Optical and DC conductivity in the *d=2* Hubbard model Including Vertex Corrections

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arXiv:1101.4037

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Calculating transport properties

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A few things we know about resistivity

- From Bloch-Boltzmann theory
  - T^2 for Fermi-liquid
  - T for AFM QCP in $d=2$ (Moriya 1990)
  - T^2 with cold spots (Hlubina-Rice 1995)
- From Mott-Ioffe-Regel (wave nature)
  - Maximum metallic resistivity
- From DMFT
  - Limit can be exceeded with linear T (Palsson, Kotliar 2001)

Mott-Ioffe-Regel limit

$$\sigma = \frac{ne^2\tau}{m}$$

$$n = \frac{k_F^2}{2\pi d}$$

$$\ell = v_F\tau$$

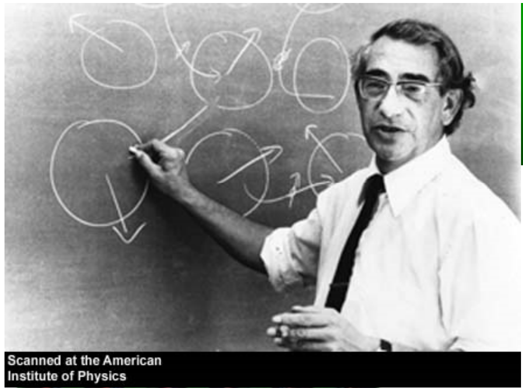
$$k_F\ell = 1$$

$$\sigma_{MIR} = \frac{1}{d}\frac{e^2}{h}$$

Vertex corrections

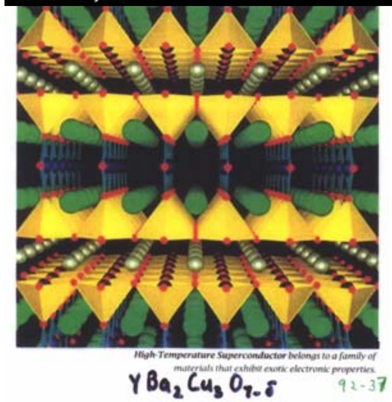
- Single particle excitations (ARPES) measures single particle scattering rate
- Resistivity measurement: particle-hole pair
  - Lifetime counts (self-energy)
  - Interaction between excited particle and hole counts (vertex correction)
  - The two must be evaluated in a consistent way (Ward identities)

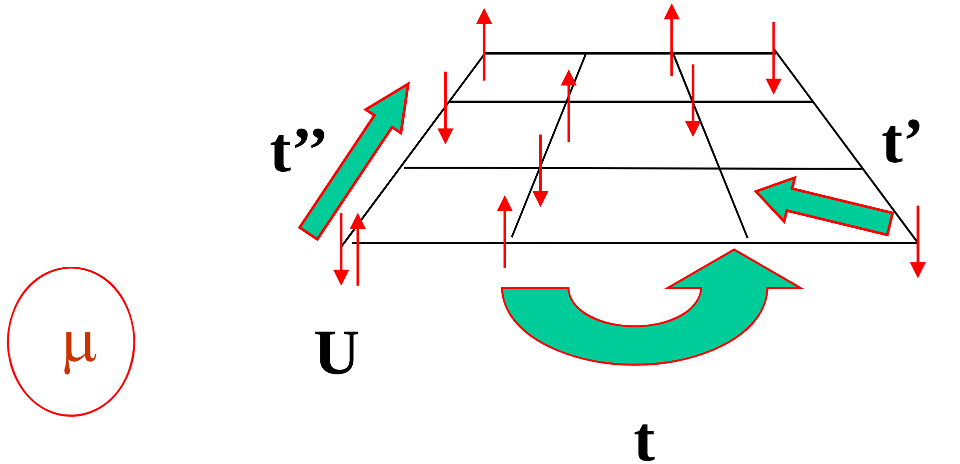
The model

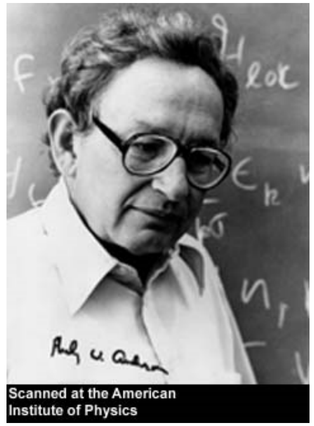


The Hubbard model

Simplest microscopic model for *Cu O* planes.







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

No mean-field factorization for d-wave superconductivity

Weak to intermediate coupling

T. Moriya, Y. Takahashi, and K. Ueda, Journal of the Physical Society of Japan, **59**, 2905 (1990/08). R. Hlubina and T. Rice, Physical Review B (Condensed Matter), **51**, 9253 (1995/04/01).	Boltzmann
A. Rosch, Phys. Rev. Lett., **82**, 4280 (1999). H. v. Löhneysen, A. Rosch, M. Vojta, and P. Wölfle, Rev. Mod. Phys., **79**, 1015 (2007).	Boltzmann disordered
S. Wermbter and L. Tewordt, Phys. Rev. B, **48**, 10514 (1993).	T-matrix
T. Dahm, L. Tewordt, and S. Wermbter, Physical Review B (Condensed Matter), **49**, 748 (1994/01/01).	FLEX
H. Kontani, Journal of the Physical Society of Japan, **76**, 074707 (2007/07). H. Kontani, K. Kanki, and K. Ueda, Physical Review B (Condensed Matter), **59**, 14723 (1999/06/01).	FLEX with MT-VC
Y. Yanase, Journal of the Physical Society of Japan, **71**, 278 (2002/01/).	
H. Kontani, Reports on Progress in Physics, **71**, 026501 (2008/02/).	Review
H. Maebashi and H. Fukuyama, Journal of the Physical Society of Japan, **66**, 3577 (1997/11/). H. Maebashi and H. Fukuyama, Journal of the Physical Society of Japan, **67**, 242 (1998/01/).	Vertex within FL

Strong coupling

F. Mancini and A. Avella, Advances in Physics, **53**, 537 (2004).

Composite operators

T. A. Maier, ArXiv Condensed Matter e-prints (2003), arXiv:cond-mat/0312447.
M. H. Hettler, M. Mukherjee, M. Jarrell, and H. R. Krishnamurthy, Phys. Rev. B, **61**, 12739 (2000).
K. Haule and G. Kotliar, Physical Review B (Condensed Matter and Materials Physics), **76**, 104509 (2007).
K. Haule and G. Kotliar, Europhysics Letters, **77**, 6 pp. (2007/01/), ISSN 0295-5075.

Quantum cluster no vertex

N. Lin, E. Gull, and A. J. Millis, Phys. Rev. B, **80**, 161105 (2009), arXiv:0909.1625 [cond-mat.str-el].
S. Okamoto, D. Sénéchal, M. Civelli, and A.-M. S. Tremblay, Phys. Rev. B, **82**, 180511 (2010).

DCA,with vertex

Methodology

Weak to intermediate coupling approaches

Two-Particle Self-Consistent
TPSC

TPSC: general ideas

- General philosophy
  - Drop diagrams
  - Impose constraints and sum rules
    - Conservation laws
    - Pauli principle ($\langle n_\sigma^2 \rangle = \langle n_\sigma \rangle$)
    - Local moment and local density sum-rules
- Get for free:
    - Mermin-Wagner theorem
    - Kanamori-Brückner screening
    - Consistency between one- and two-particle $\Sigma G = U\langle n_\sigma n_{-\sigma} \rangle$

Vilk, AMT J. Phys. I France, **7**, 1309 (1997);
Theoretical methods for strongly correlated electrons also (Mahan, 3rd)

TPSC equations

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

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

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

Kanamori-Brückner screening

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

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

Internal accuracy check

$$\frac{1}{2}\mathrm{Tr}\left(\Sigma^{(2)}G^{(1)}\right) = U\langle n_\uparrow n_\downarrow \rangle = \frac{1}{2}\mathrm{Tr}\left(\Sigma^{(2)}G^{(2)}\right)$$

