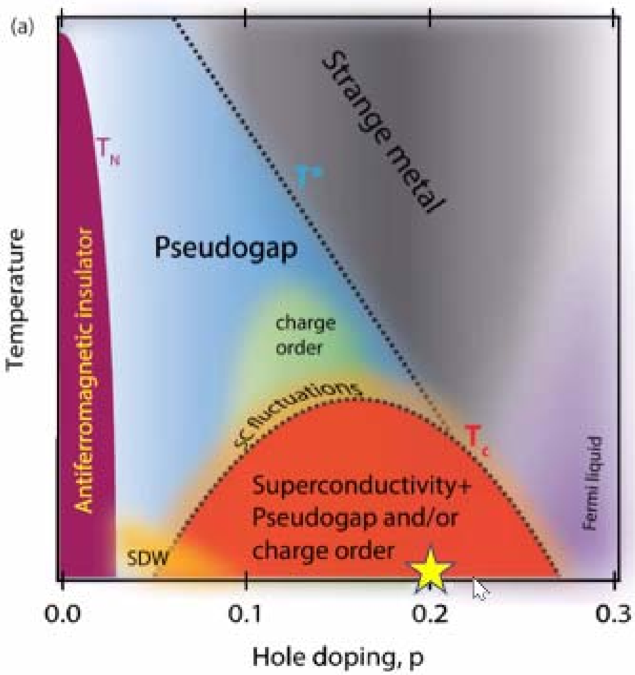
A unified theoretical perspective on the cuprate phase diagram

A.-M.S. Tremblay

Harvard CMSA, high-T_c series
May 12, 10:30

Institut quantique

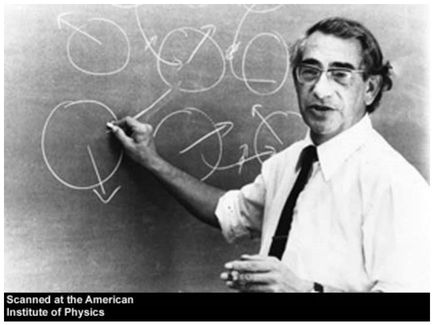
- Who ordered this?



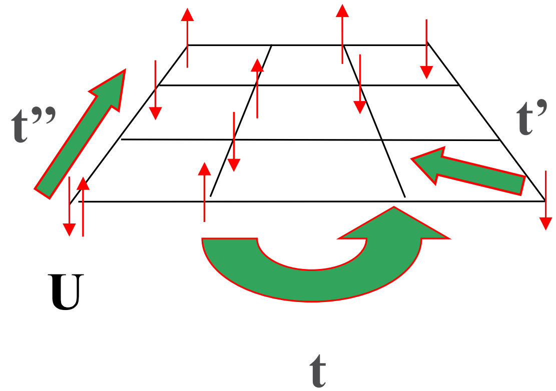
Vishik, Rep. Prog. Phys. (2018)

- Mott insulator
- Pseudogap
- Strange metal
- Quantum critical point (QCP)
- Superconductivity in the presence of strong repulsion
- Competing ground states

Hubbard model

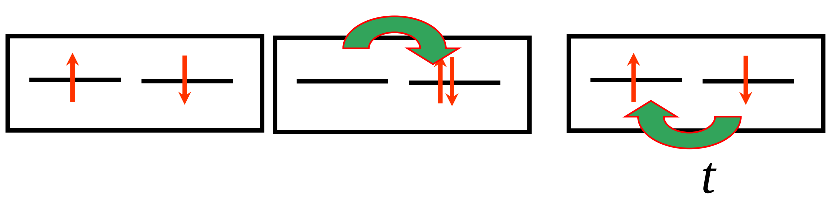


μ



1931-1980

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

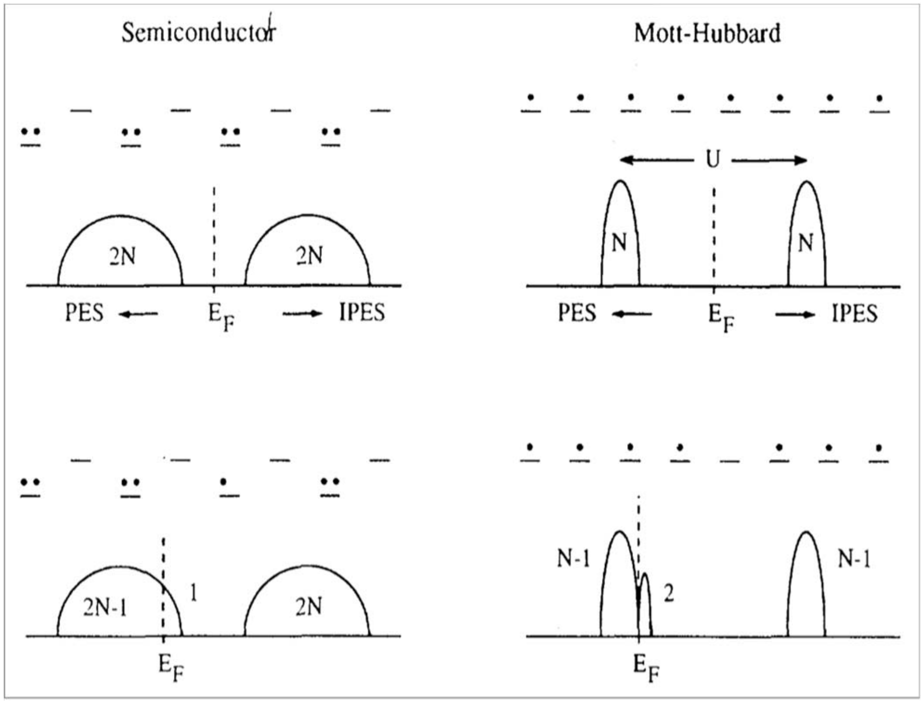


Effective model, Heisenberg: $J = 4t^2/U$

Attn: Charge transfer insulator

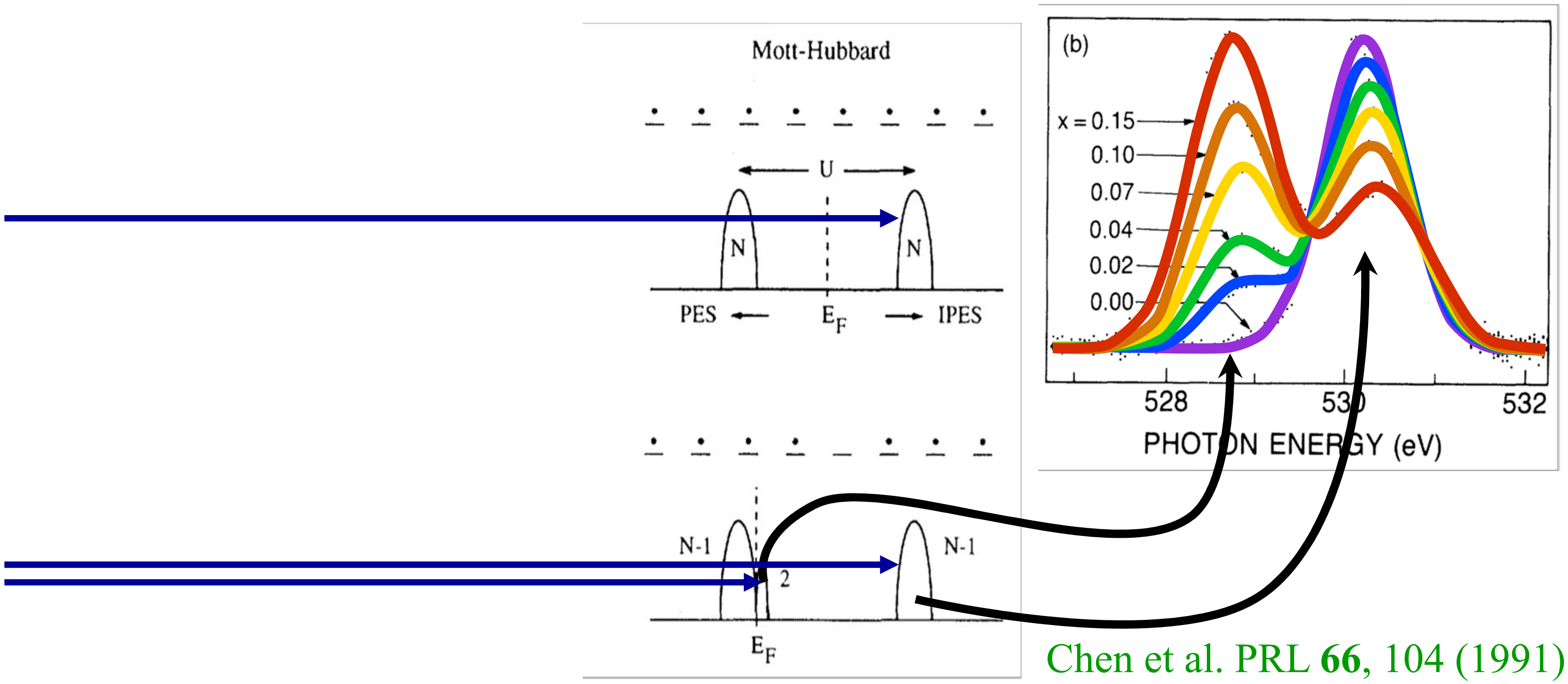
Mott Insulator : X-Ray absorption

Meinders *et al.* PRB **48**, 3916 (1993)



