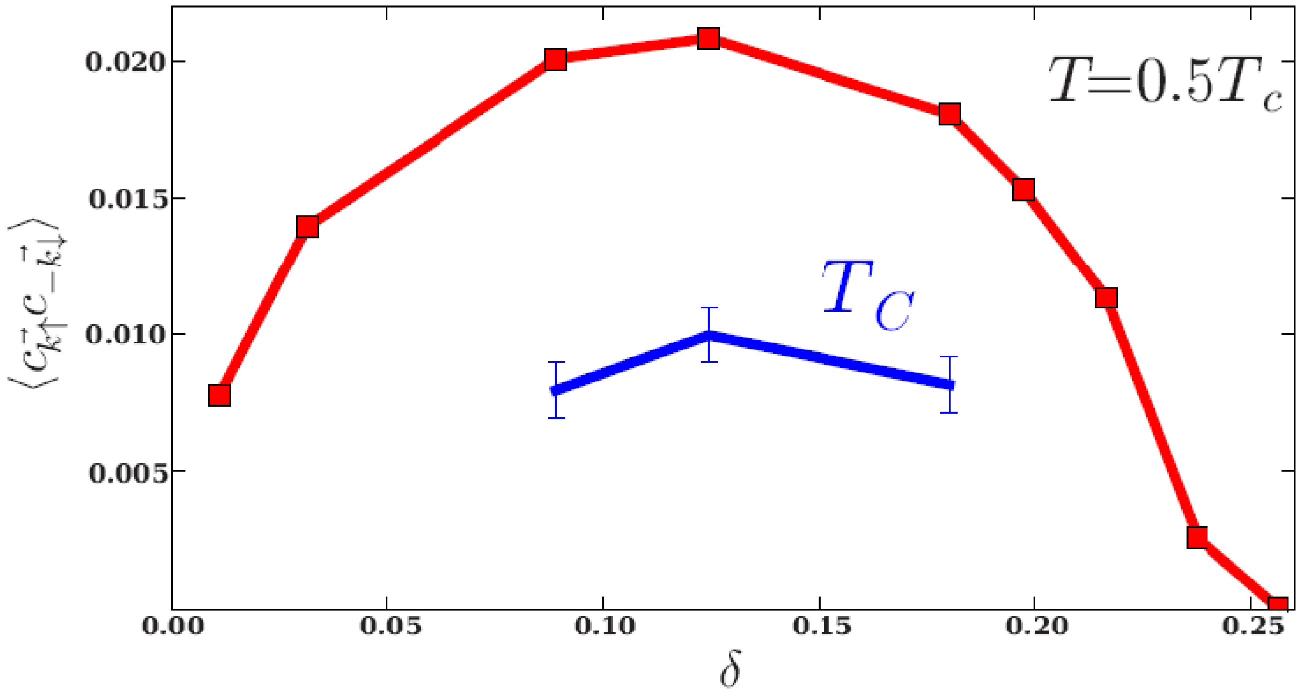
- In CDMFT + ED
  - Yes for *U < 0, s-wave (BCS)*
  - No for *U > 0*
- Reconciling Retarded and Instantaneous views



Maier, Poilblanc, Scalapino, PRL (2008)

Order parameter scales like T_c

Haule and Kotliar Phys. Rev. B (2007)



Frequencies relevant for the order parameter : Dynamics of the pairs

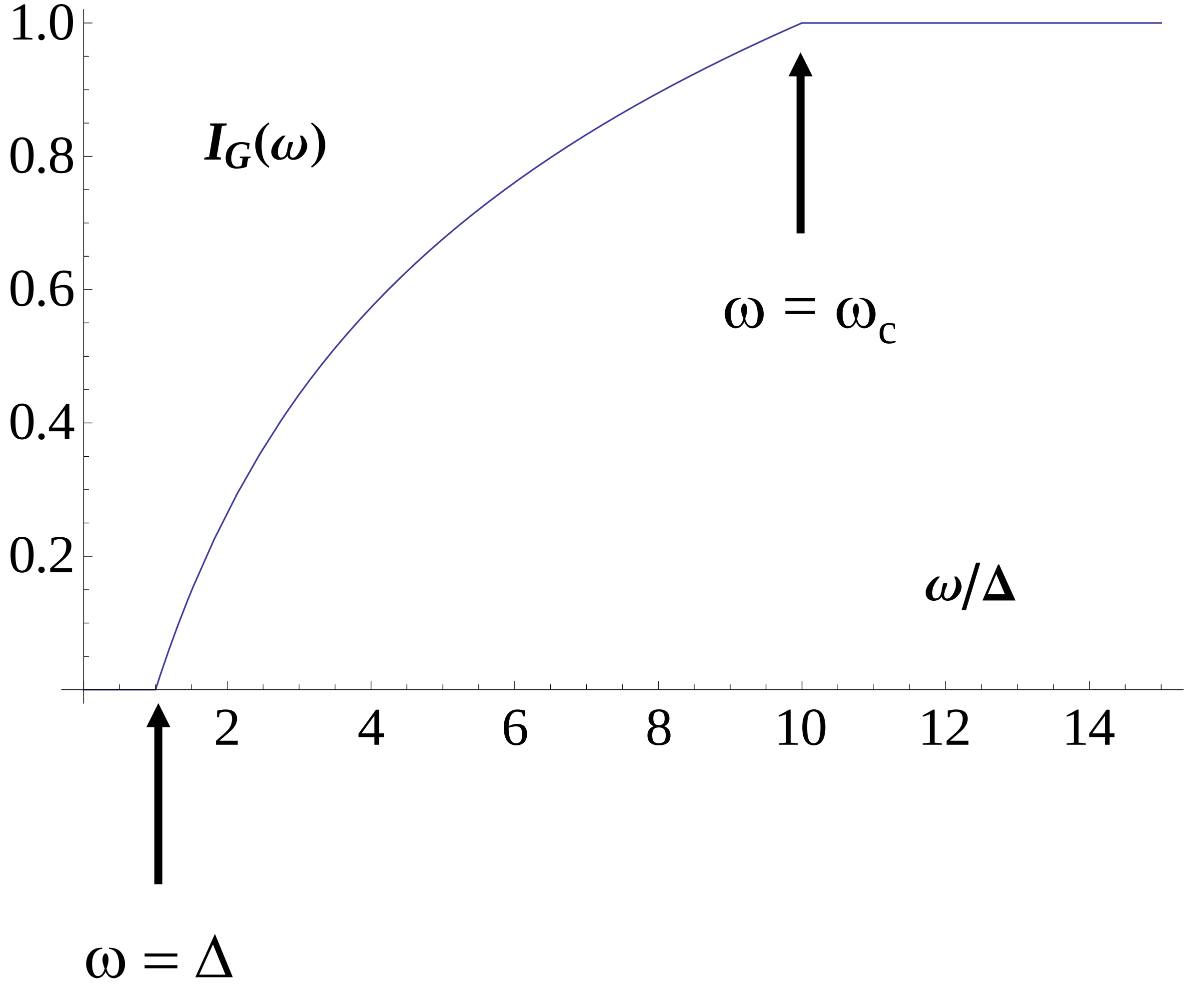
$$\langle c_{i\uparrow} c_{j\downarrow} \rangle = I_G(\infty) = -\int_0^{\infty} \frac{d\omega'}{\pi} \operatorname{Im} F^R(\mathbf{r}_i, \mathbf{r}_j; \omega')$$

$$I_G(\omega) \equiv -\int_0^{\omega} \frac{d\omega'}{\pi} \operatorname{Im} F^R(\mathbf{r}_i, \mathbf{r}_j; \omega')$$

$$I_G(\omega) = \sum_m \langle 0|c_{i\uparrow}|m\rangle\langle m|c_{j\downarrow}|0\rangle \,\theta(\omega - (E_m - E_0))$$