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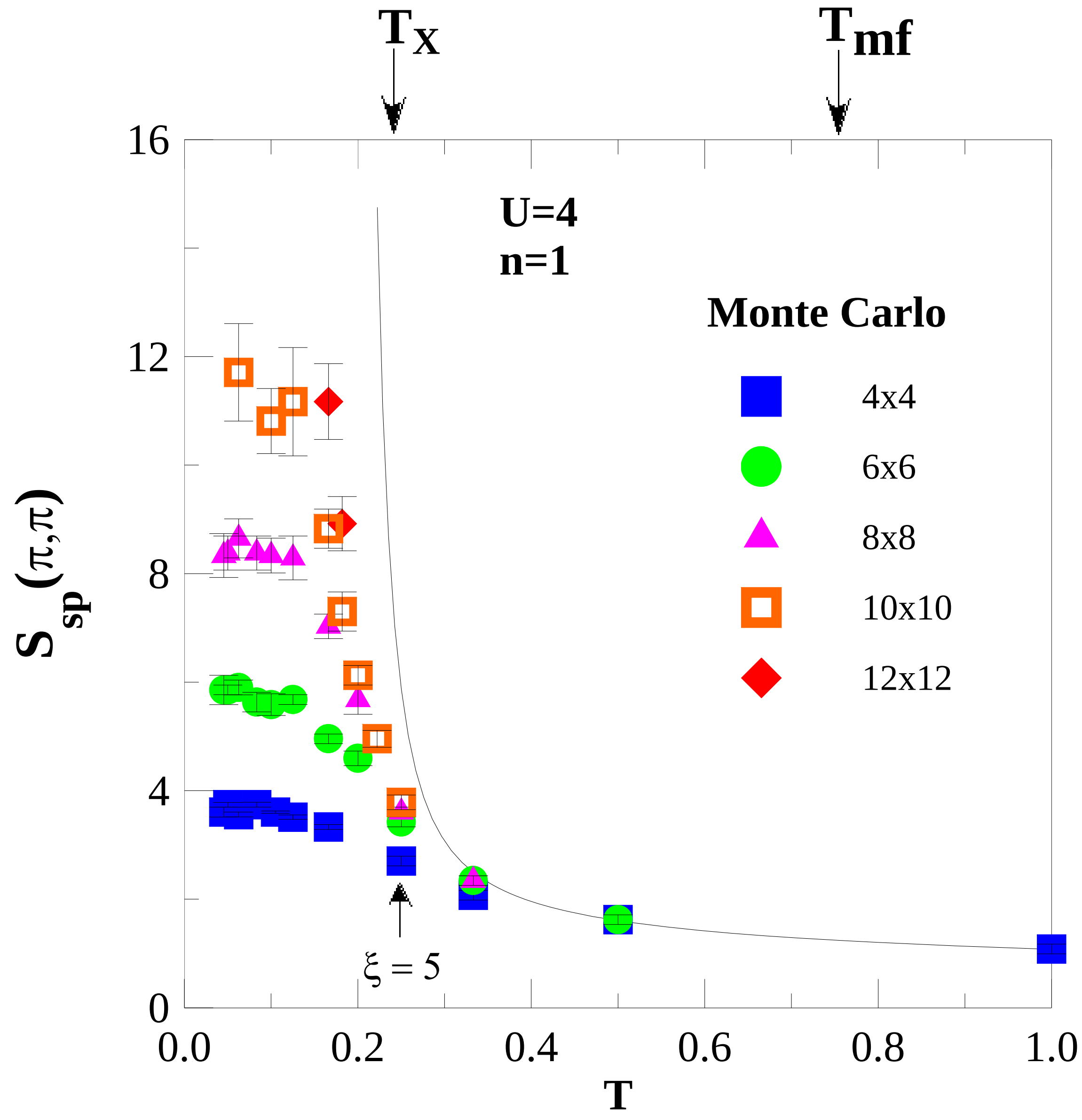
Benchmark TPSC with Quantum Monte Carlo

n=1

$$\xi \sim \exp\left(C(T)/T\right)$$



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

QMC: S. R. White, et al. Phys. Rev. **40**, 506 (1989).

$O(N=\infty)$ A.-M. Daré, Y.M. Vilk and A.-M.S.T Phys. Rev. B **53**, 14236 (1996)

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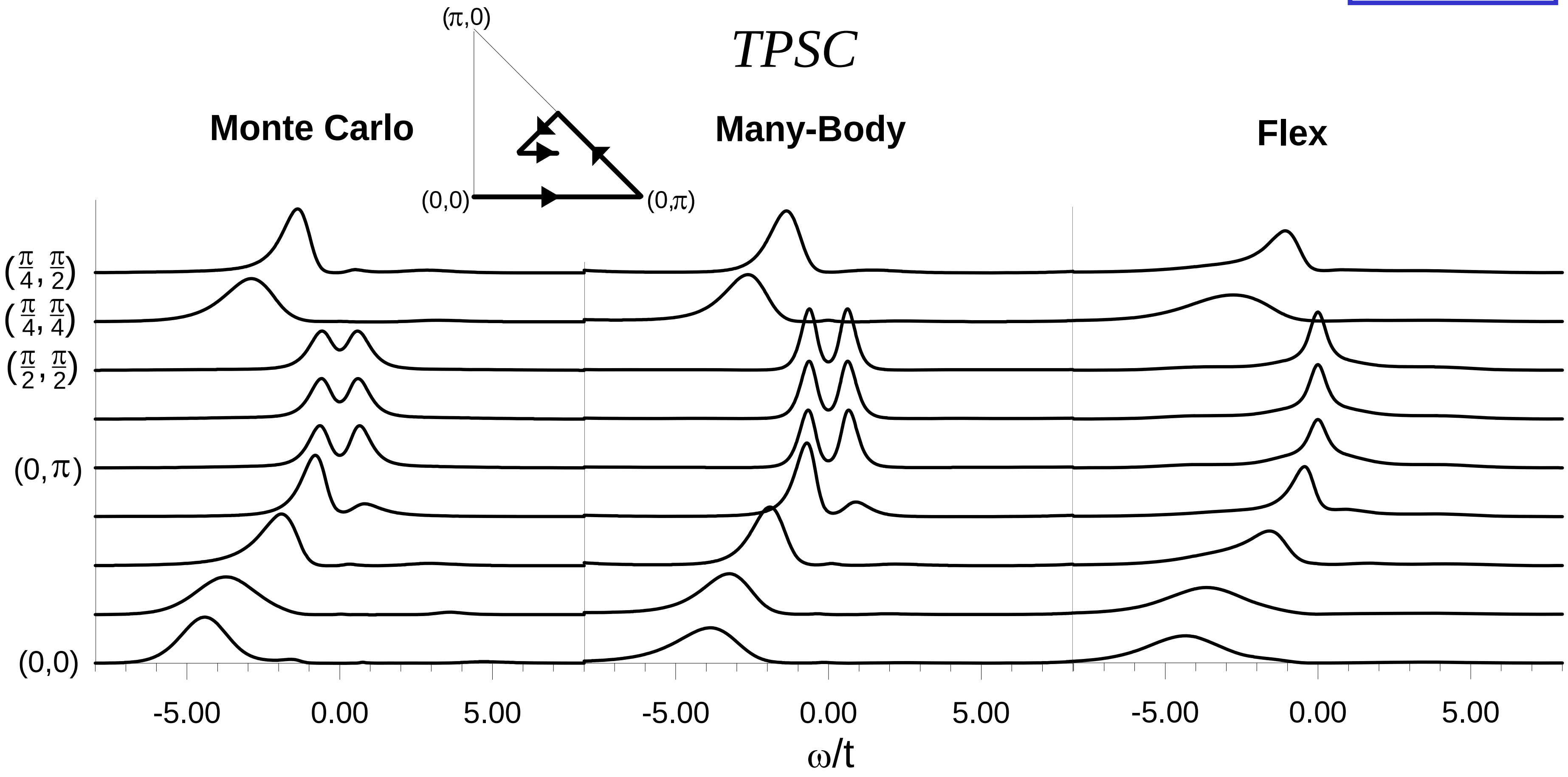
Proofs...

U = + 4
β = 5



Calc. + QMC: Moukouri et al. P.R. B 61, 7887 (2000).