Mott Insulator : X-Ray absorption

Meinders *et al.* PRB **48**, 3916 (1993)



Chen et al. PRL **66**, 104 (1991)

Take home messages

- Most of the main features of the phase diagram follow from the Hubbard model.
- This physics is continuously connected to the Mott transition at half-filling
- We need to look beyond traditional tools of solid state physics to work this out.

Outline

- Method

- One-band Hubbard model
  - Pseudogap
  - Quantum Critical Point
  - d-wave superconductivity

- Three-band Hubbard model
  - Pseudogap
  - d-wave superconductivity

Method :
The precursors

Hohenberg-Kohn : Exchange correlation

Kohn-Sham : Basis set

Density Functional Theory

Method

Metzner, Vollhardt PRL **62**, 324 (1989)
Georges, Kotliar, PRB **45,** 6479 (1992)
Jarrell PRL **69,** 168 (1992)
Review: Georges, Kotliar, Krauth, Rozenberg, RMP **68**, 13 (1996)

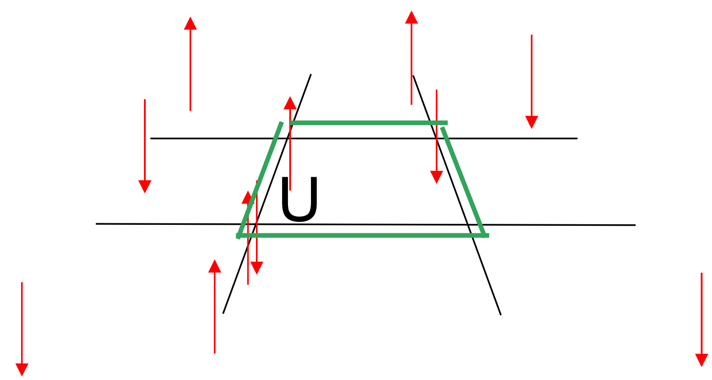
Dynamical Mean-Field Theory : DMFT

For additionnal physical intuition: Compare with more analytical approaches

- Pseudogap
  - Wei Wu, Scheurer, Chatterjee, Sachdev, Georges, Ferrero PRX 8, 021048 (2018)
  - Scheurer, Chatterjee, Wu, Ferrero, Georges, Sachdev, PNAS **115**, E3665 (2018).

Localized and delocalized pictures

Localized



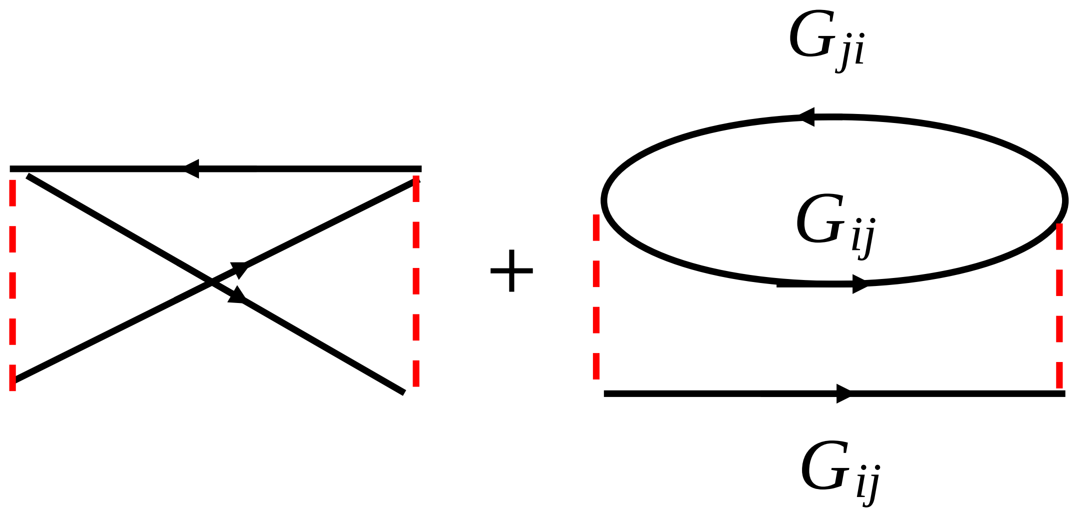
Lichtenstein *et al.*,PRB 2000
Kotliar *et al.*, PRB 2000
M. Potthoff, EJP 2003

$$(G^{-1})_{ij} = (G_0^{-1})_{ij} - \Sigma_{ij}$$

REVIEWS
Maier, Jarrell et al., RMP. (2005)
Kotliar *et al.* RMP (2006)
AMST *et al.* LTP (2006)

Skeleton expansion for the Anderson impurity problem

$\Sigma_{ij} =$

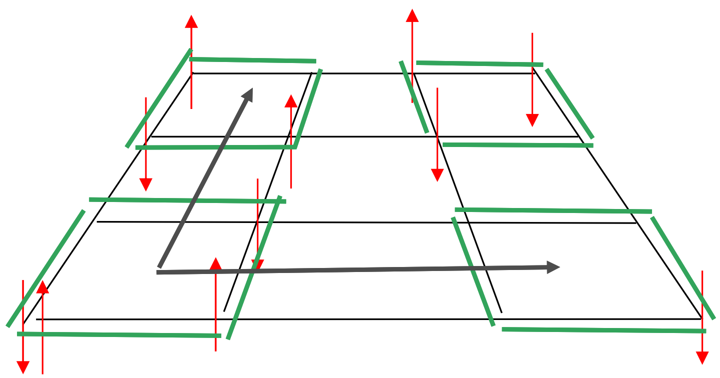


$+ \ldots$

$$(G^{-1})_{ij} = (G_0^{-1})_{ij} - \Sigma_{ij}$$

Localized and delocalized pictures

Delocalized

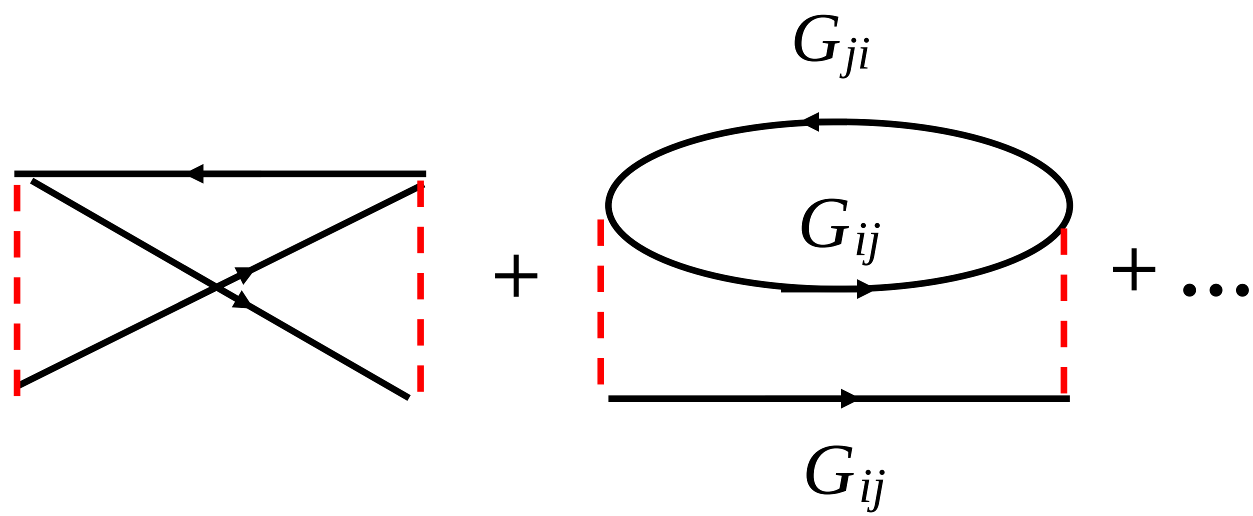


$$\mathbf{R} \longrightarrow \tilde{k}$$

$$G_{ij}\left(\tilde{k}\right) = \left(\frac{1}{(i\omega_n+\mu)I-\varepsilon\left(\tilde{k}\right)-\Sigma}\right)_{ij}$$