This is a good way to see « mechanism » in BCS

- Phonon frequency (cutoff) comes in as prefactor in gap (isotope effect) but…

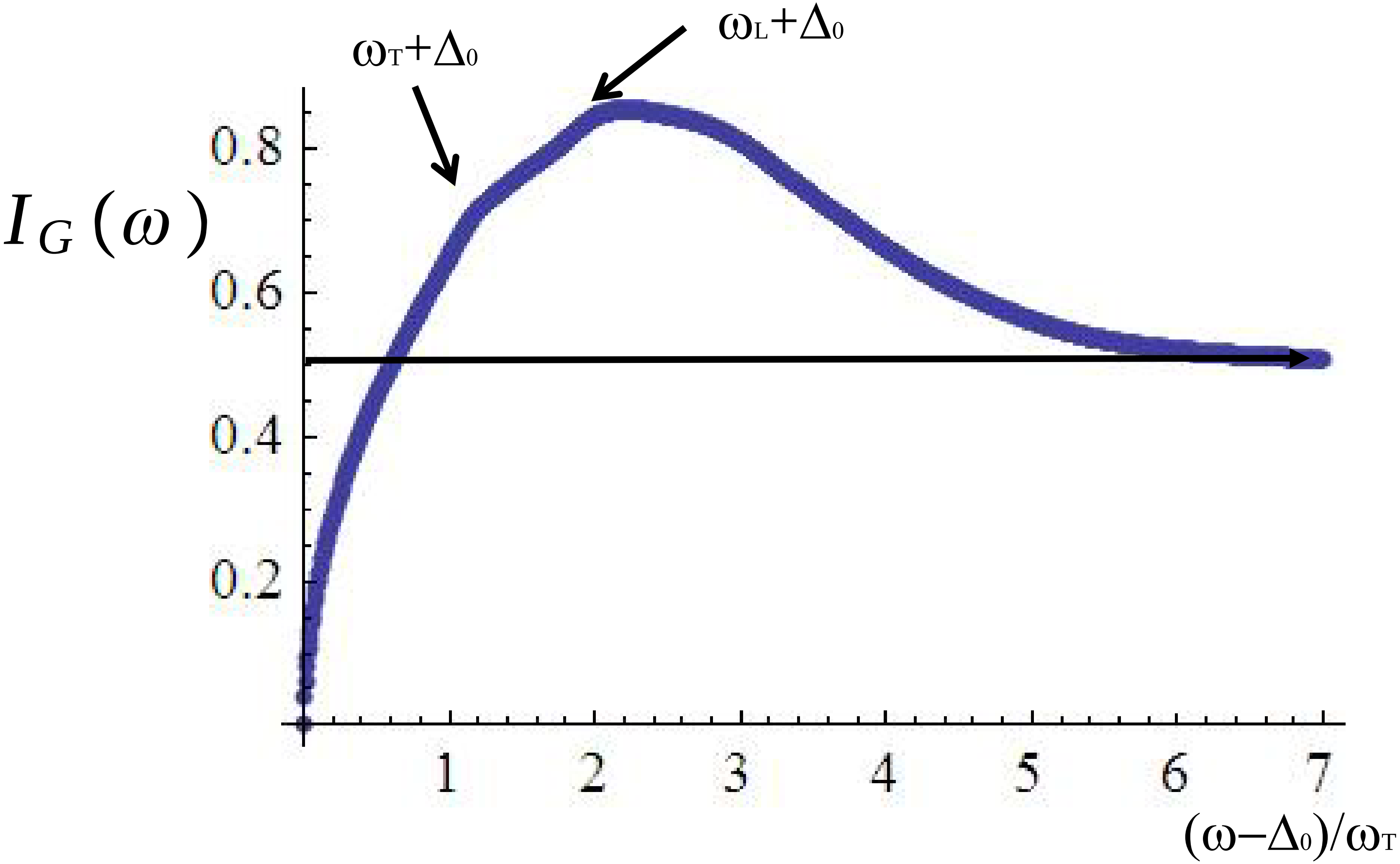


Can be calculated from known results for lead

$$I_G(\omega) = N(0)\int_0^{\omega} \mathrm{Re}\left[\frac{\Sigma_{an}(\omega')}{\sqrt{(Z(\omega')\omega')^2 - \Sigma_{an}(\omega')^2}}\right] d\omega'$$

Scalapino, Schrieffer, Wilkins PR (1966)

The case of lead



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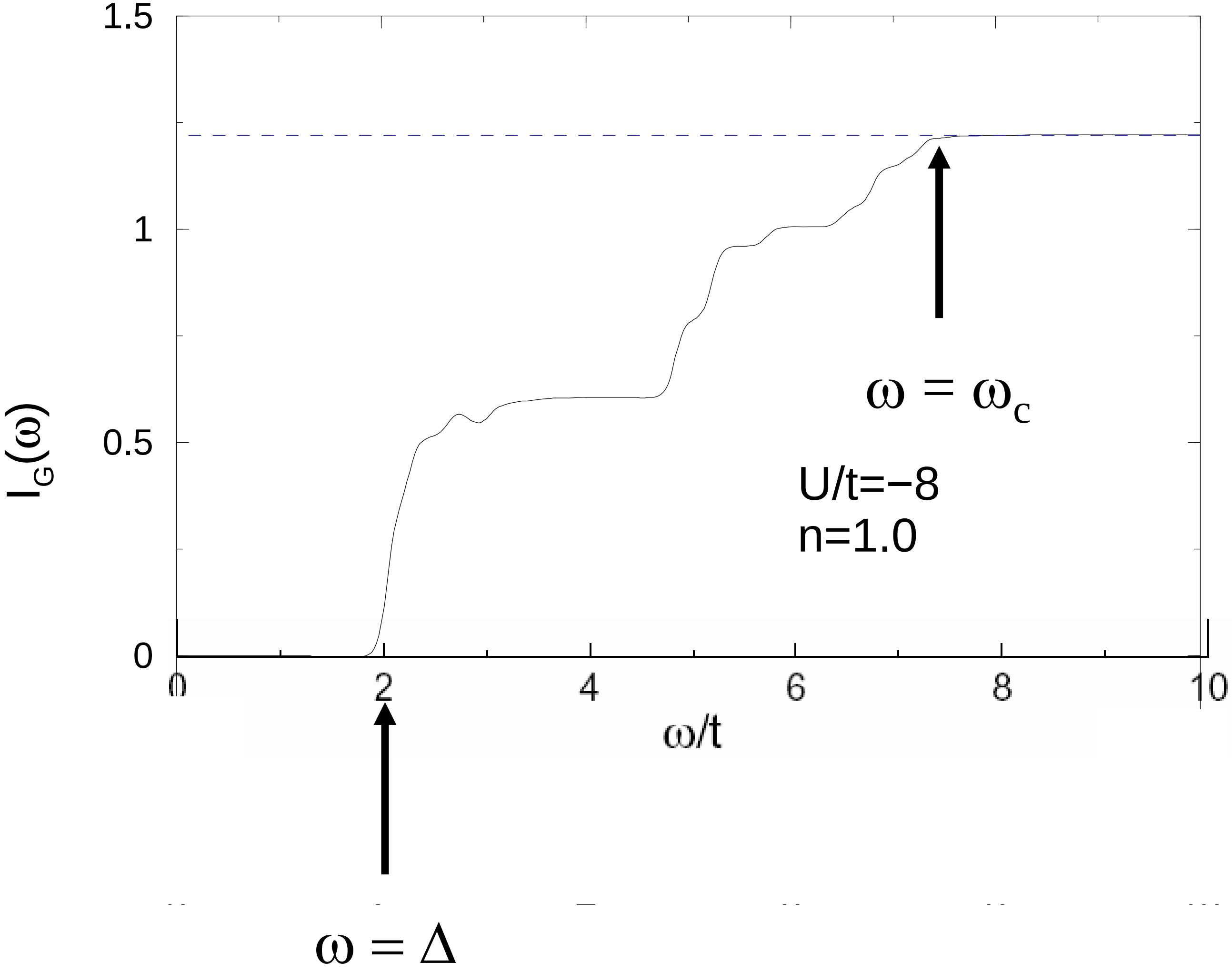
Attractive model, *s*-wave, *U* = -8