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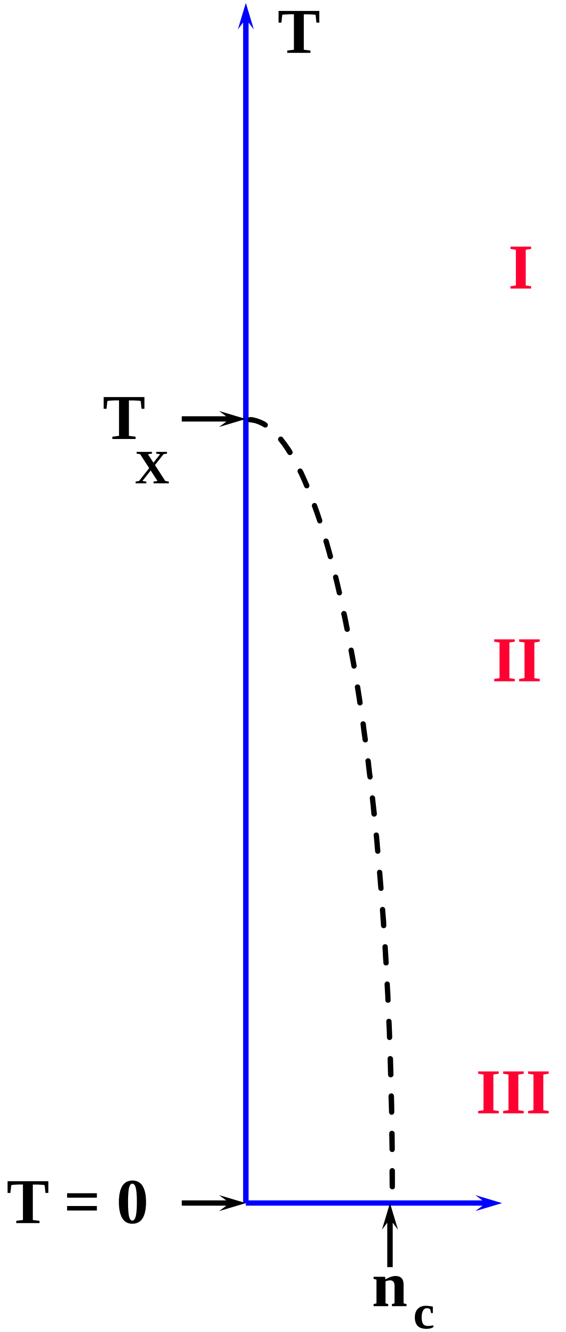
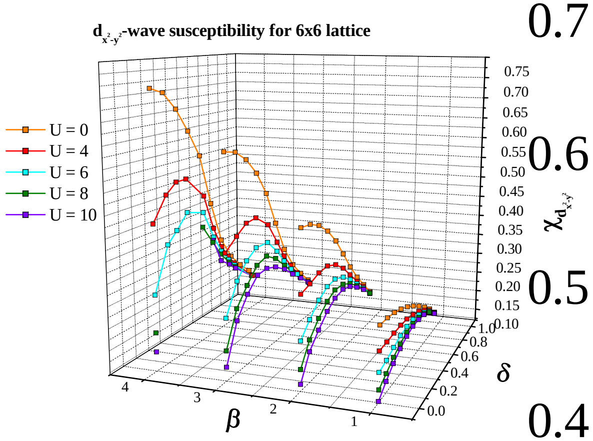
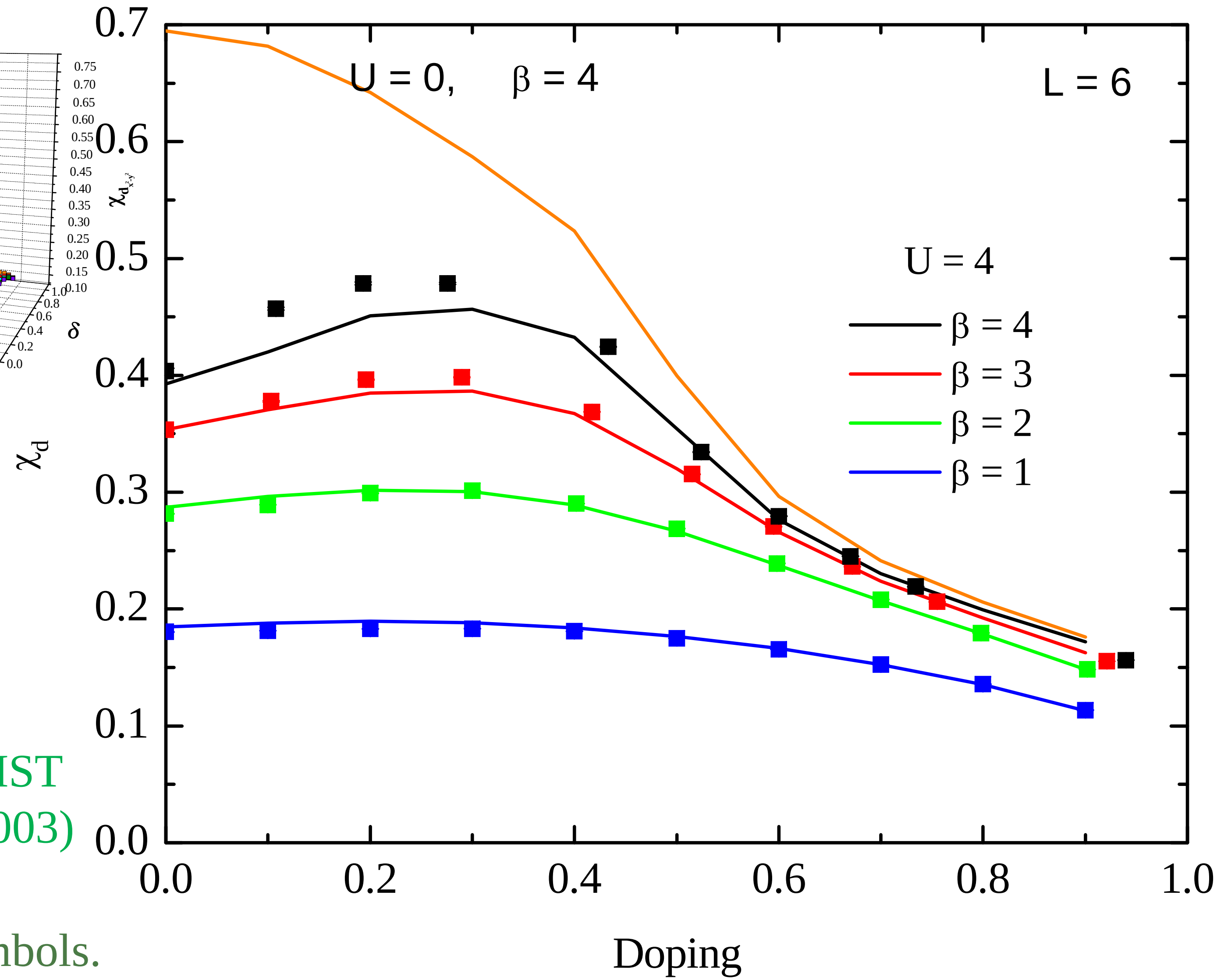

T
I
T
X
II
III
T = 0
n
c





Kyung, Landry AMST
PRB **68**, 174502 (2003)

QMC: symbols.
Solid lines analytical.

Kyung, Landry, A.-M.S.T.

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The pseudogap in electron-doped cuprates

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Analytically :

effect of critical fluctuations on particles (RC regime)

$\hbar\omega_{sf} << k_B T$

Imaginary part: compare Fermi liquid, $\lim_{T\to 0}\Sigma_R''(\mathbf{k}_F,0) = 0$

$$\Sigma_R''(\mathbf{k}_F,0) \propto \frac{T}{v_F}\int d^{d-1}q_\perp \frac{1}{q_\perp^2+\xi^{-2}} \propto \frac{T}{v_f}\xi^{3-d} \underset{d=2}{\propto} \frac{\xi}{\xi_{th}}$$

$$\Delta\ \varepsilon \approx \nabla\ \varepsilon_k \cdot \Delta\ k \approx v_F\hbar\Delta\ k = k_B T$$

$$\mathrm{Im}\Sigma^R(\mathbf{k}_F,0) \propto -U\xi/(\xi_{th}\xi_0^2) > 1$$

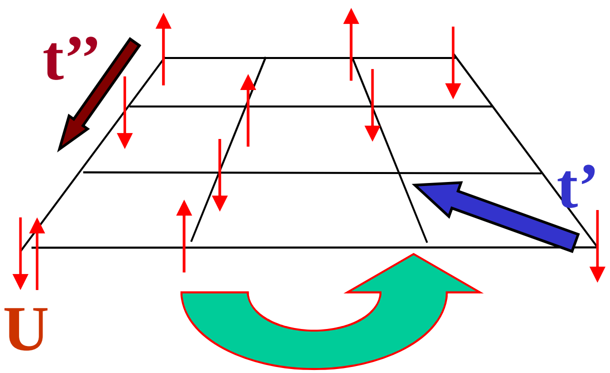
Why leads to pseudogap

$$A(\mathbf{k},\omega) = \frac{-2\Sigma_R''}{(\omega-\varepsilon_{\mathbf{k}}-\Sigma_R')^2+\Sigma_R''^2}$$

Y.M. Vilk and A.-M.S. Tremblay, J. Phys. Chem. Solids **56**, 1769 (1995).
Y.M. Vilk and A.-M.S. Tremblay, Europhys. Lett. **33**, 159 (1996);