Skeleton expansion for the connected clusters

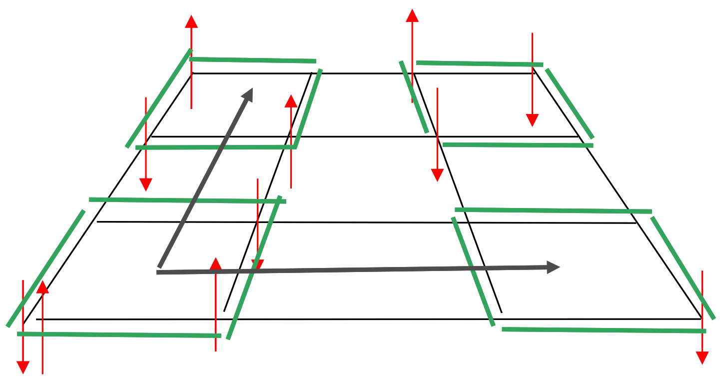
$$\Sigma_{ij} =$$



$$G_{ij}\left(\widetilde{k}\right) = \left(\frac{1}{(i\omega_n+\mu)I-\varepsilon\left(\widetilde{k}\right)-\Sigma}\right)_{ij} \longrightarrow G_{ij} = \int \frac{d^d\widetilde{k}}{(2\pi)^d} G_{ij}\left(\widetilde{k}\right)$$

Localized and delocalized pictures C-DMFT

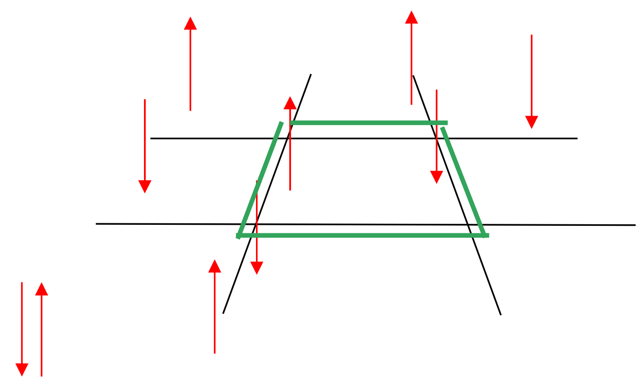
Delocalized



$$\mathbf{R} \rightarrow \tilde{k}$$

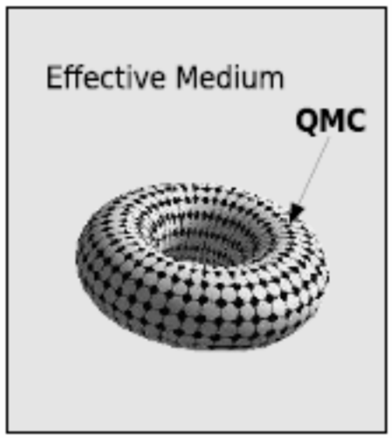
$$G_{ij} = \int \frac{d^d\tilde{k}}{(2\pi)^d} \left(\frac{1}{(i\omega_n+\mu)I-\varepsilon(\tilde{k})-\Sigma} \right)_{ij}$$

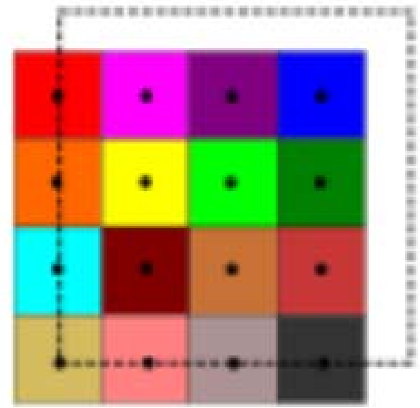
Localized



$$(G^{-1})_{ij} = (G_0^{-1})_{ij} - \Sigma_{ij}$$

Dynamical cluster approximation (DCA)

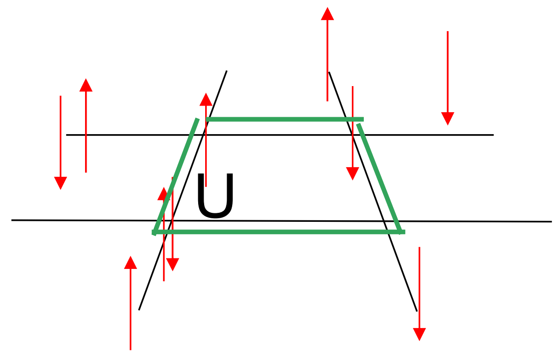




Hettler …Jarrell…Krishnamurty PRB **58** (1998)

Impurity solvers

Impurity solver (Exact diagonalisation)



Caffarel, Krauth, PRL **72** 1545 (1994)

QCM David Sénéchal

Impurity solver : continuous-time quantum Monte Carlo

$$Z = \int \mathcal{D}[\psi^\dagger, \psi]\, \mathrm{e}^{-S_c - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{\mathbf{K}} \psi^\dagger_{\mathbf{K}}(\tau)\Delta_{\mathbf{K}}(\tau,\tau')\psi_{\mathbf{K}}(\tau')}$$

Hybridization expansion :

Werner Millis PRB **74**, 155107 (2006)
Werner Millis B **75**, 085108 (2007)
Haule, PRB **75**, 155113 (2007)
Sémon, Sordi, AMST PRB **89**, 165113 (2014)
Sémon, Yee, Haule, AMST PRB **90**, 075149 (2014)

triqs **ALPSCore / CT-HYB** **iQIST** **ComCTQMC**

Impurity solver : continuous-time quantum Monte Carlo

$$S = \int_0^\beta \mathrm{d}\tau \mathrm{d}\tau' \sum_{\sigma=\uparrow,\downarrow} \xi^*_\sigma(\tau) \left[g^{-1}_{0\sigma}(\tau-\tau') \right] \xi_\sigma(\tau') + U \int_0^\beta \mathrm{d}\tau \left(n_\uparrow(\tau) n_\downarrow(\tau) - \frac{n_\uparrow(\tau) + n_\downarrow(\tau)}{2} \right)$$

CT-AUX : Gull, Werner, Parcollet, Troyer, 2008, Europhys. Lett. **82**, 57003 (2008)

DCA++

Review of these methods

Gull, Millis, Lichtenstein, Rubtsov, Troyer, Werner RMP **83,** 349 (2011)

Some groups using these methods for cuprates

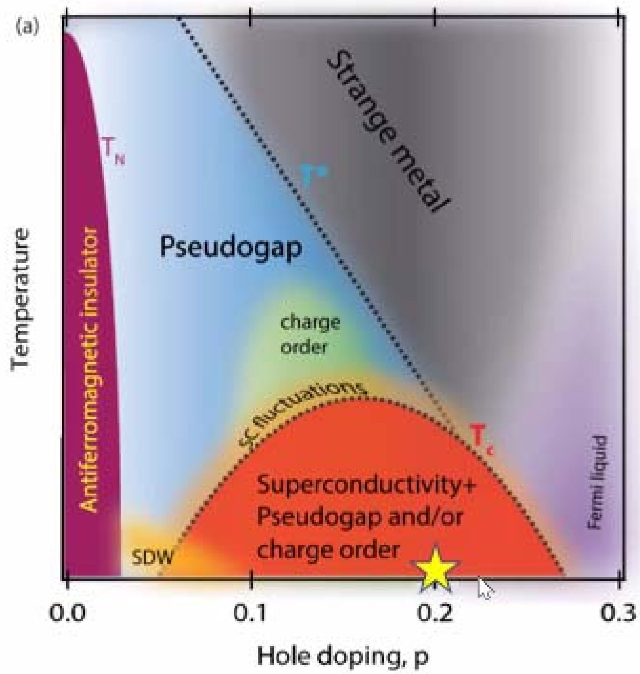
- Europe:
  - Georges, Parcollet, Ferrero, Civelli, Wu (Paris)
  - Lichtenstein, Potthoff, (Hamburg) Aichhorn (Graz), Liebsch (Jülich) de Medici (Grenoble) Capone (Italy)
- USA:
  - Gull (Michigan) Millis (Columbia)
  - Kotliar, Haule (Rutgers)
  - Jarrell (Louisiana)
  - Maier, Okamoto (Oakridge)
- Japan
  - Imada (Tokyo) Sakai, Tsunetsugu, Motome