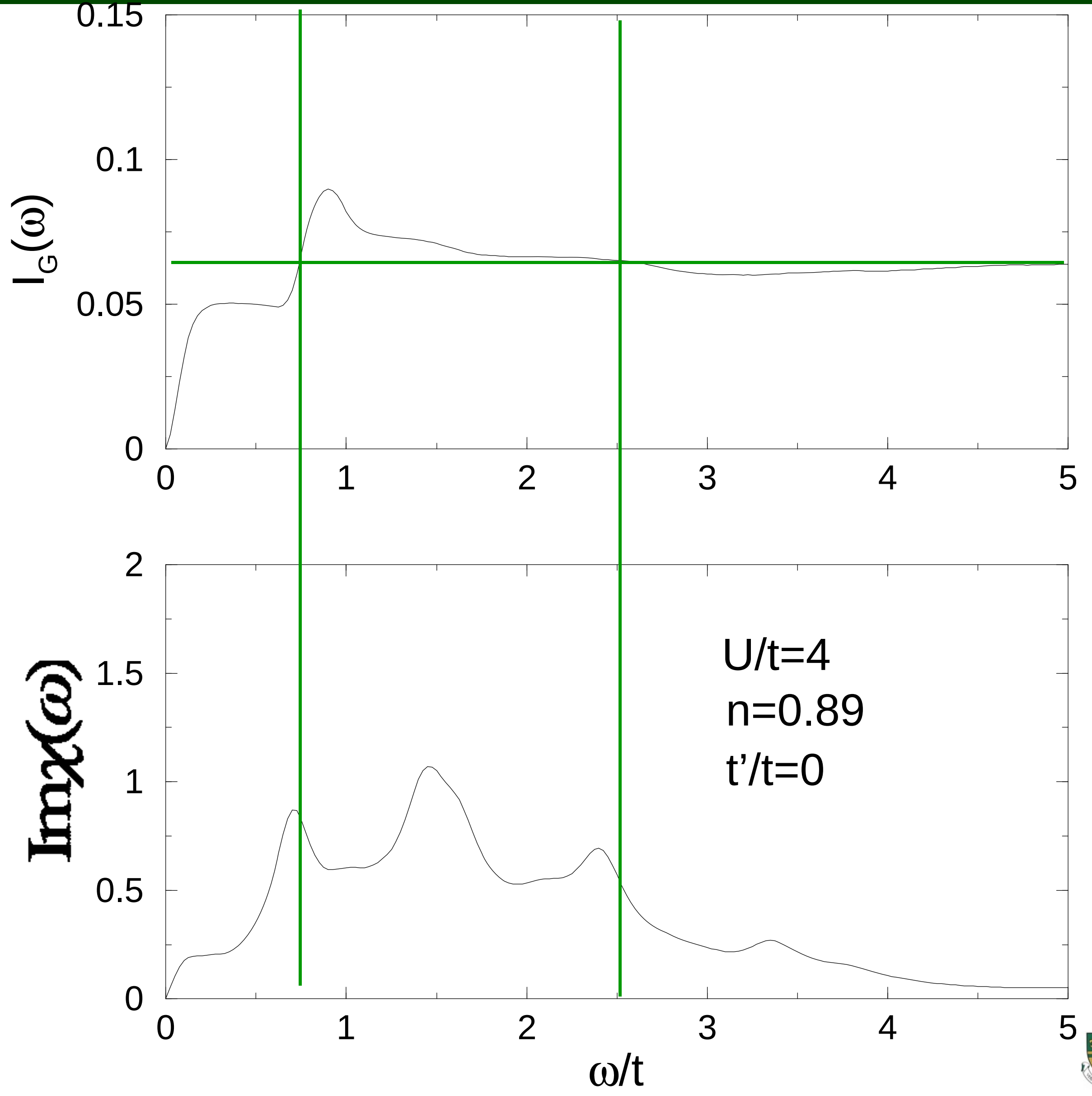


Relevant frequencies

Effect of U

$t' = t'' = 0$

$U = 4 \quad \delta = 0.11$



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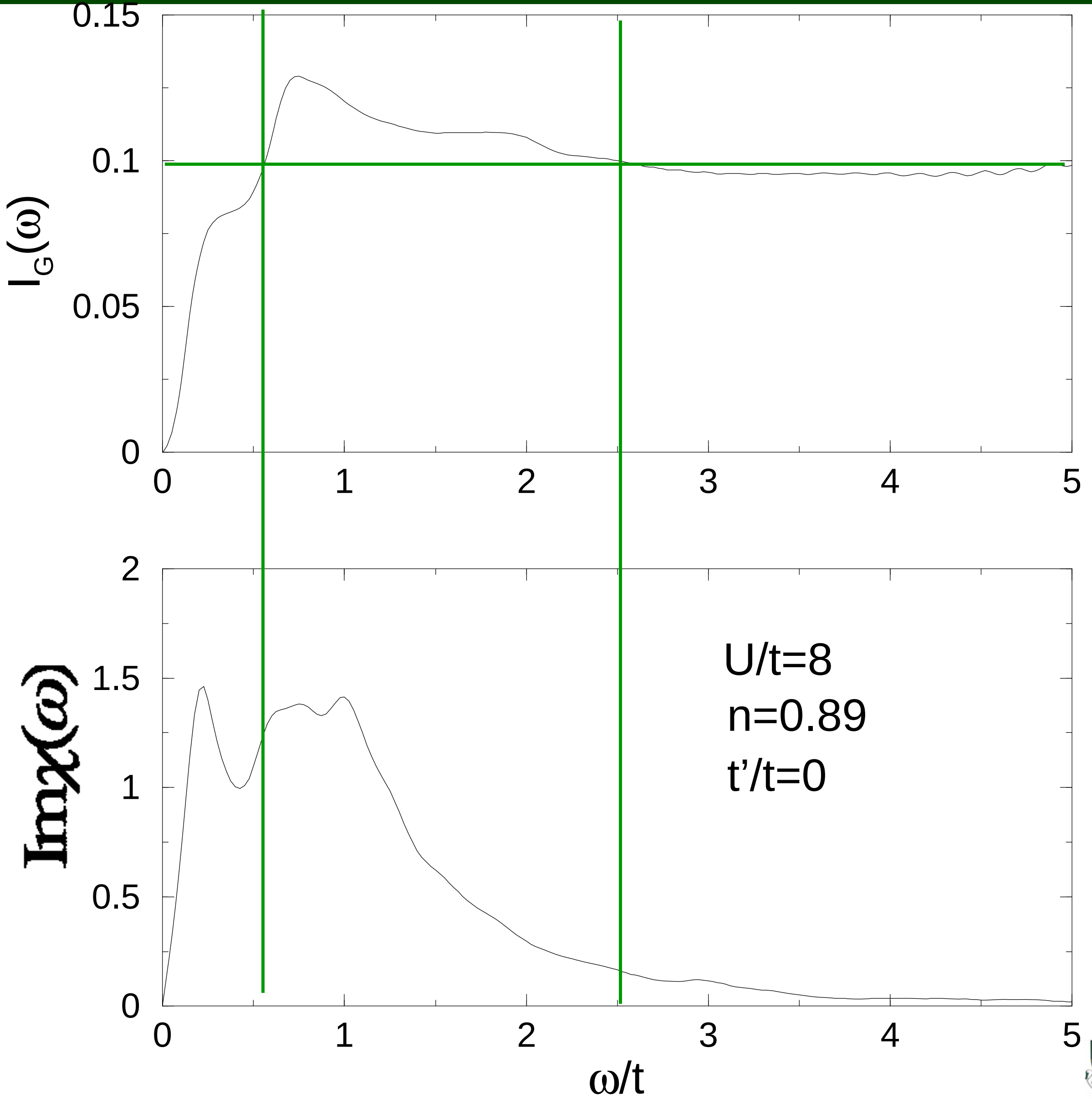
$U = 8 \quad \delta = 0.11$



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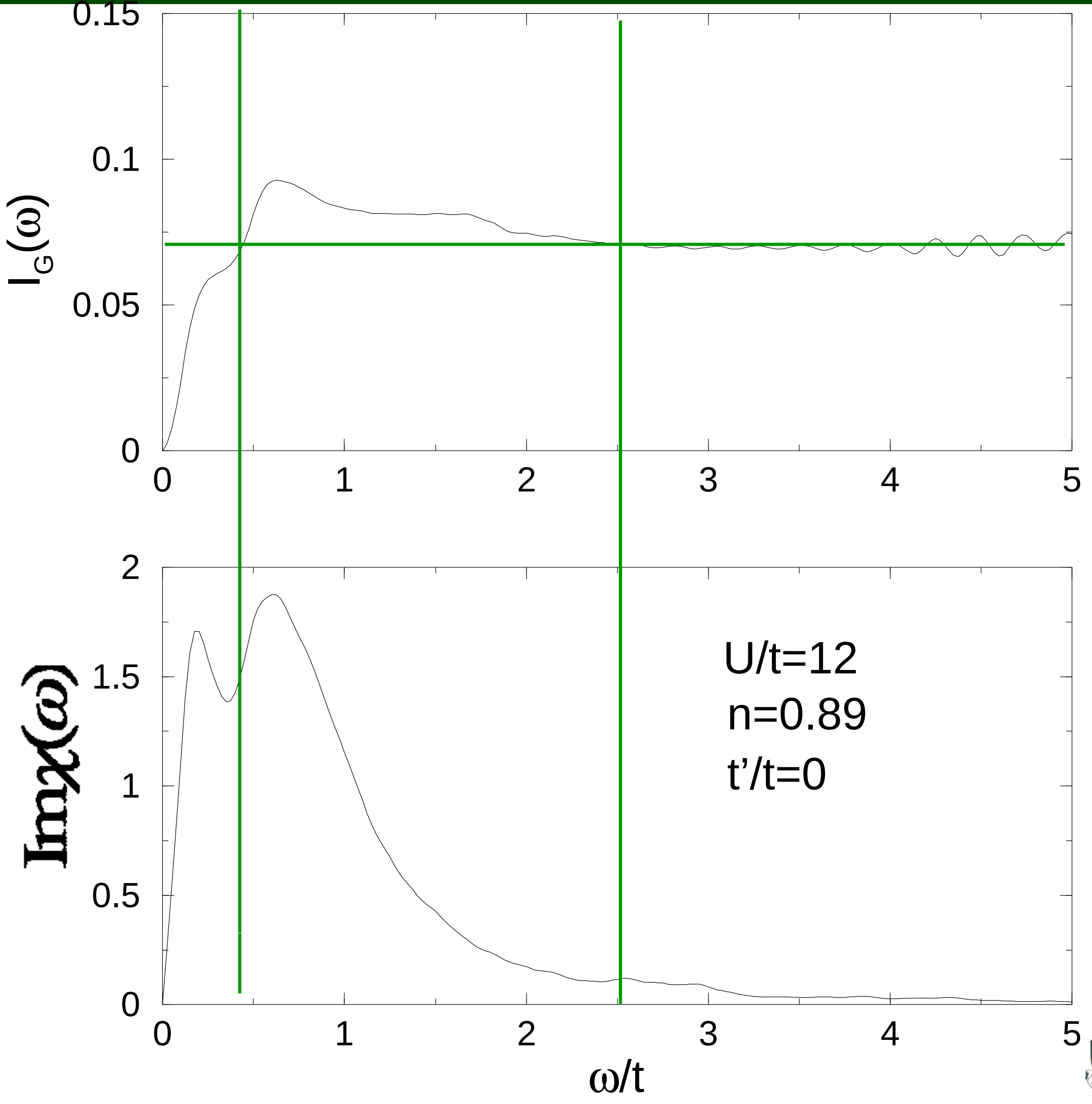
$U = 12 \quad \delta = 0.11$