Parameters for electron-doped near optimal δ

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

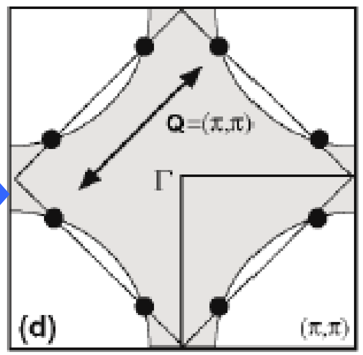


U=6t

fixed

t’=-0.175t, t”=0.05t

t=350 meV, T=200 K

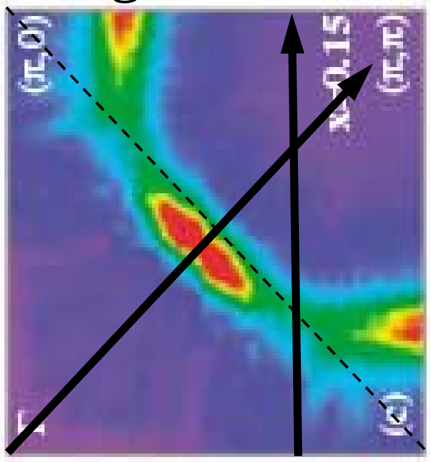


Weak coupling *U<8t*

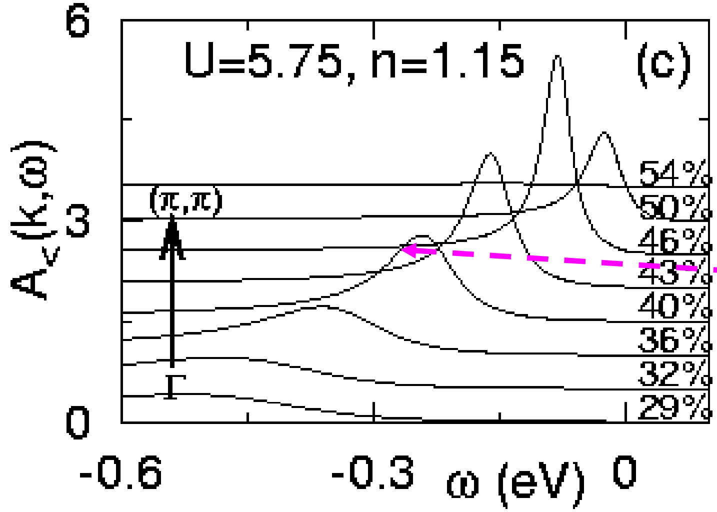
n=1+x – electron filling

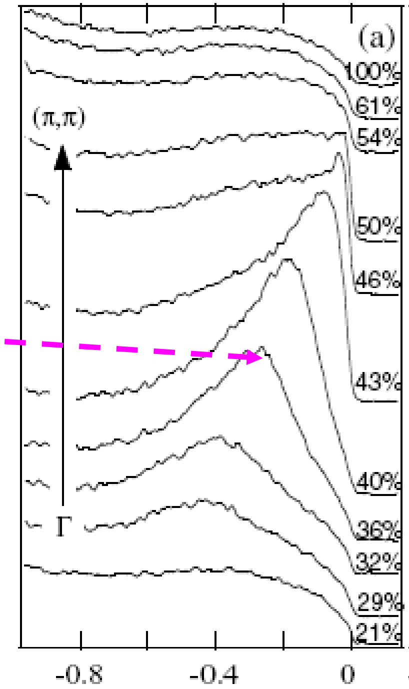
15% doped case: EDCs in two directions

Armitage et al. PRL 2001



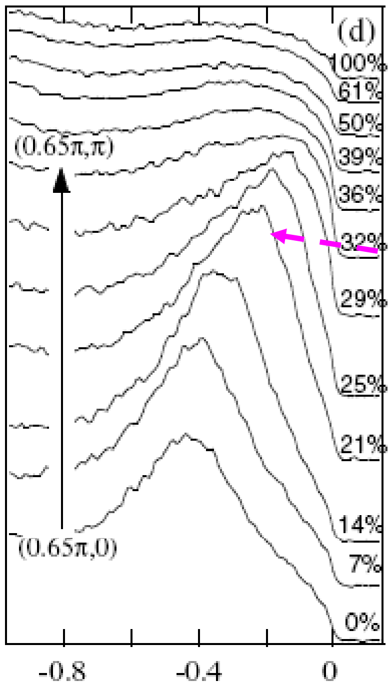
TPSC

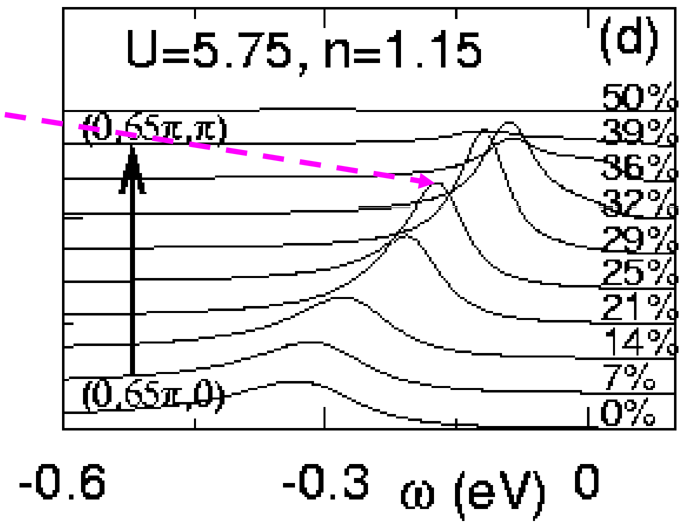




Exp

Exp





Hankevych, Kyung, A.-M.S.T., PRL (2004).

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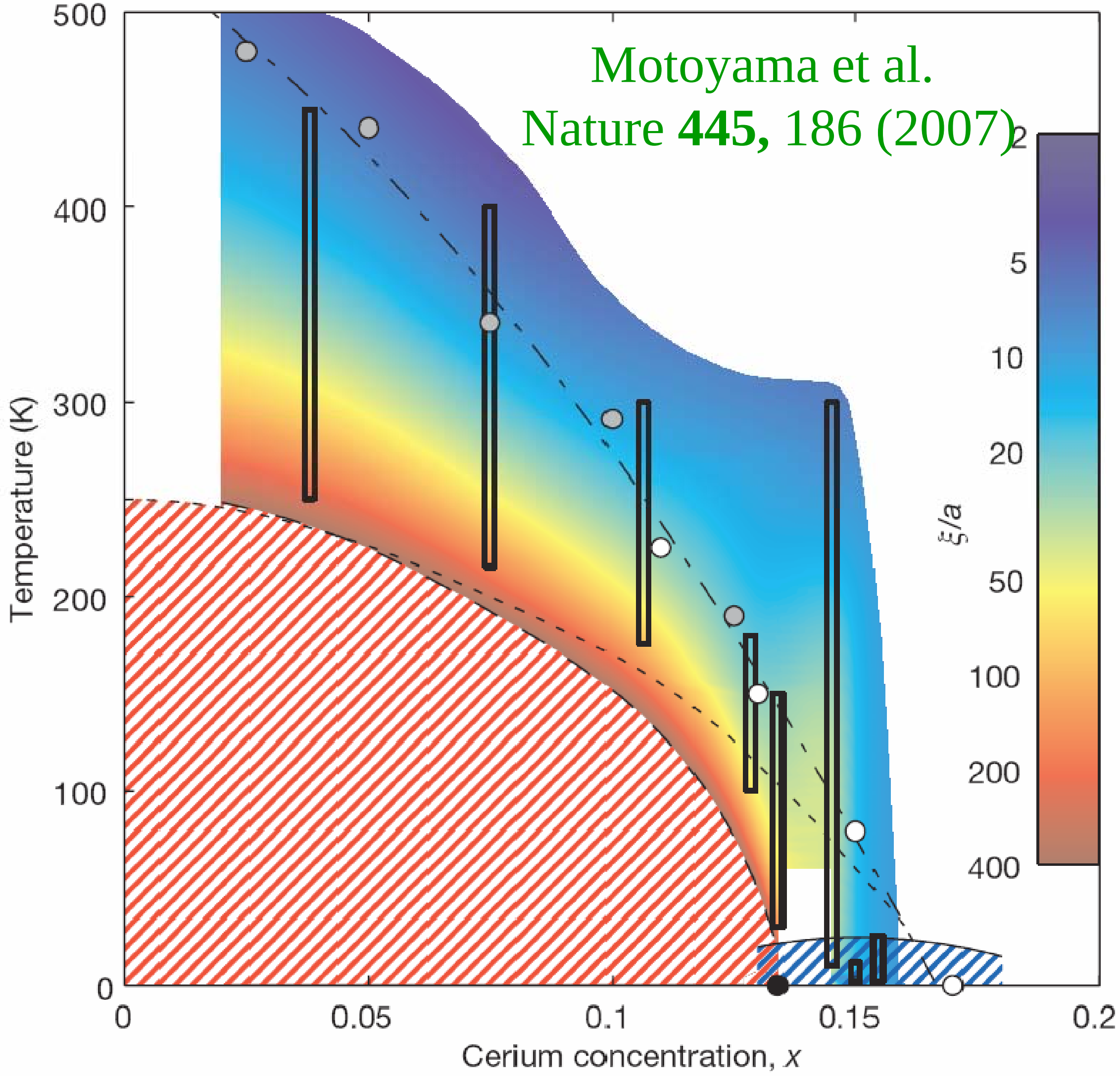
Electron doped Neutron scattering



Motoyama et al.
Nature **445,** 186 (2007)

$$\xi^\star = 2.6(2)\xi_{th}.$$

Vilk, A.-M.S.T (1997)

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

Semi-quantitative fits of both ARPES and neutron

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Precursor of SDW state
(dynamic symmetry breaking)

- Y.M. Vilk and A.-M.S. Tremblay, J. Phys. Chem. Solids **56**, 1769-1771 (1995).
- Y. M. Vilk, Phys. Rev. B 55, 3870 (1997).
- J. Schmalian, *et al*. Phys. Rev. B **60**, 667 (1999).
- B.Kyung *et al*.,PRB **68**, 174502 (2003).
- Hankevych, Kyung, A.-M.S.T., PRL, sept 2004
- R. S. Markiewicz, cond-mat/0308469.

Dominic Bergeron

Calculation of the conductivity

Bumsoo Kyung

Vasyl Hankevych

Linear response : No quasiparticle assumption

- Linear response theory:

$$Re\,\sigma_{xx}(\omega) = \frac{\chi''_{j_x j_x}(\omega)}{\omega}$$

- $\chi_{j_x j_x}(q_x,\omega)$ is the *current-current* correlation fonction:

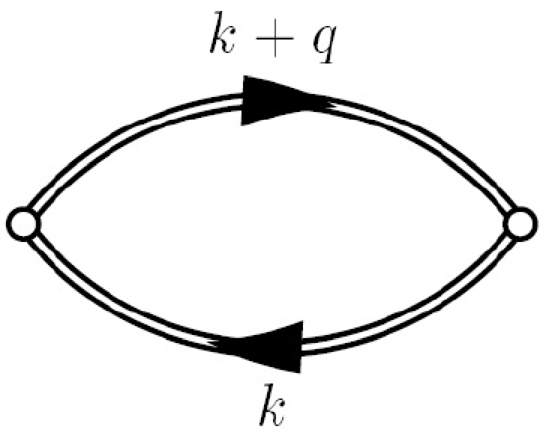
$$\chi_{j_x,j_x}(\mathbf{r}-\mathbf{r}',t-t') = \frac{\delta\langle j_x(\mathbf{r},t)\rangle}{\delta A_x(\mathbf{r}',t')} = i\langle[j_x(\mathbf{r},t),j_x(\mathbf{r}',t')]\rangle\theta(t-t')$$

- $\chi_{j_x j_x}$ can be calculated with vertex corrections obtained from

$$\frac{\delta U_{sp}}{\delta A_x}\Big|_{A_x=0,\mathbf{q}=\mathbf{0}} = \frac{\delta U_{ch}}{\delta A_x}\Big|_{A_x=0,\mathbf{q}=\mathbf{0}} = 0 \qquad \boxed{\frac{\delta\Sigma^{(2)}}{\delta A_x}}$$