Critique

+ and -

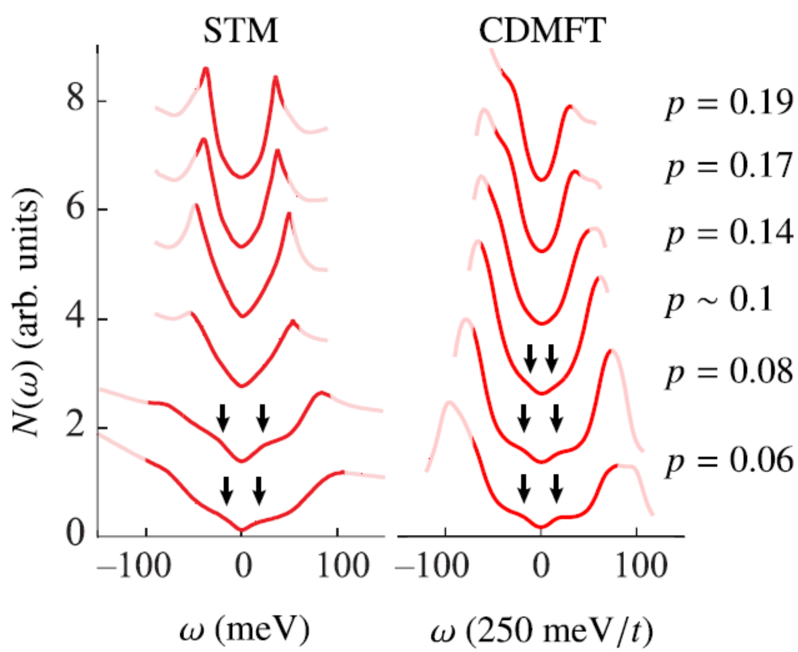
- Long range order:
  - No mean-field factorization on the cluster
  - Symmetry breaking allowed in the bath
- Included exactly:
  - Short-range dynamical and spatial correlations

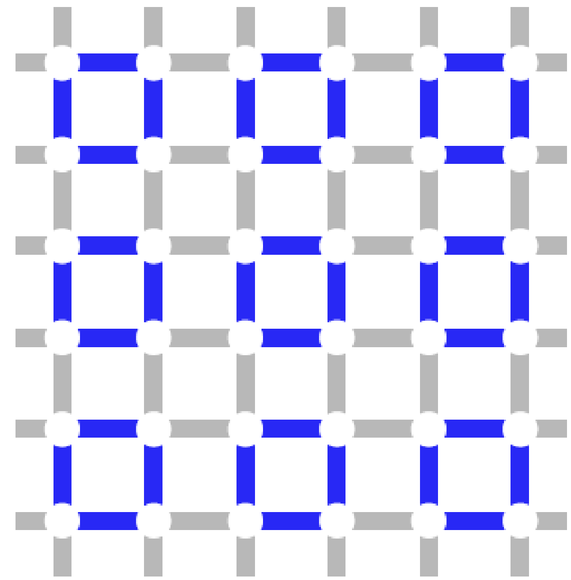
- Missing:
  - Long wavelength p-h and p-p fluctuations
  - Hence good when the correponding correlation lengths are small



Vishik, Rep. Prog. Phys. (2018)

Possible artefacts





Verret, Roy, Foley, Charlebois, Sénéchal, A.-M.S.T, RPB **100**, 224520 (2019)

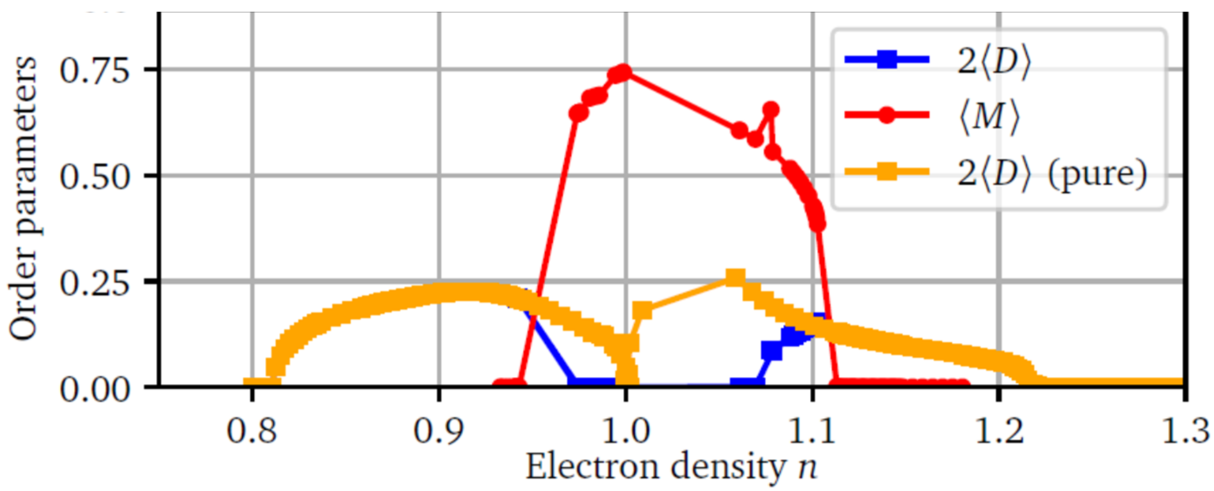
STM Kohsaka, … Davis, Nature (London) **454**, 1072 (2008).

What to do

- Exact in the infinite size limit of the cluster
  - Compare different cluster sizes
  - Compare real-space (CDMFT) and momentum space (DCA) clusters

A bird's eye overview of the *T = 0* phase diagram

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



A. Foley *et al.* Phys. Rev. B **99**, 184510 (2019)
S. S. Kancharla, *et al.* Phys. Rev. B **77**, 184516 (2008)
D. Sénéchal, *et al.* Phys. Rev. Lett. **94**, (2005)
M. Jarrell *et al.* EPL **56** 563, (2001)

CDMFT 4 sites

Competing ground states

PHYSICAL REVIEW X **10,** 031016 (2020)