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Repulsive Hubbard model
Relevant frequencies

Effect of doping $U = 8t$

$t' = t'' = 0$

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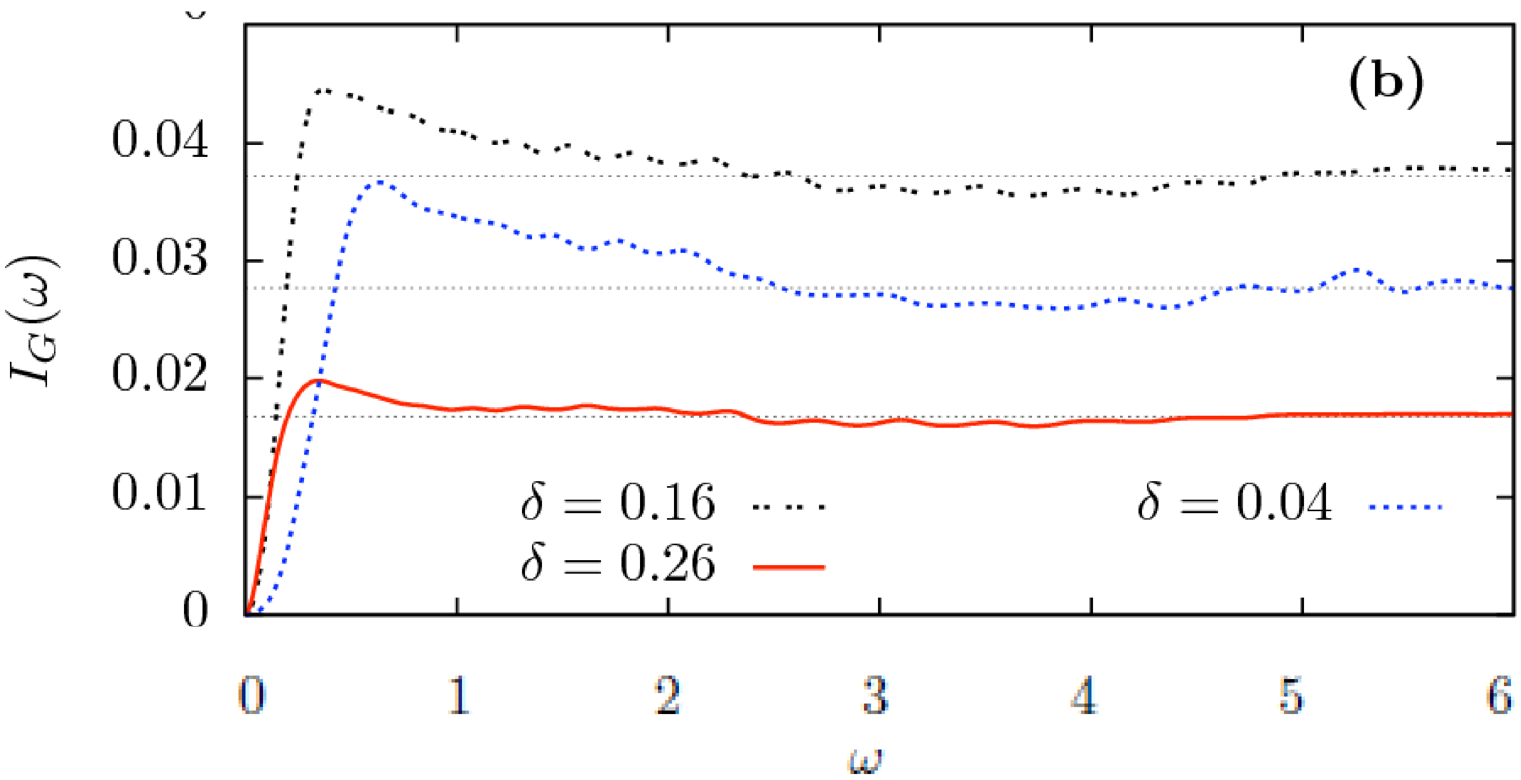
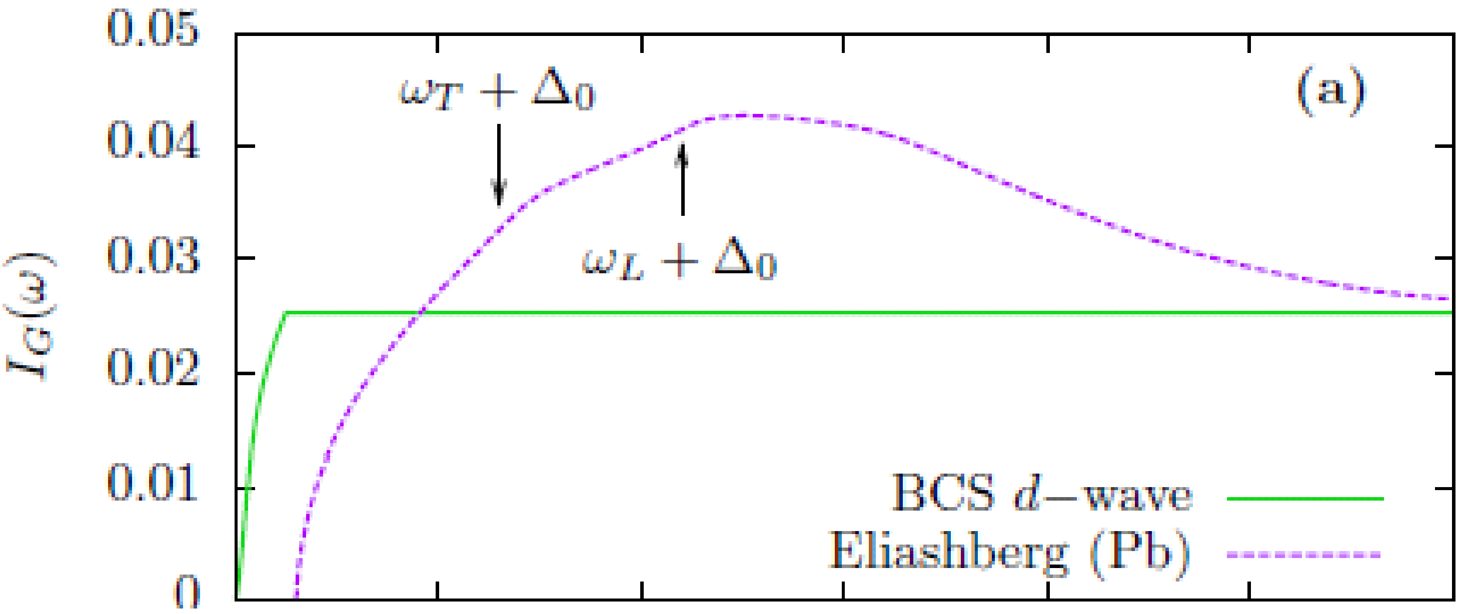
Doping dependence