Bubble

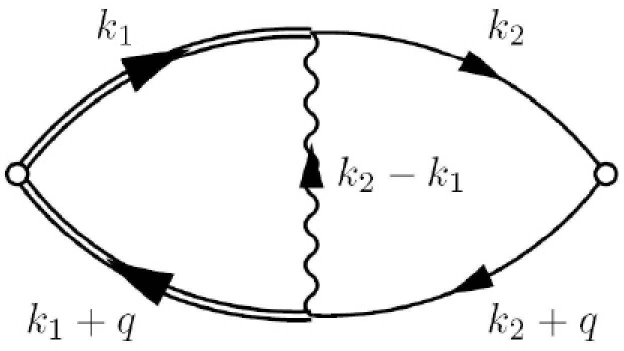
$$\chi^{b}_{j_x j_x}(iq_n, \mathbf{q}=0) = -\frac{2T}{N}\sum_k \left(\frac{\partial \varepsilon_k}{\partial k_x}\right)^2 G^{(2)}(k)G^{(2)}(k+iq_n)$$



Maki Thomson

$$\chi^{vc1}_{j_x j_x}(iq_n) = -\frac{U}{4}\left(\frac{T}{N}\right)^2 \sum_{k_1 k_2} G^{(2)}(k_1)G^{(2)}(k_1+iq_n)G^{(1)}(k_2)G^{(1)}(k_2+iq_n)$$

$$\frac{\partial \varepsilon_k}{\partial k_x}(k_1)\frac{\partial \varepsilon_k}{\partial k_x}(k_2)\left[3U_{sp}\chi_{sp}(k_2-k_1)+U_{ch}\chi_{ch}(k_2-k_1)\right]$$



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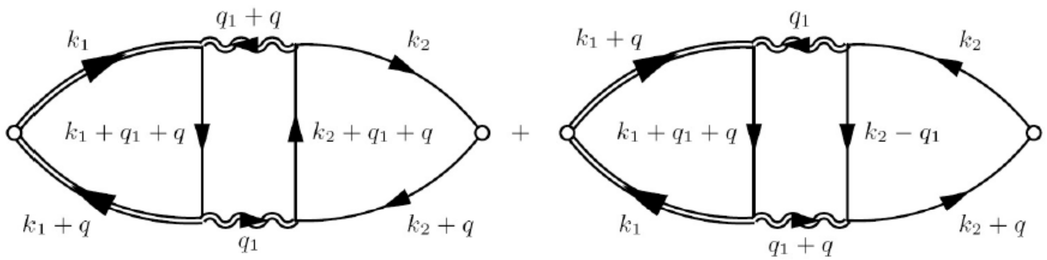
Aslamasov-Larkin

$$\chi^{vc2}_{j_x j_x}(iq_n) = \frac{U}{2}\left(\frac{T}{N}\right)^3 \sum_{k_1,k_2,q_1} \frac{\partial \varepsilon_k}{\partial k_x}(k_1)\frac{\partial \varepsilon_k}{\partial k_x}(k_2) G^{(2)}(k_1) G^{(2)}(k_1+iq_n)$$
$$\times G^{(1)}(k_2)G^{(1)}(k_2+iq_n)\left[G^{(1)}(k_2+q_1+iq_n)+G^{(1)}(k_2-q_1)\right]$$
$$\times G^{(1)}(k_1+q_1+iq_n)\left(3U_{sp}\frac{1}{1-\frac{U_{sp}}{2}\chi_0(q_1)}\frac{1}{1-\frac{U_{sp}}{2}\chi_0(q_1+iq_n)}\right.$$
$$\left.+U_{ch}\frac{1}{1+\frac{U_{ch}}{2}\chi_0(q_1)}\frac{1}{1+\frac{U_{ch}}{2}\chi_0(q_1+iq_n)}\right)$$



Dominic Bergeron

3 loops : at 10 Gflops, *T=0.01 t*

400 billion years for 100 frequencies

Fast Fourier transforms

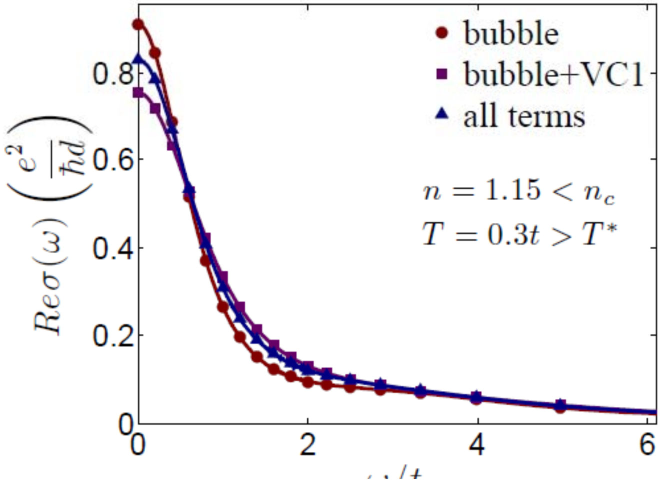
Analytical continuation

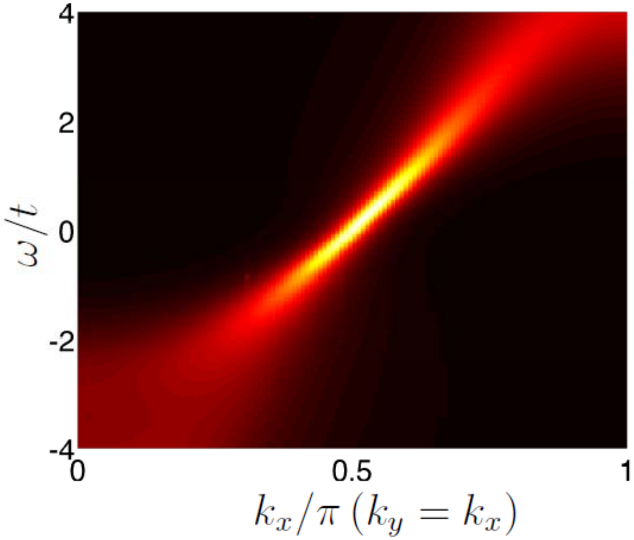
- Analytical continuation of Matsubara conductivity
  - For 10^{-6} precision, Padé not enough
  - Maximum Entropy
    - Checked with model spectral densities

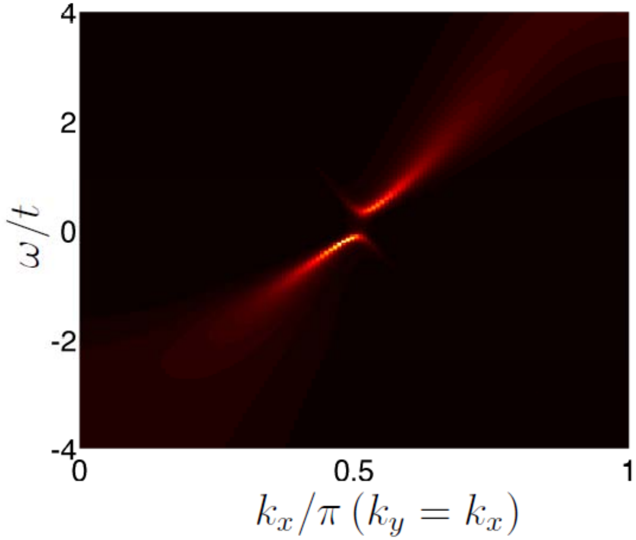
Optical conductivity

Optical conductivity $n < n_c$

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







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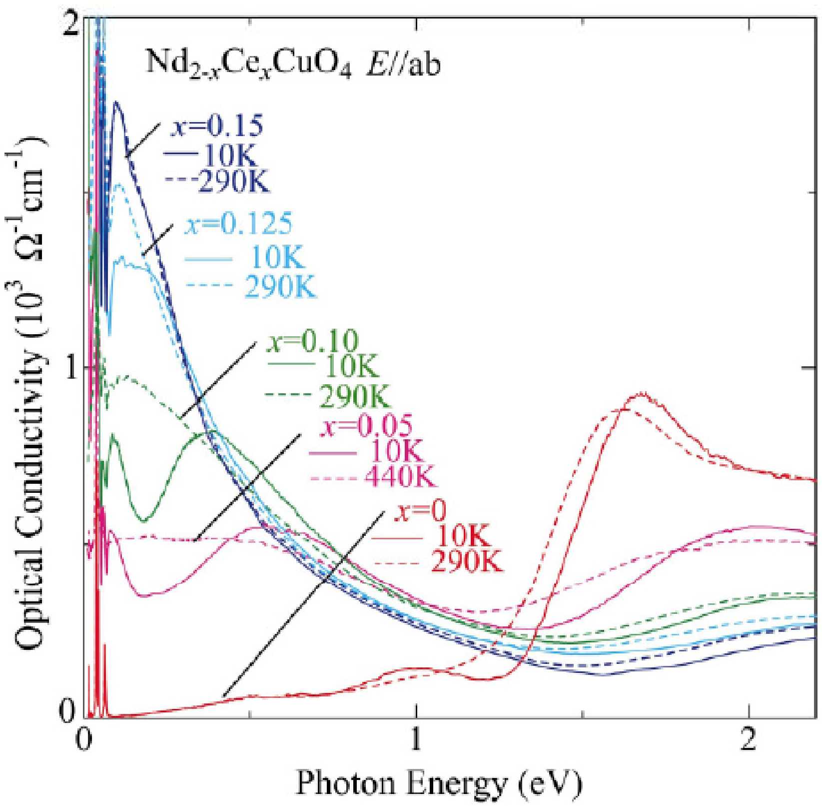
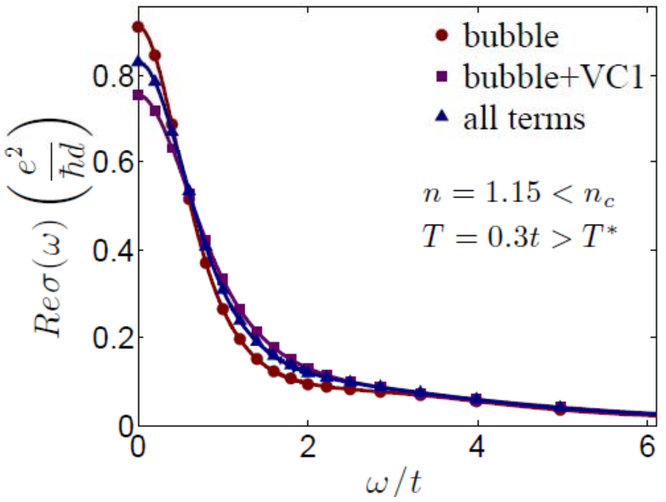
Optical conductivity in NCCO