Absence of Superconductivity in the Pure Two-Dimensional Hubbard Model

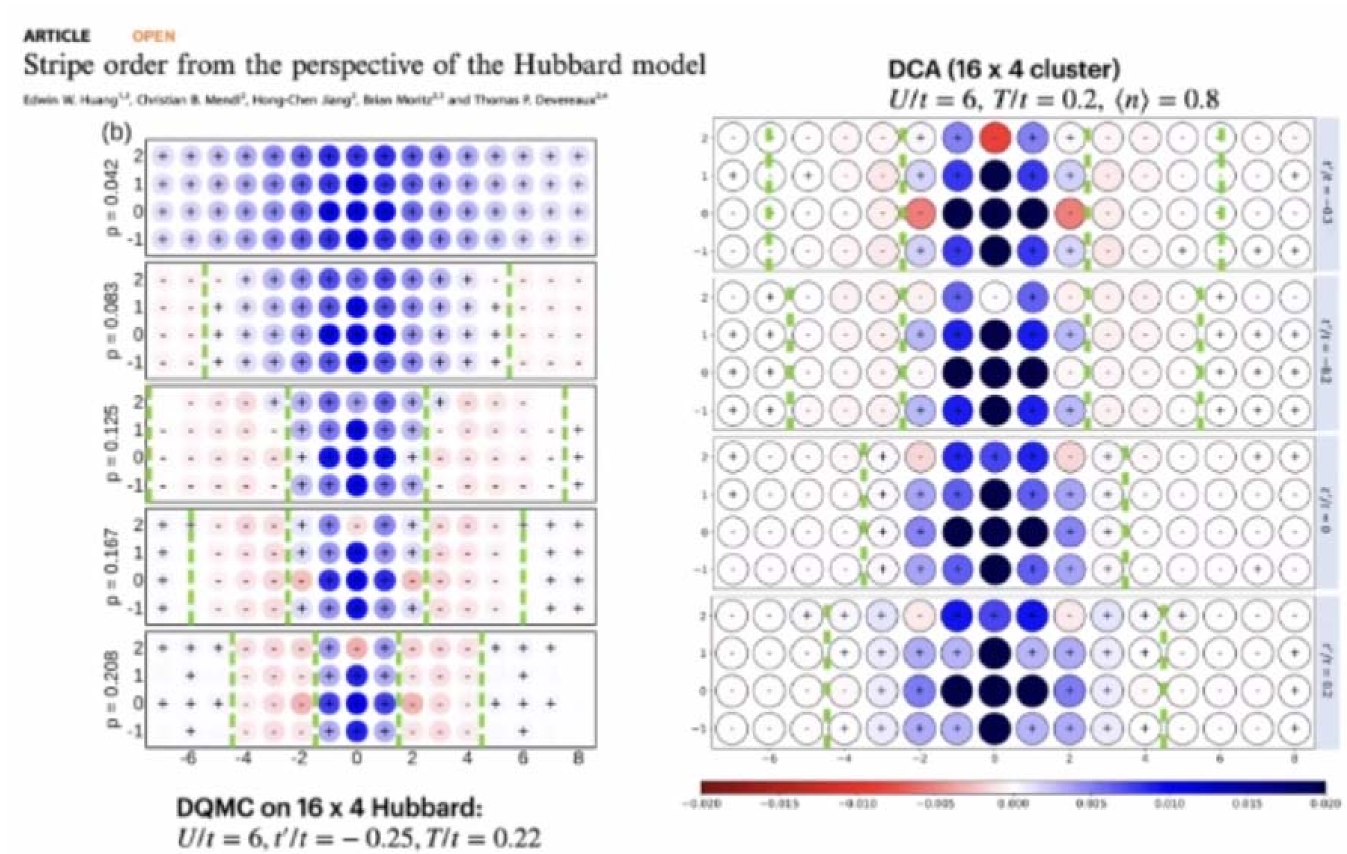
Mingpu Qin,[1,2,*] Chia-Min Chung,[3,4,*] Hao Shi,[5] Ettore Vitali,[6,2] Claudius Hubig,[7]
Ulrich Schollwöck,[3,4] Steven R. White,[8] and Shiwei Zhang[5,2]

PRL **113,** 046402 (2014) PHYSICAL REVIEW LETTERS week ending 25 JULY 2014

Competing States in the *t*-*J* Model: Uniform *d*-Wave State versus Stripe State

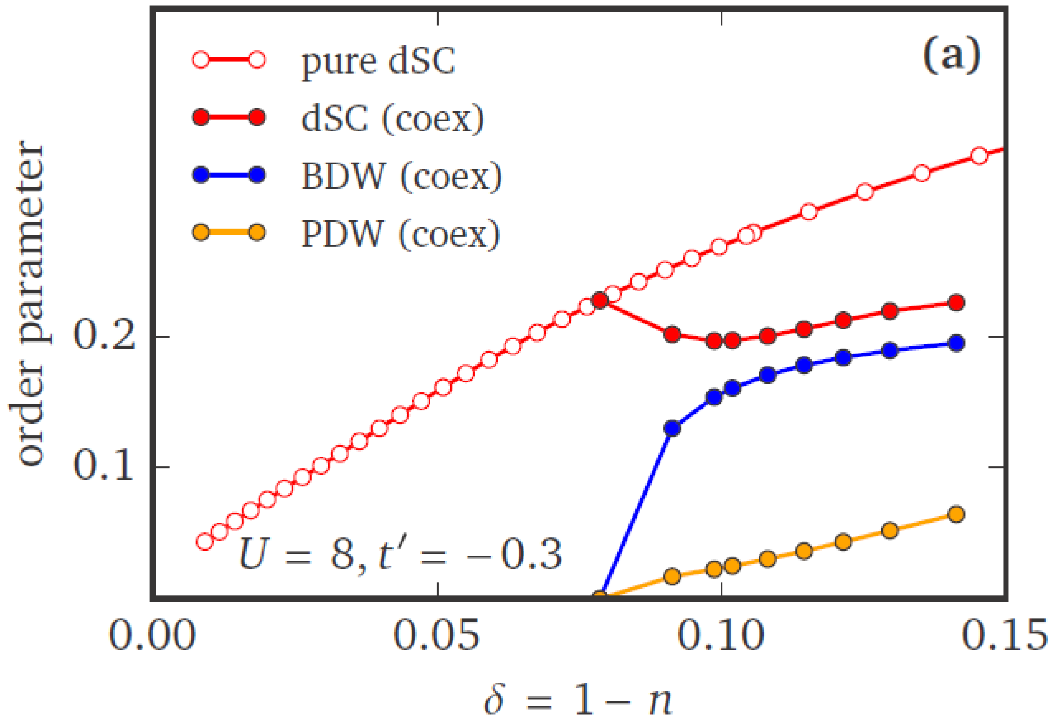
Philippe Corboz,[1,2] T. M. Rice,[1] and Matthias Troyer[1]

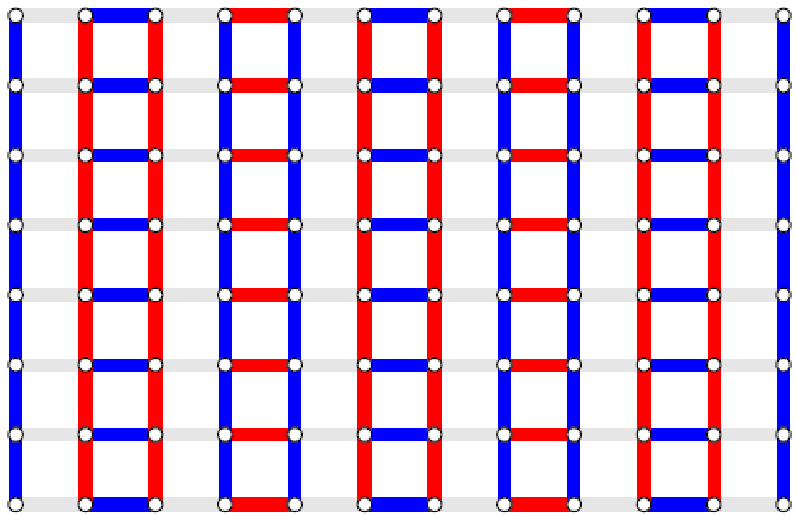
Competing ground states



P. Mai, S. Karakuzu, S. Johnston & TAM, in preparation

Competing states





VCA

Faye Sénéchal, PRB **95** (2017)