BCS vs Eliashberg



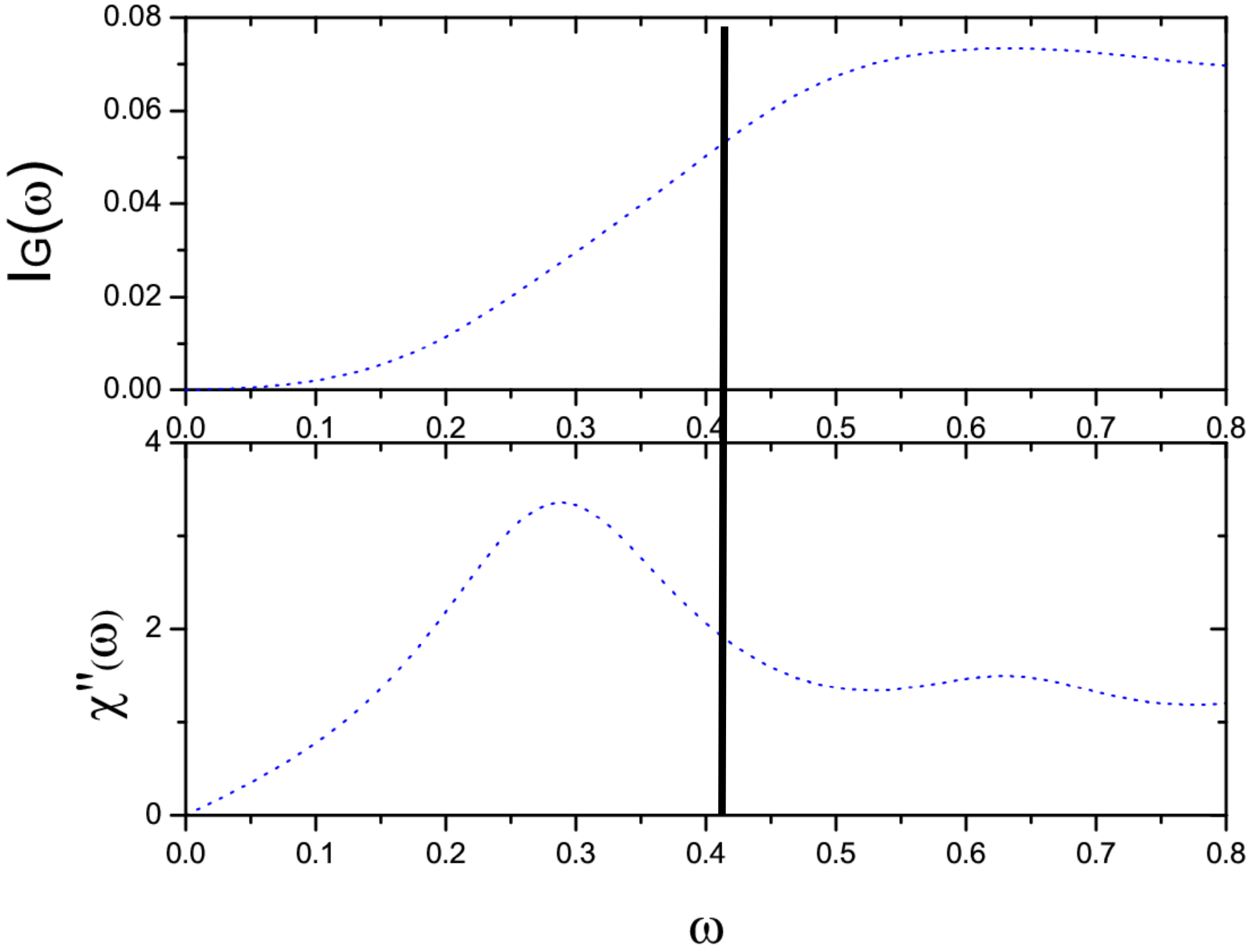
Repulsive Hubbard model
Relevant frequencies

Effect of doping (again) $U = 8t$

$t' = t'' = 0$

arXiv:0812.1228

Relevant frequencies (small ω)



δ=0.04

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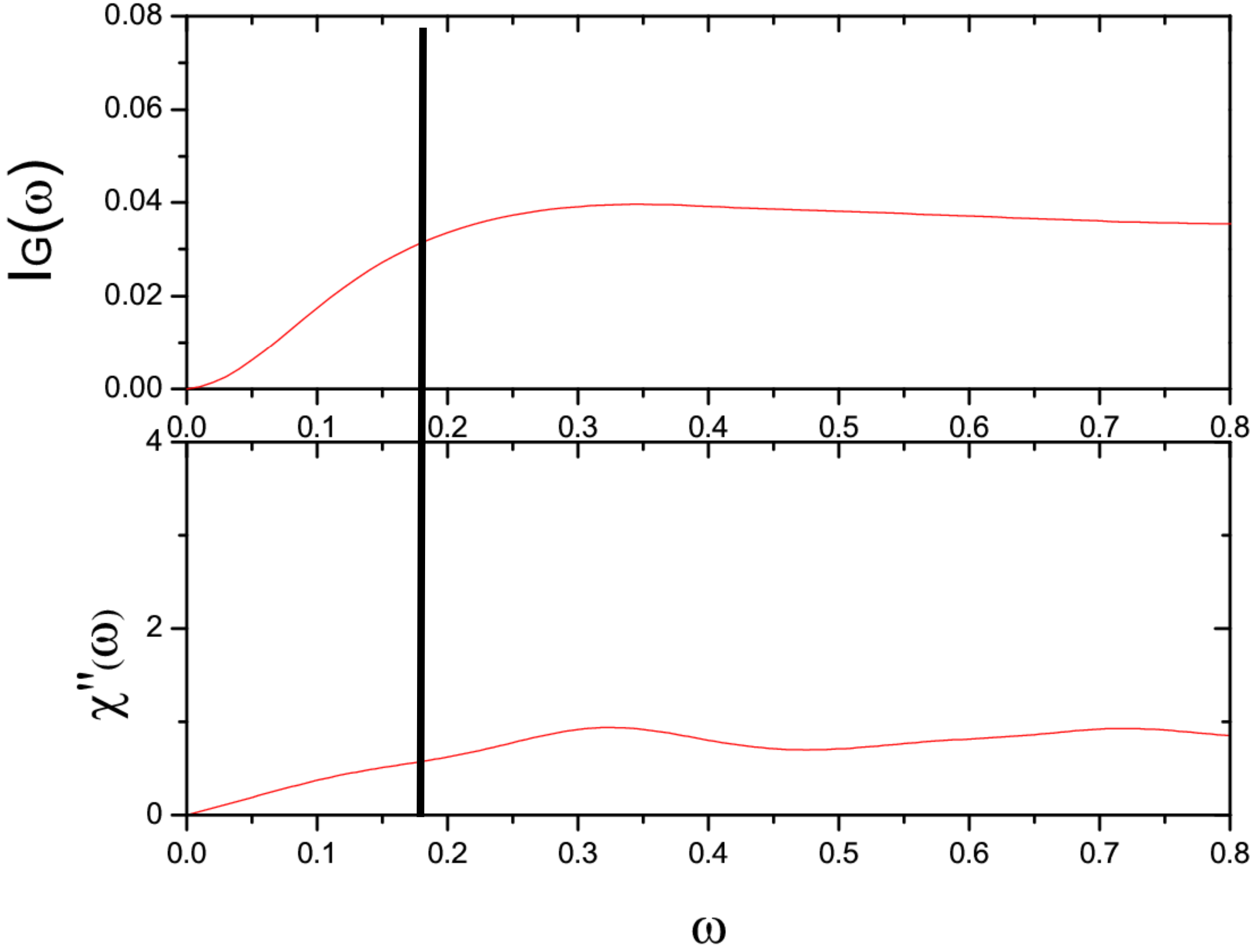
Relevant frequencies (small ω)