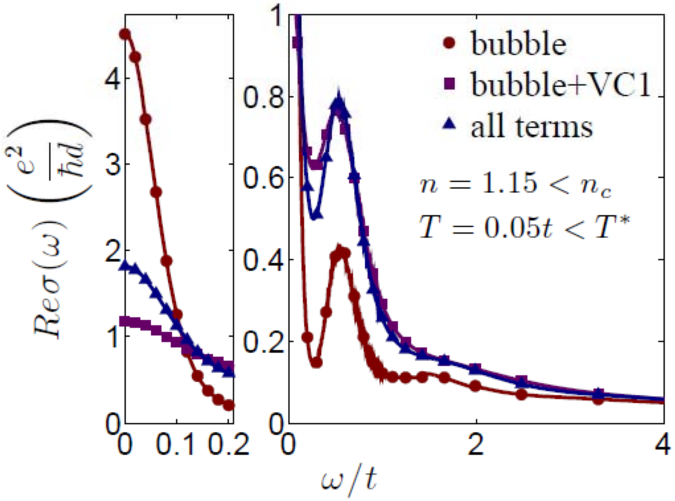


Y. Onose *et al.*, Phys. Rev. B, 69, 24504 (2004)

Optical conductivity $n < n_c$ and $n > n_c$

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





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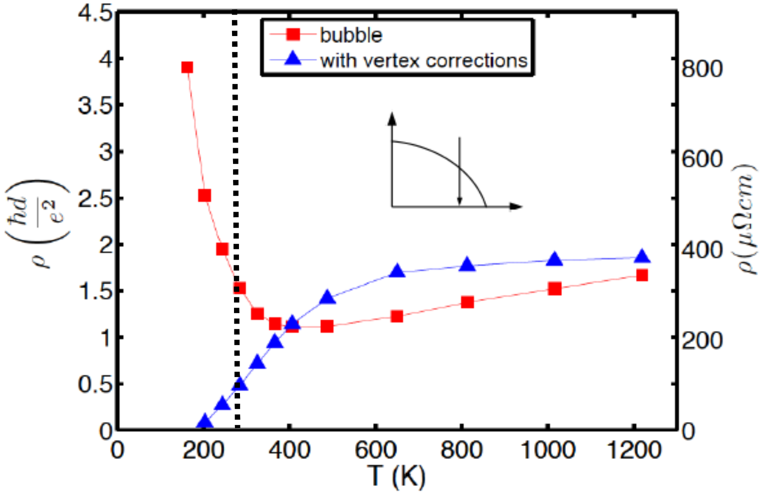
Results : DC resistivity