Pseudogap


Alexis Reymbaut

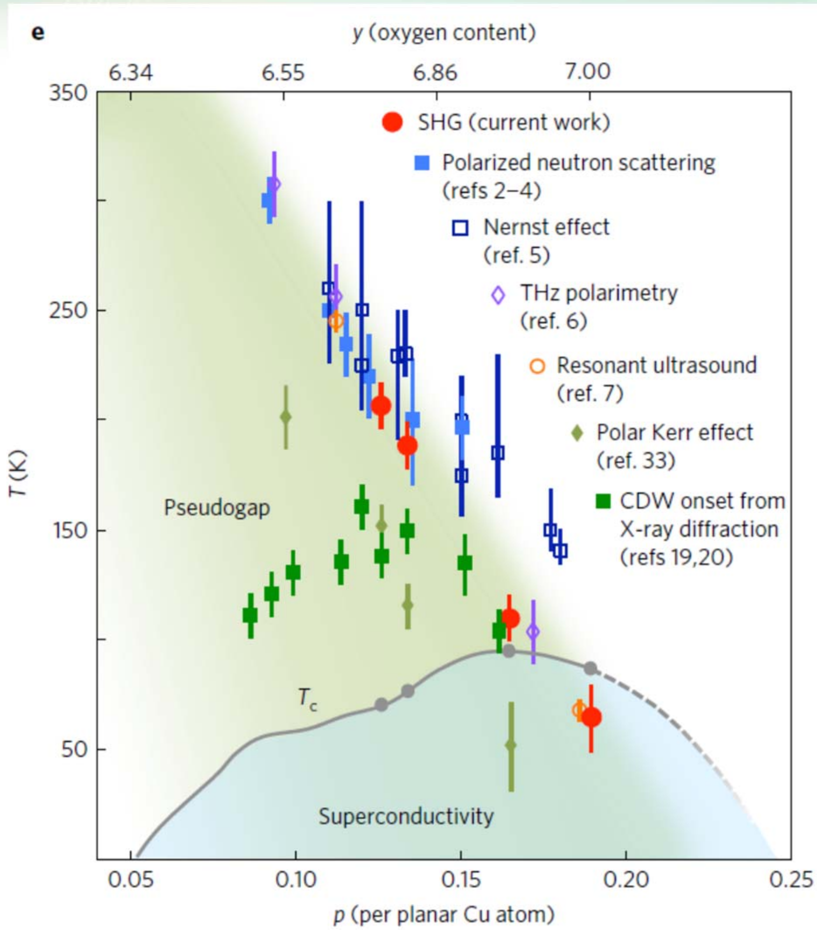

Simon Bergeron


Maxime Charlebois


Patrick Sémon

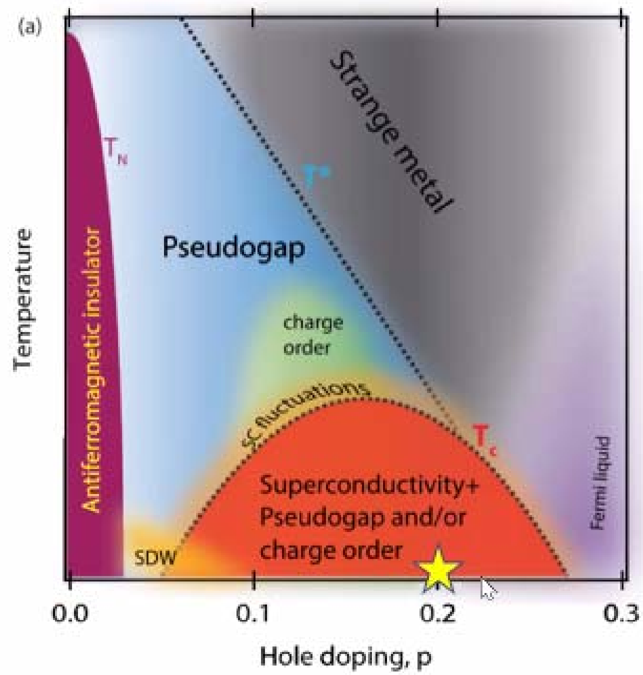

Marion Thénault

Reymbaut, *et al.*
Phys. Rev. Research **1**, 023015 (2019)

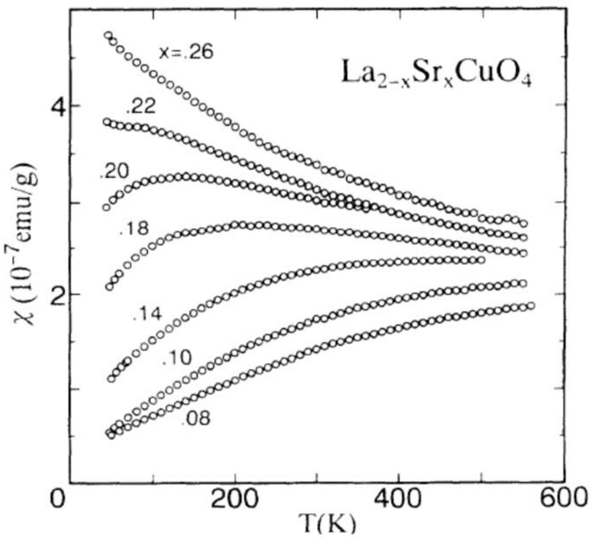


Zhao *et al.* Nat. Phys. 13, 250 (2017).

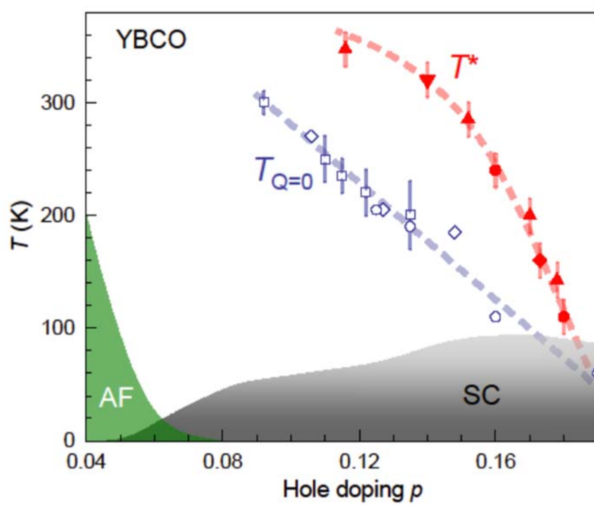
Pseudogap



Vishik, Rep. Prog. Phys. (2018)



Nakano *et al.* Phys. Rev. B **49**, 16000 (1994)
Alloul *et al* (1989)



T^* from NMR Knight shift
Alloul *et al.*
Curro *et al.*
Berthier *et al.*
Julien *et al.*

$T_{Q=0}$ from
Neutron scattering (Bourges *et al.*)
Torque (Matsuda *et al.*)
SHG (Hsieh *et al.*)

Knight shift   (Q=0 spin susceptibility)

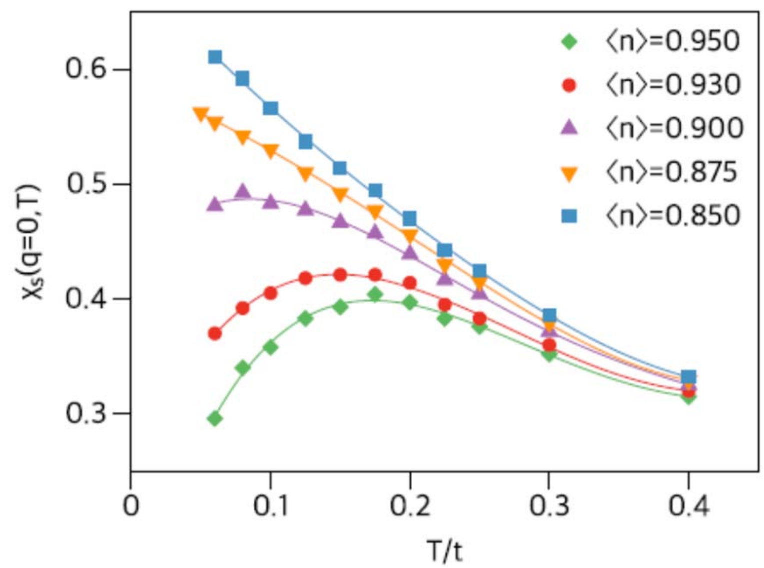
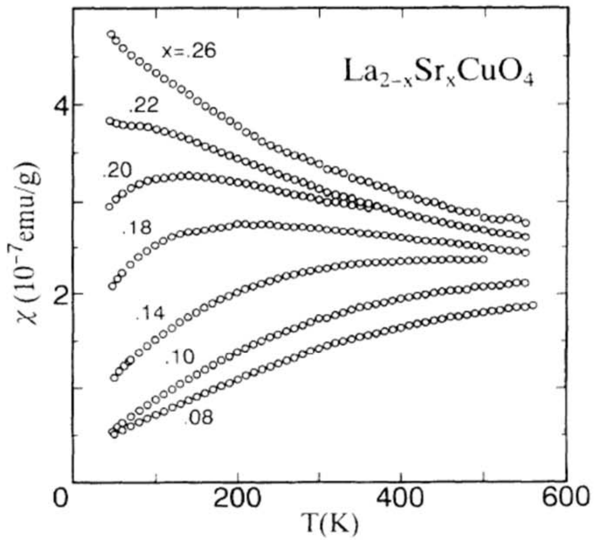


Fig. 3 Temperature and doping dependence of the $q = 0$ spin susceptibility. At the smaller dopings (larger filling $\langle n \rangle$), $\chi_s(T)$ exhibits a peak in the temperature dependence indicating the opening of a PG

DCA 12 sites, *t'=0, U = 7*

T.A. Maier, D.J. Scalapino, npj Quantum Materials (2019)