δ=0.26

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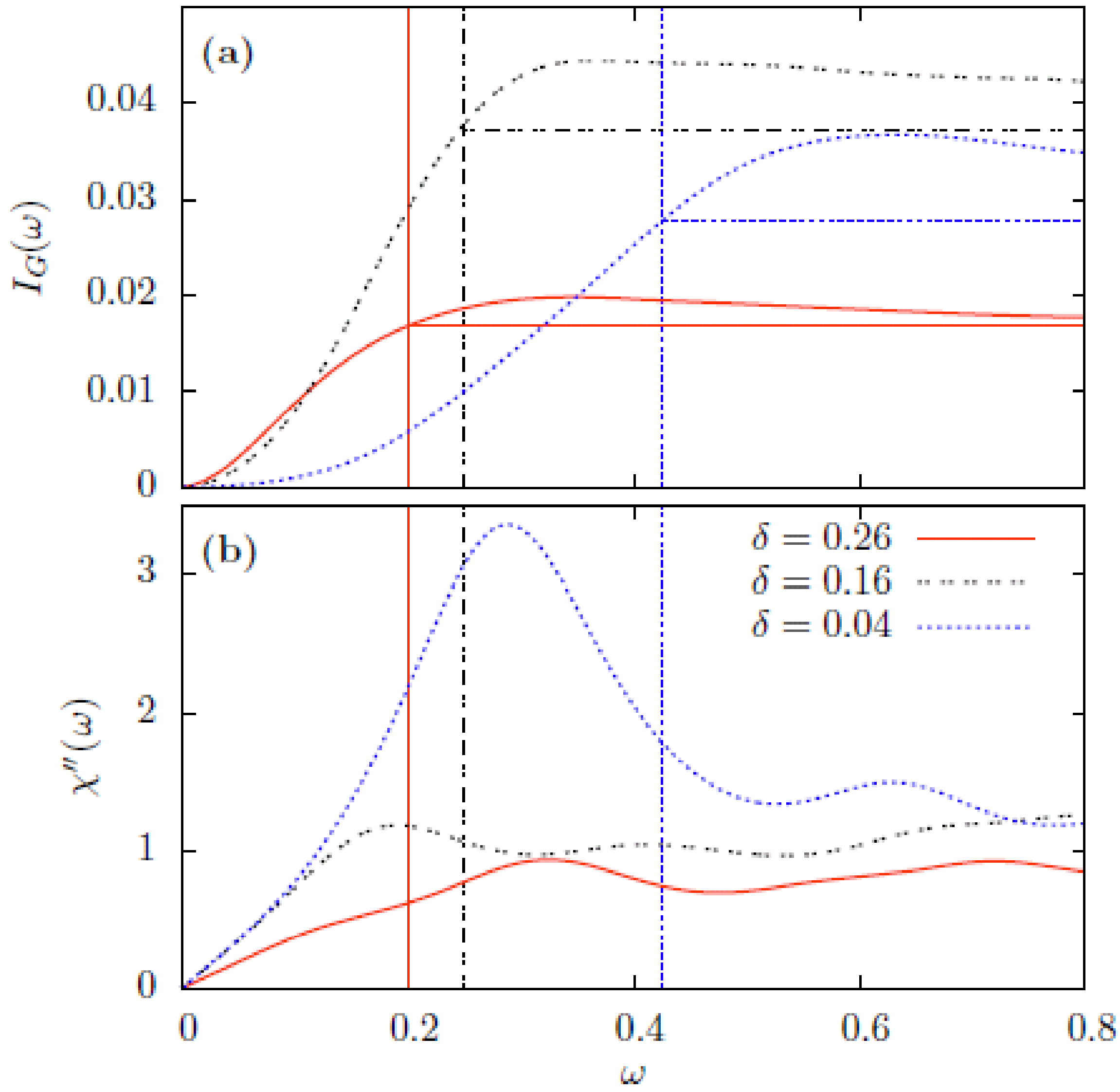
Relevant frequencies (small ω)



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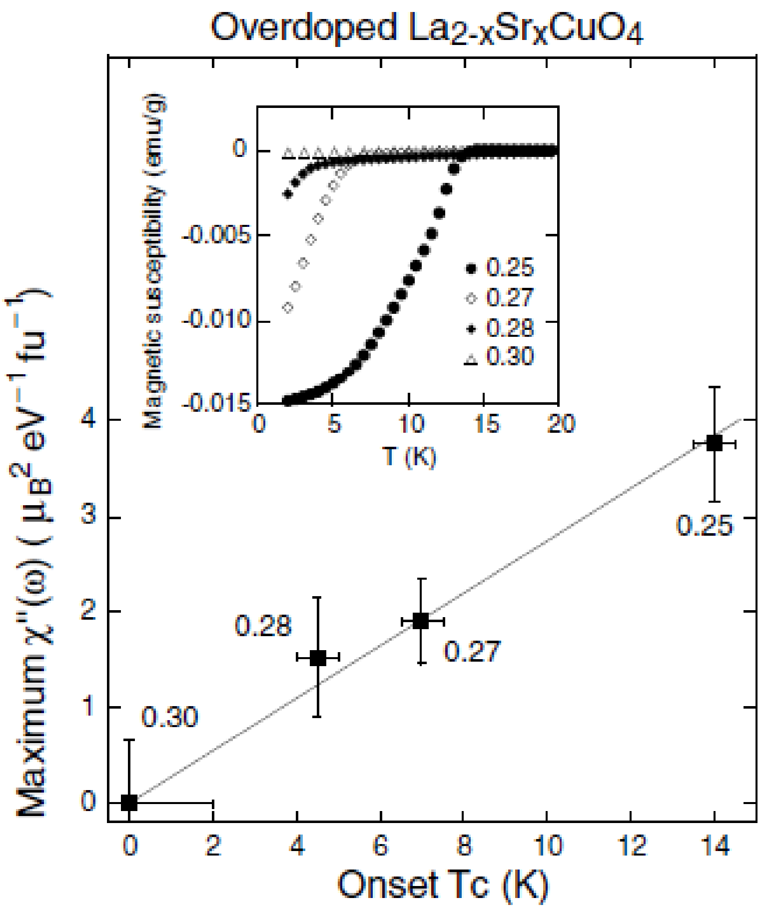
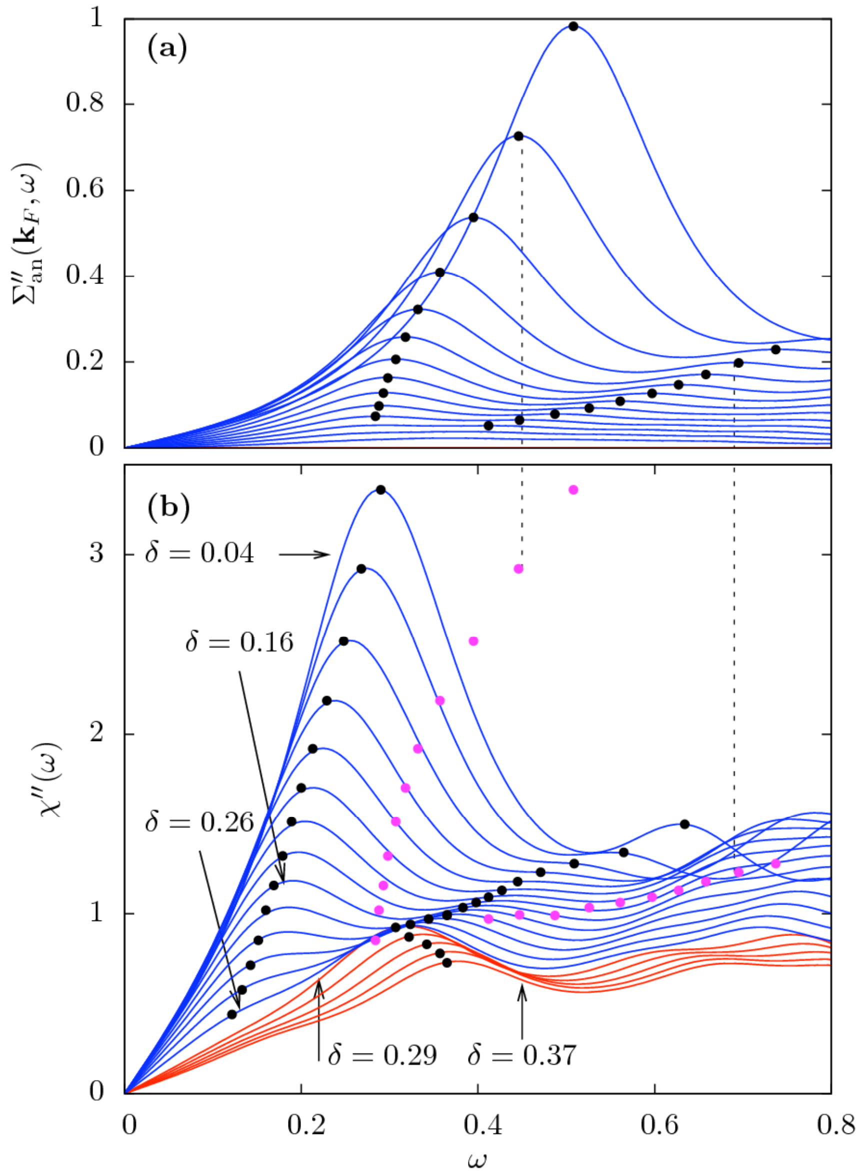
Experiment and the glue

Neutron scattering and Tc



Wakimoto … Birgeneau
PRL (2004)