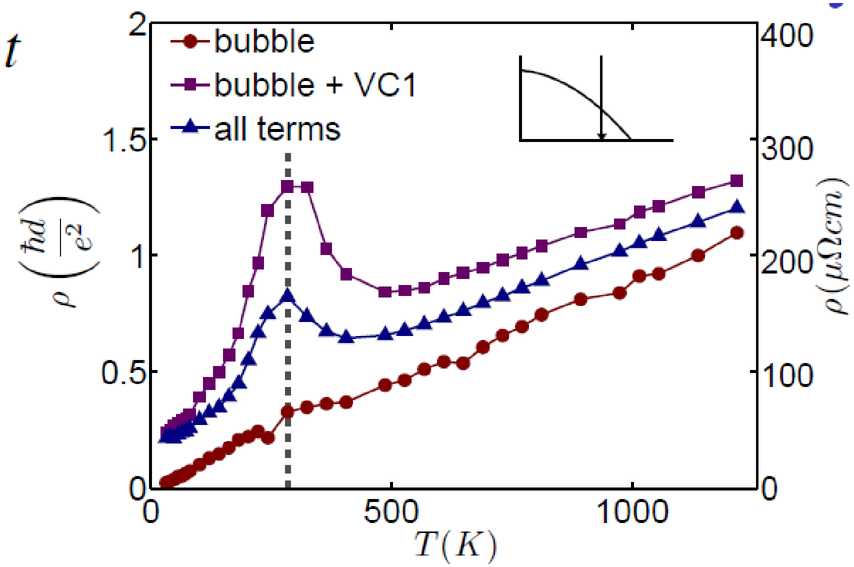
Entering the pseudogap

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

U=6t, t'=0

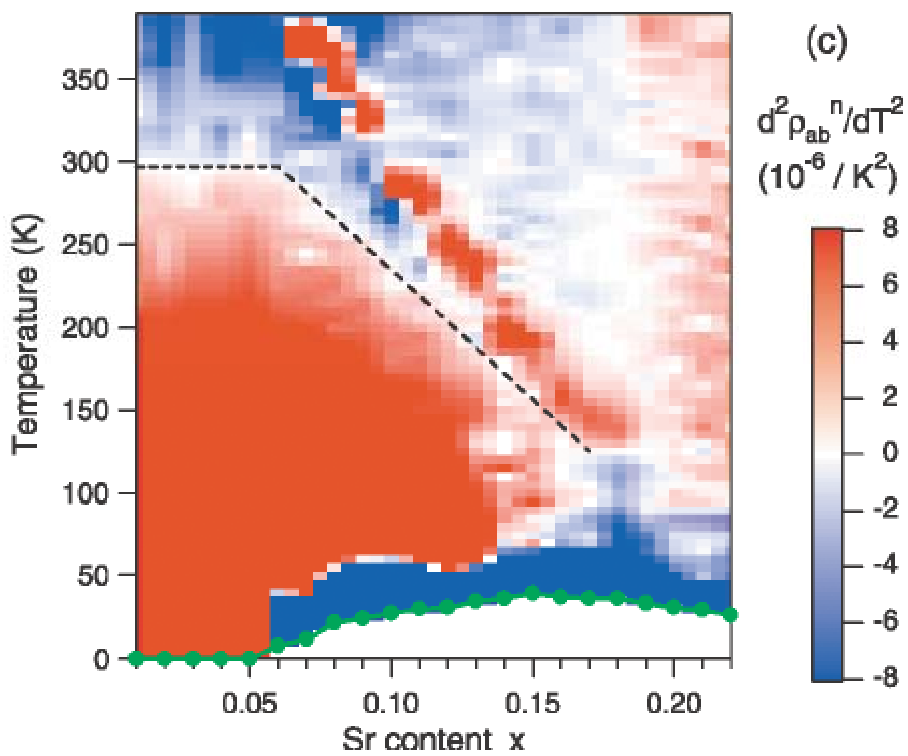
$p = 0.15$



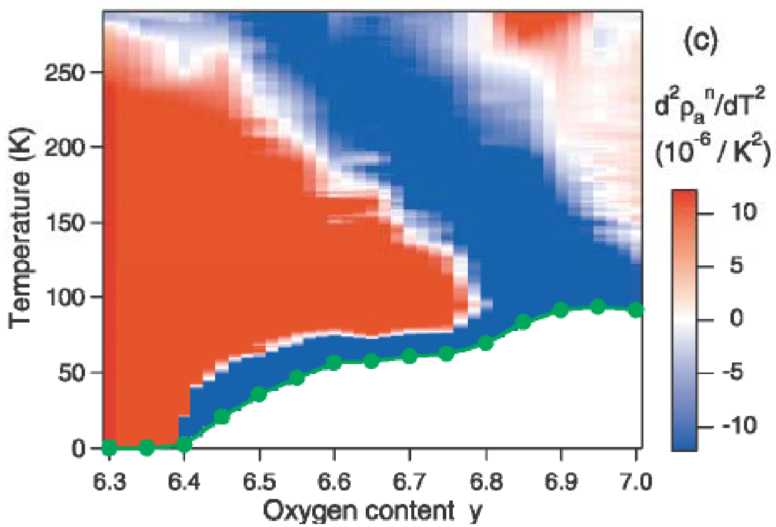


$(t = 0.35eV \text{ and } d = 5\text{Å})$

Curvature maps



LSCO



YBCO

Ando et. Al. PRL **93,** 267001 **(2004)**

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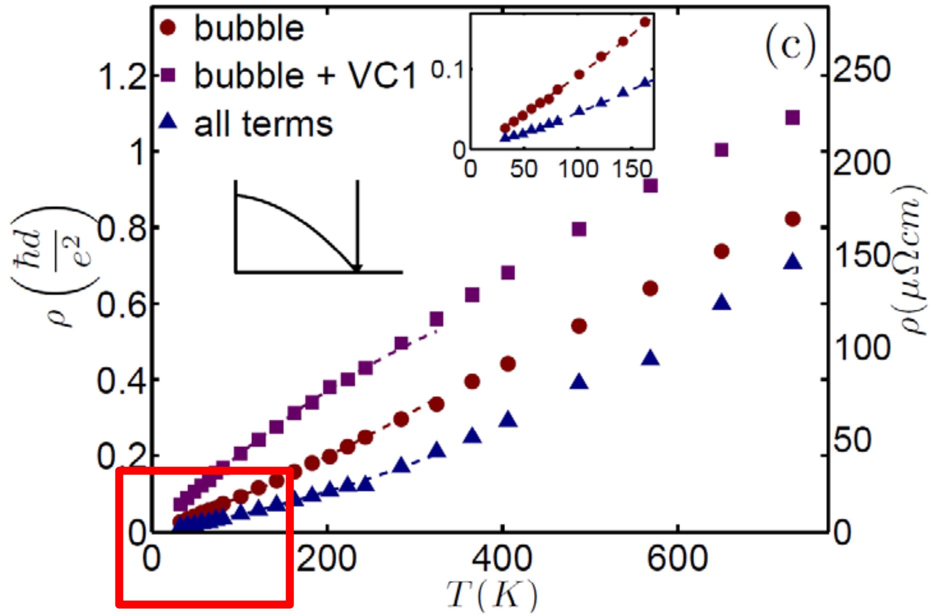
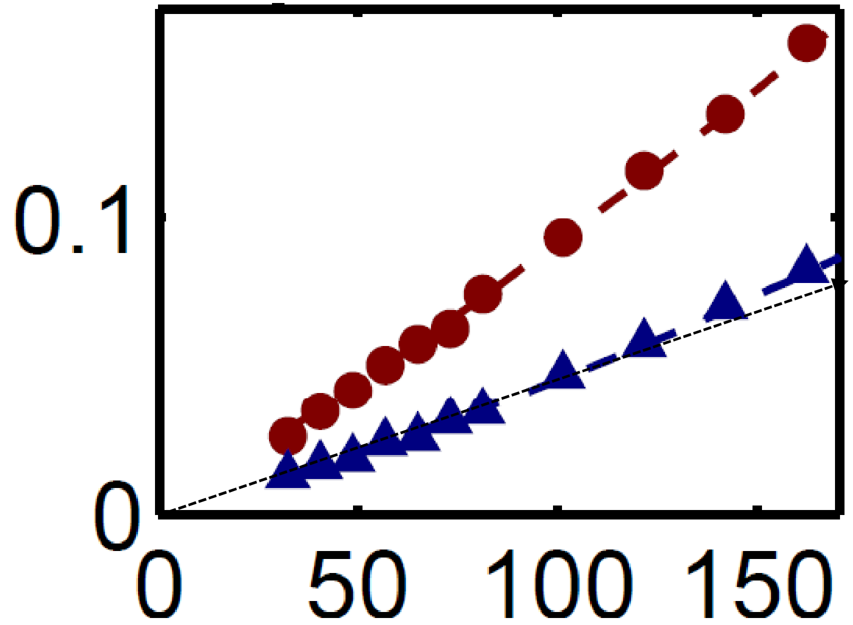
At the quantum critical point

U=6t, t'=0





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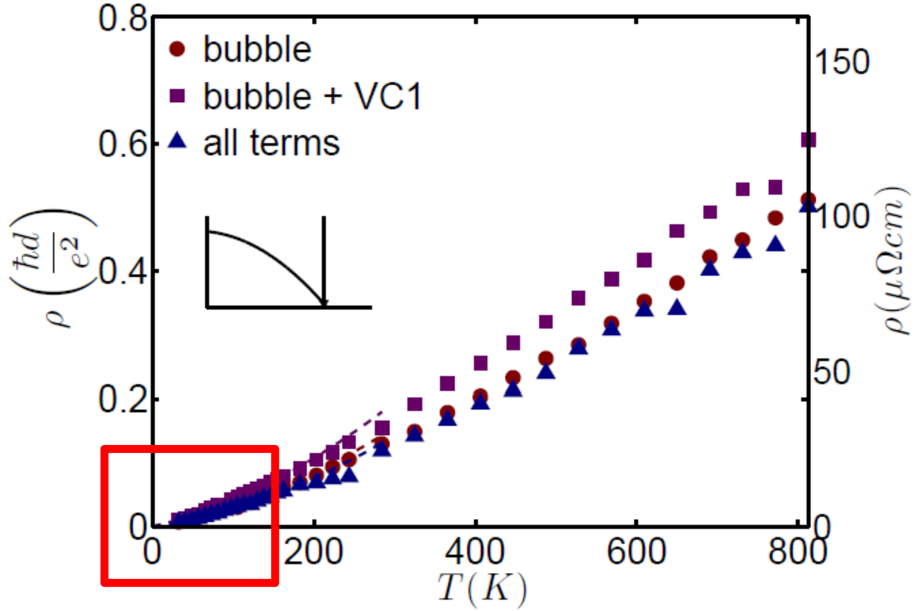
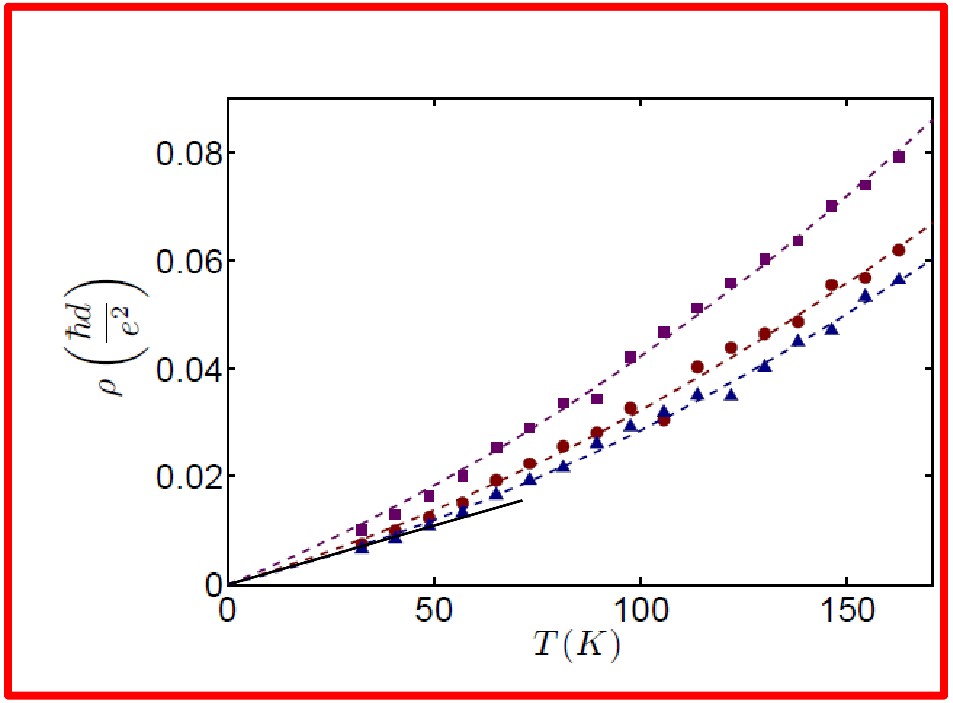
At the QCP for finite *t'*

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





$$\rho(T) = AT + BT^2$$

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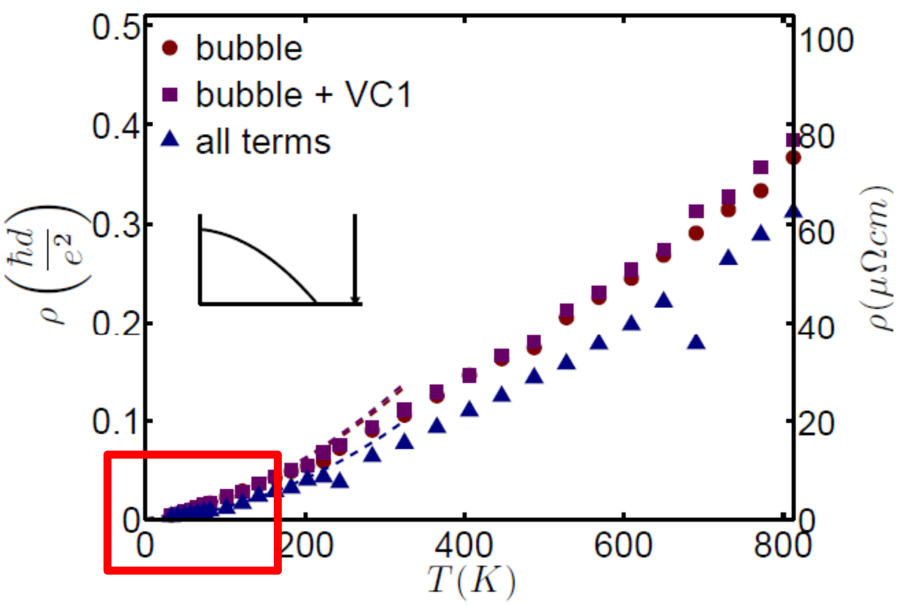
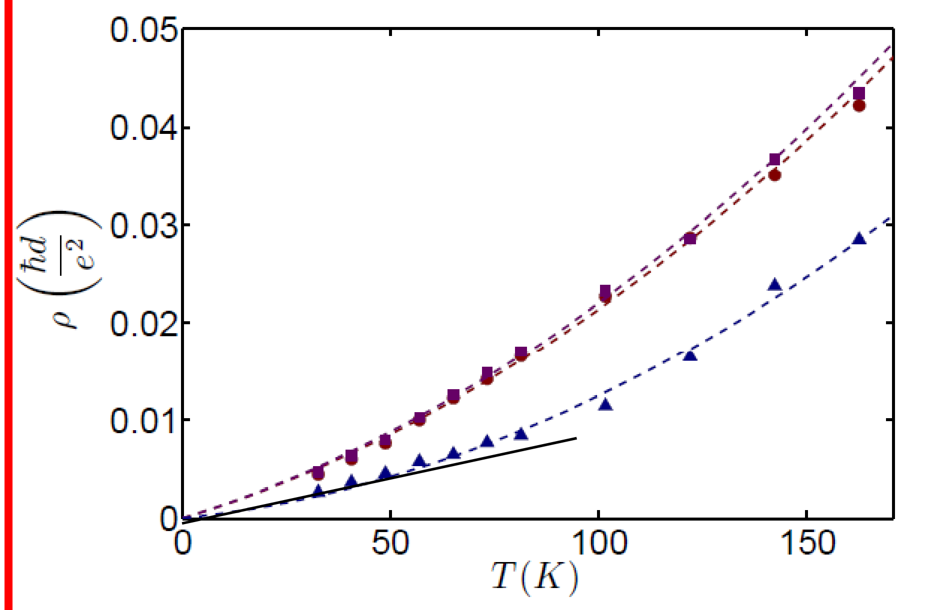
Right of the QCP