Comparison



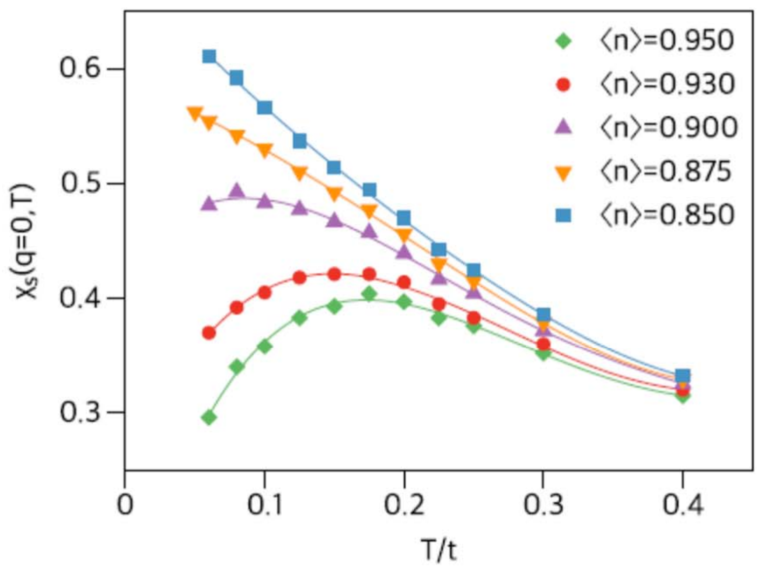
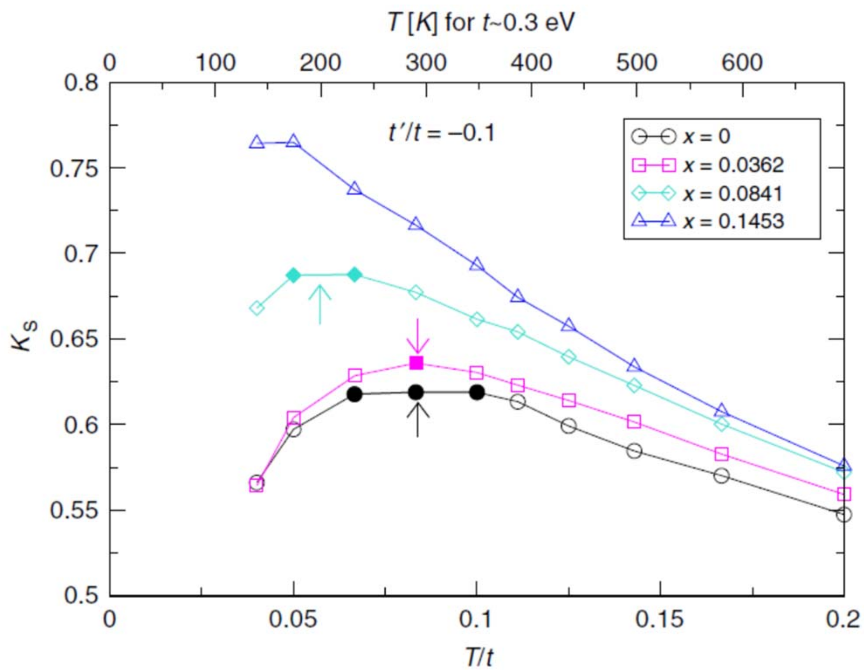


Fig. 3 Temperature and doping dependence of the $q = 0$ spin susceptibility. At the smaller dopings (larger filling $\langle n \rangle$), $\chi_s(T)$ exhibits a peak in the temperature dependence indicating the opening of a PG

Knight shift



DCA 8 sites, *U = 6, t' = -0.1t*

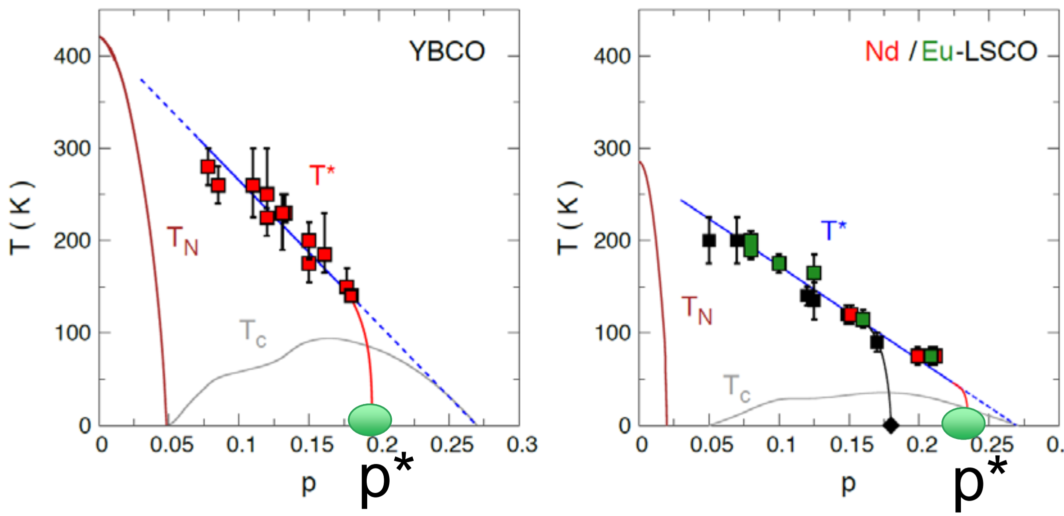
Chen, LeBlanc, Gull, Nature Com. Apr. 2017