Neutron scattering and transition

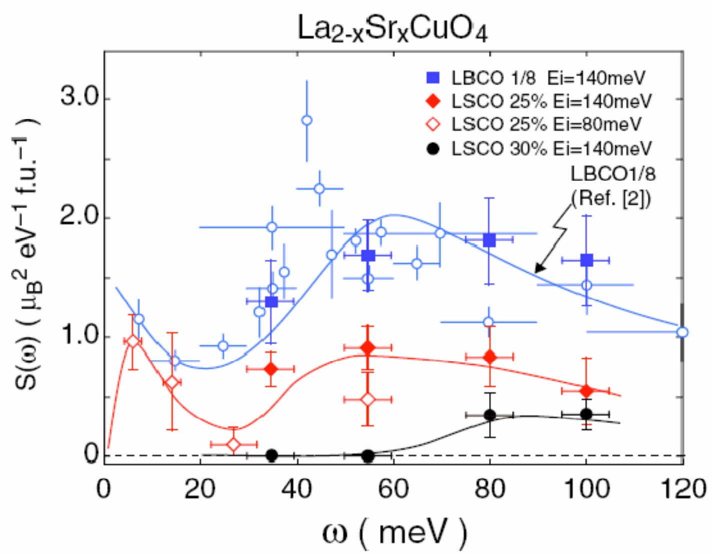
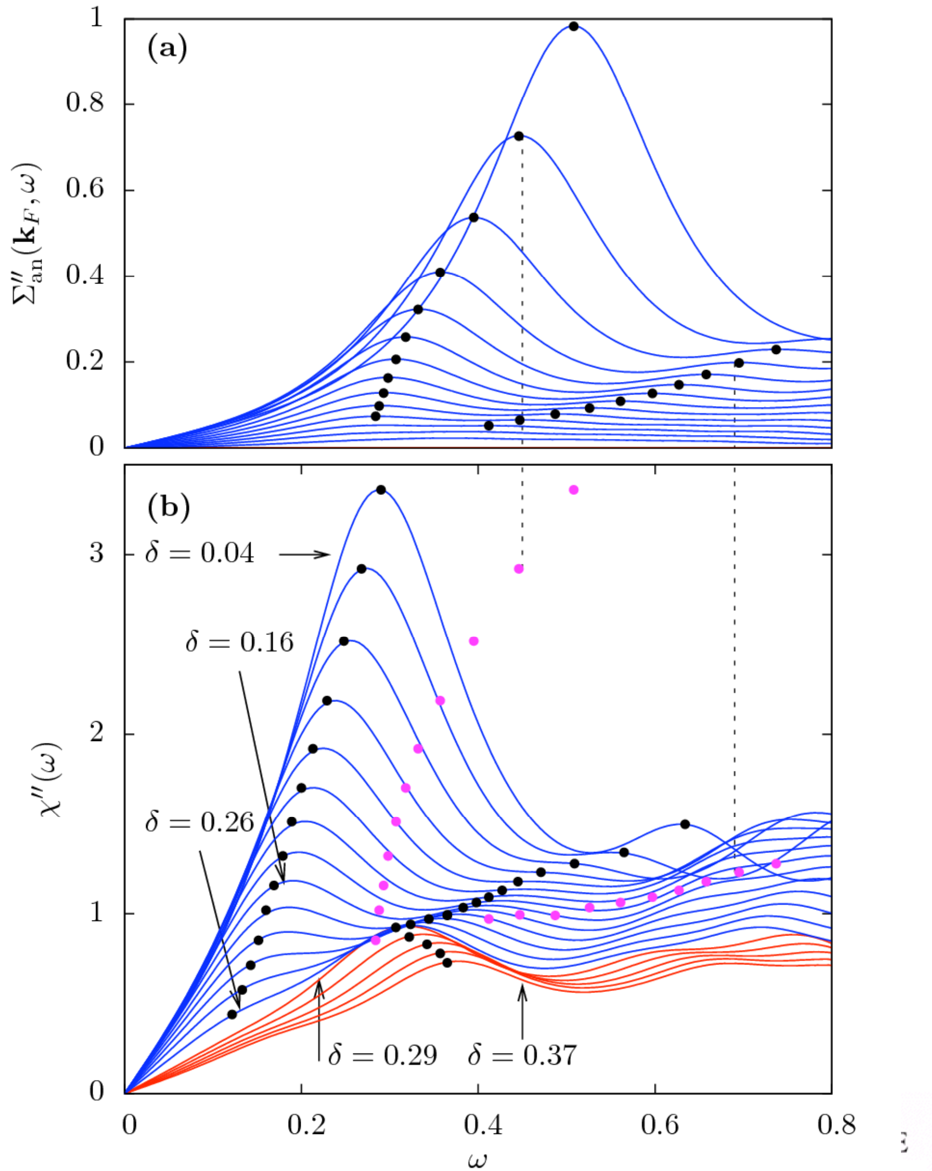


FIG. 3 (color online). **Q**-integrated dynamic structure factor $S(\omega)$ which is derived from the wide-H integrated profiles for LBCO 1/8 (squares), LSCO $x = 0.25$ (diamonds; filled for E_i = 140 meV, open for E_i = 80 meV), and $x = 0.30$ (filled circles) plotted over $S(\omega)$ for LBCO 1/8 (open circles) from [2]. The solid lines following data of LSCO $x = 0.25$ and 0.30 are guides to the eyes.



Wakimoto … Birgeneau PRL (2007);
PRL (2004)

Glue function, optical conductivity

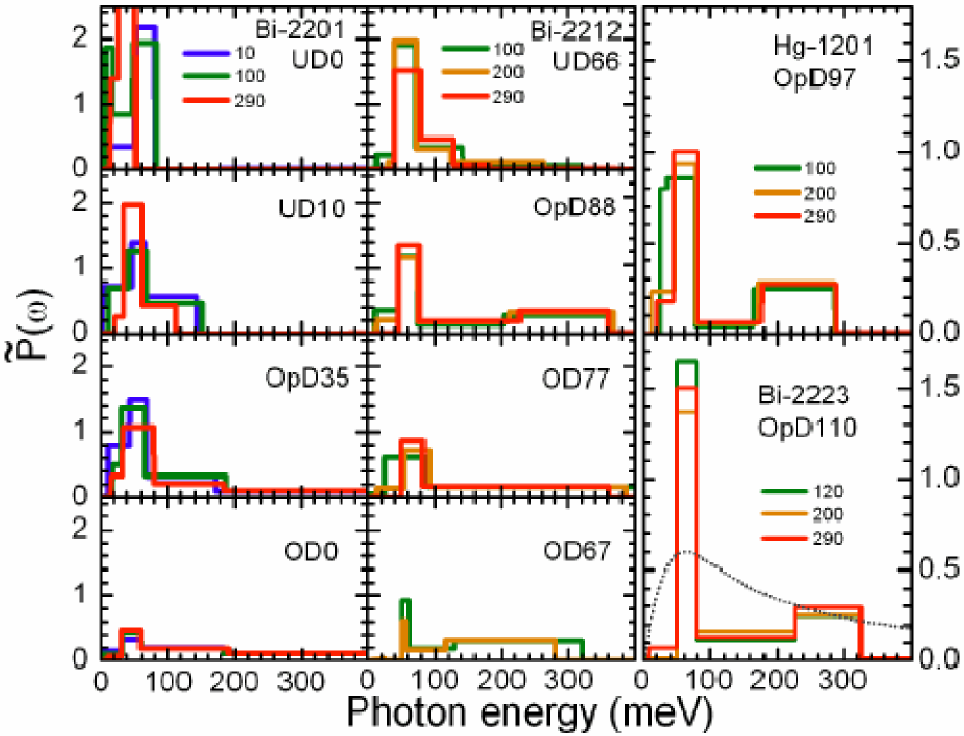
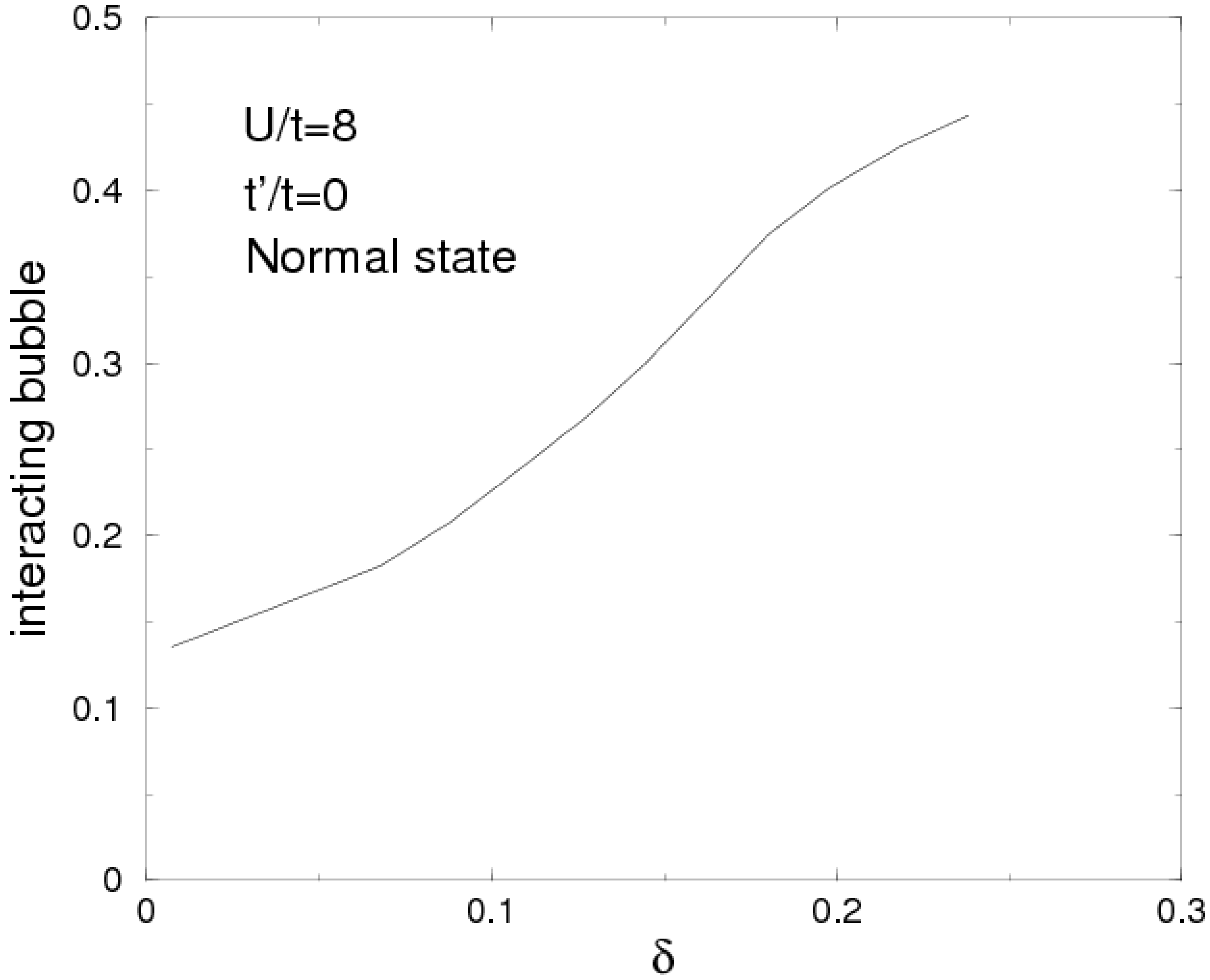