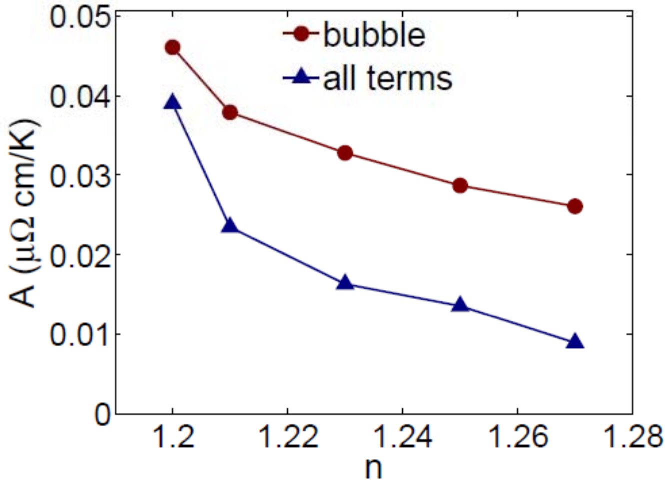
$$U = 6t,\ t' = -0.175t,\ t'' = 0.05t$$

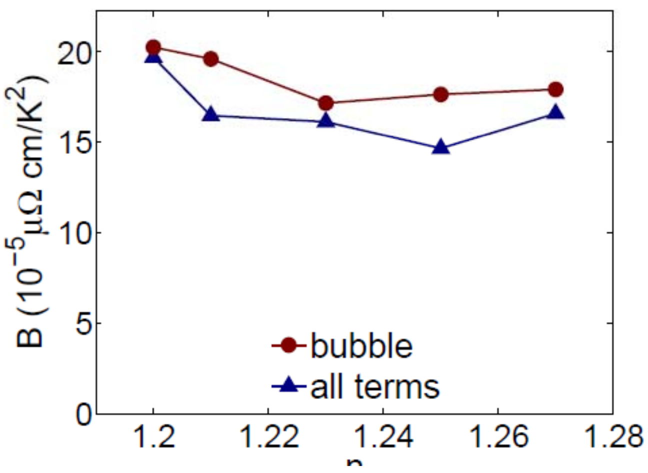




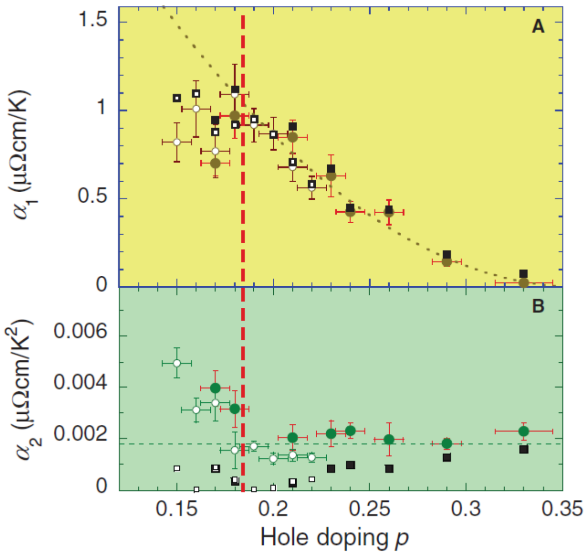
Linearity for $n > n_c$ and T_c

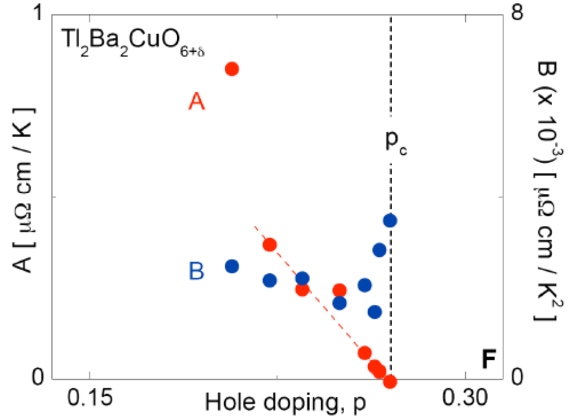
Fitting $\rho(T) = AT + BT^2$ for all dopings:





Cooper et al. Science **323** 30 (2009)





Doiron-Leyraud et al. arXiv:0905.0964

Doiron-Leyraud et al. Phys. Rev. B **80**, 214531 (2009)

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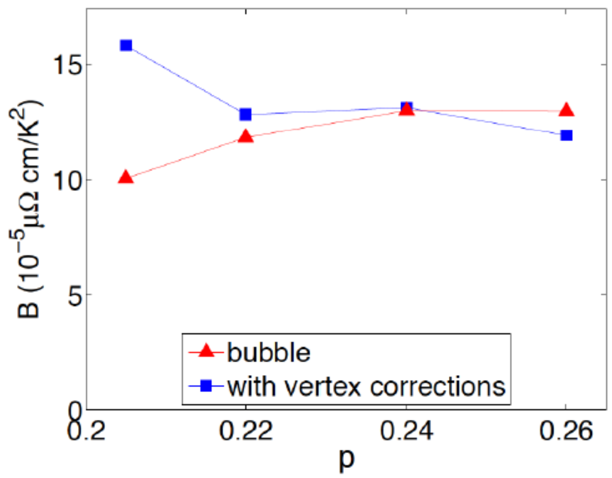
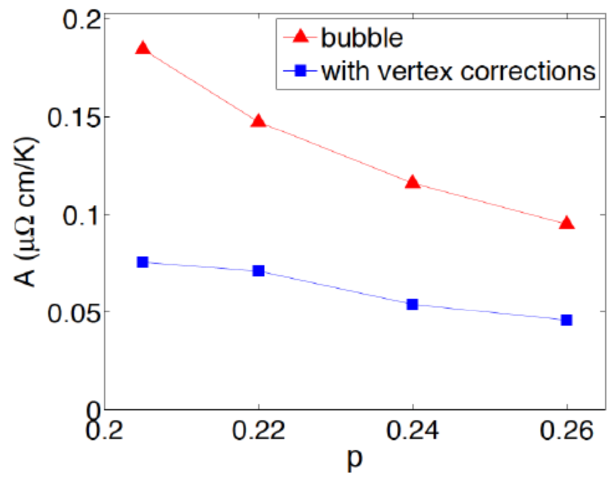
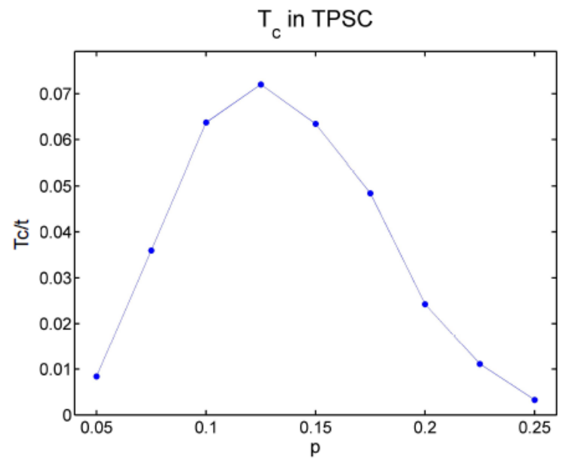
Linearity for $n > n_c$ *and* T_c

$U = 6t,\ t' = 0$

By fitting $\rho(T) = AT + BT^2$ for all dopings:



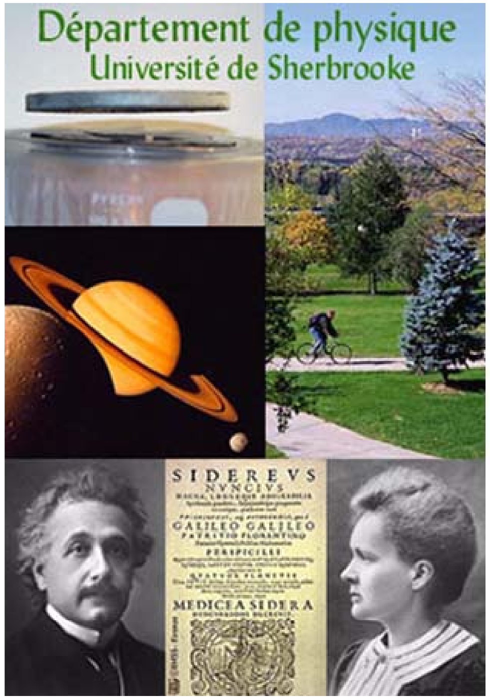




Kyung et al. PRB 68, 174502

Conclusion

- Calculation: No-QP. Ioffe-Regel saturation
  - Hubbard bands necessary to violate MIR limit
- Vertex corrections are important close to half-filling.
  - They have non-universal effect
  - Less important away from QCP. Do not remove linearity (universal).
- Linear term decreases with *n* and disappears with SC
- Optical conductivity has mid-infrared peak.



André-Marie Tremblay

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Thanks…

Merci