FIG. 2: Electron-boson coupling function $\tilde{P}(\omega)$ for Bi-2201 at 4 different charge carrier concentrations (10 K, 100 K, 290 K), Bi-2212 at 4 charge carrier concentrations, and optimally doped Bi-2223 and Hg-1201 (100 K, 200 K, 290 K). The dotted curve in the lower right panel represents the spin-fluctuation model.

Van Heumen… Van der Marel … Shen, arXiv:0807.1730

Dressed bubble *U=8* normal state

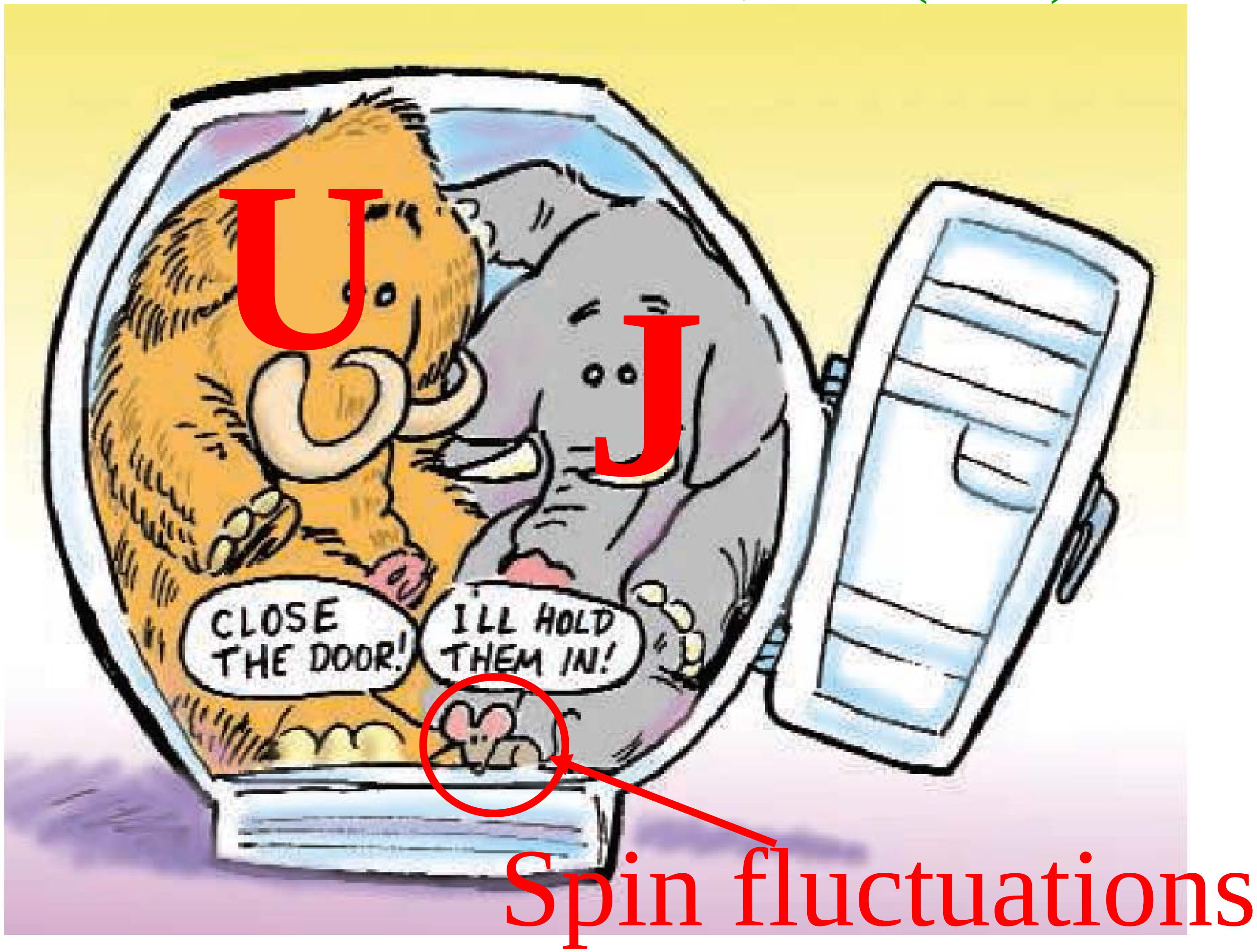
Effect of self-energy bubble, normal state



)KE

So what is the glue?

P.W. Anderson Science 317, 1705 (2007)



“We have a mammoth and an elephant in our refrigerator—do we care much if there is also a mouse?”

So what is the glue?

P.W. Anderson Science 317, 1705 (2007)

"We have a mammoth and an elephant in our refrigerator— do we care much if there is also a mouse?"

Main lessons

- Scale is *J*
- Spin dynamics reflected in pair dynamics
- Not exactly the same as simple spin fluctuations:
  - Going down in underdoped regime because of large self-energy effects in the normal part of the correlations (Mott Physics)
  - Short-range correlations suffice (Magnetic resonance has small weight) (Kee, Kivelson, Aeppli PRL (2002))
  - Anomalous self-energy increases towards half-filling

Pitfalls

- Correlation vs cause and effect
- Spin fluctuations rearrange self-consistently with the opening of the gap

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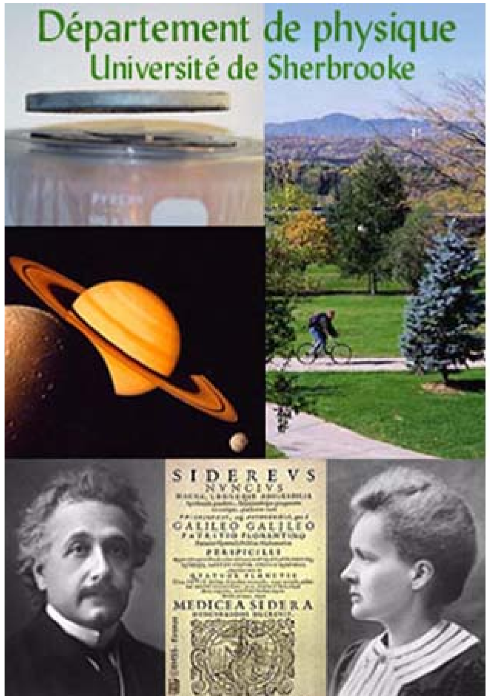

André-Marie Tremblay

CANADA RESEARCH CHAIRS
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Thanks...

Merci