See also Jarrell *et al.* 2001, 2002

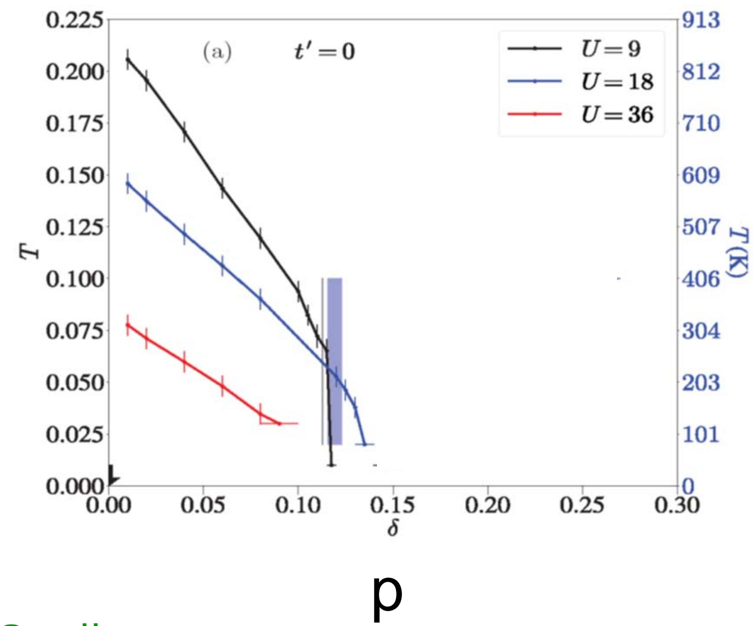
Experiments and *T**

$$\boxed{k_B T^* \sim J}$$

J = 4*t*²/*U*



Cyr-Choinières et al. Phys. Rev. B **97**, 064502

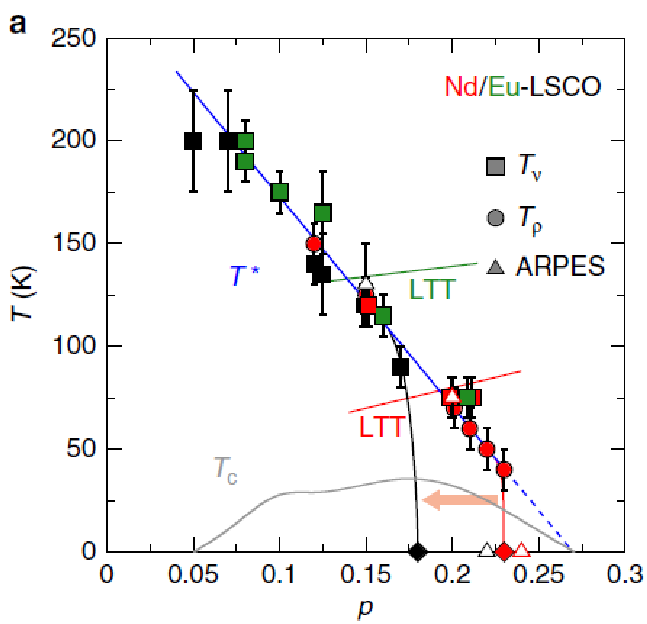


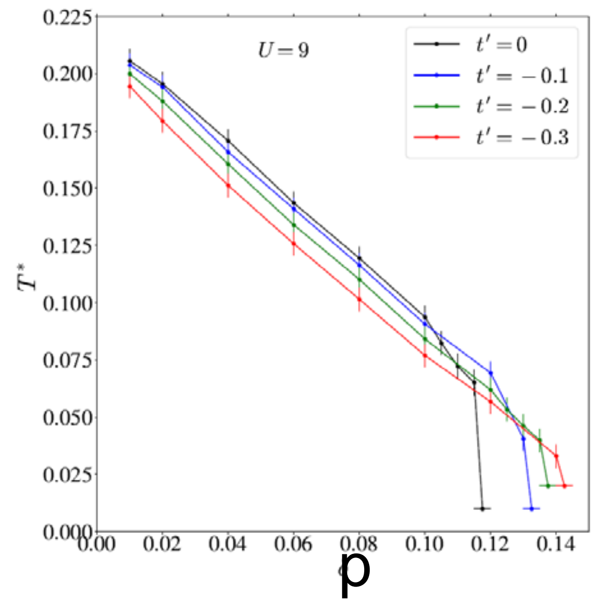
A. Reymbaut, M. Thénault, L. Fratino, G. Sordi,
P. Sémon, AMT, Phys. Rev. Research **1**, 023015 (2019)

W Wu, A Georges, M Ferrero Phys. Rev. X 8, 021048 (2018).

Bragança, Sakai, Aguiar, Civelli, PRL **120**, 067002 (2018)

Results : effect of *t'* on *T**

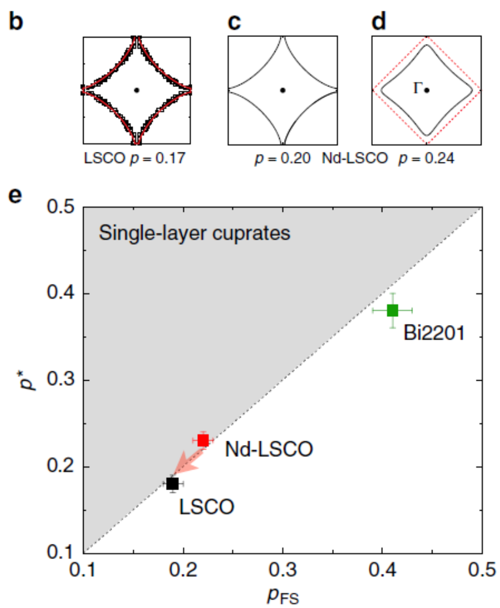


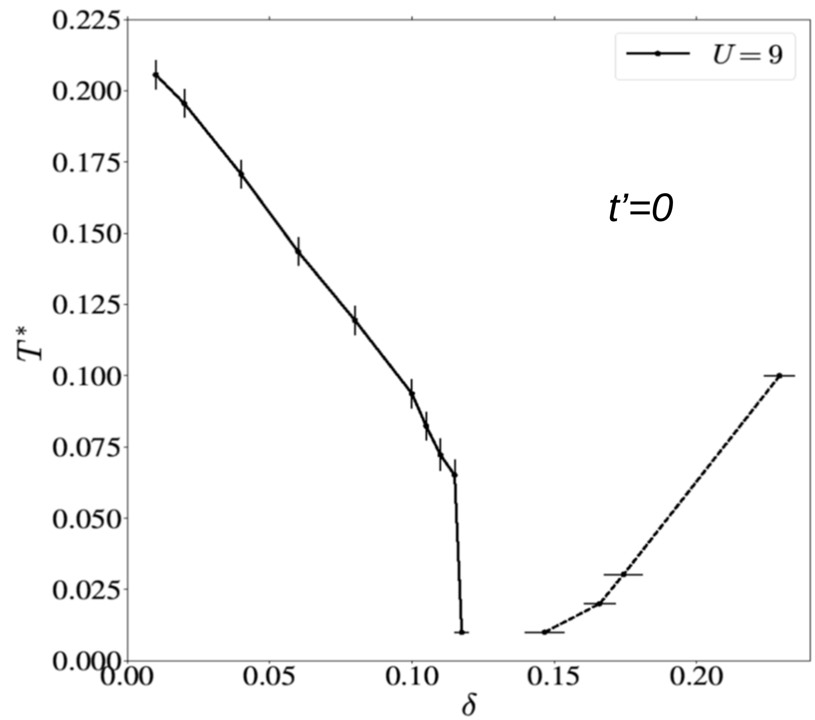


Doiron-Leyraud *et al.*
Nature Comm. **8** 2044

A.Reymbaut, *et al.*
Phys. Rev. Research **1**, 023015 (2019)

Results: van Hove singularity





$p^* < p_{fs}$

p^* p_{fs}

Doiron-Leyraud *et al.*
Nature Comm. **8** 2044

A.Reymbaut, *et al.*
Phys. Rev. Research **1**, 023015 (2019)
W Wu, A Georges, M Ferrero Phys. Rev. X 8, 021048 (2018).

Giovanni Sordi

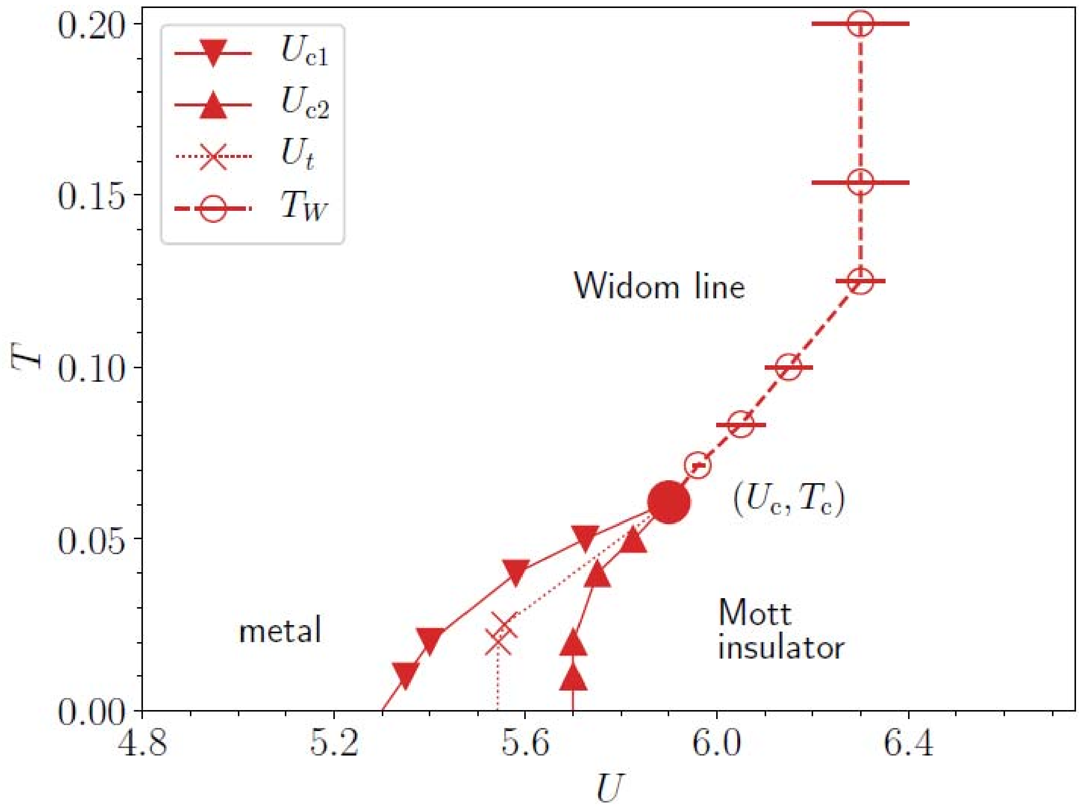
Patrick Sémon

Kristjan Haule

First-order transition, Widom line and Mott physics

G. Sordi, *et al*. Scientific Reports 2, 547 (2012)

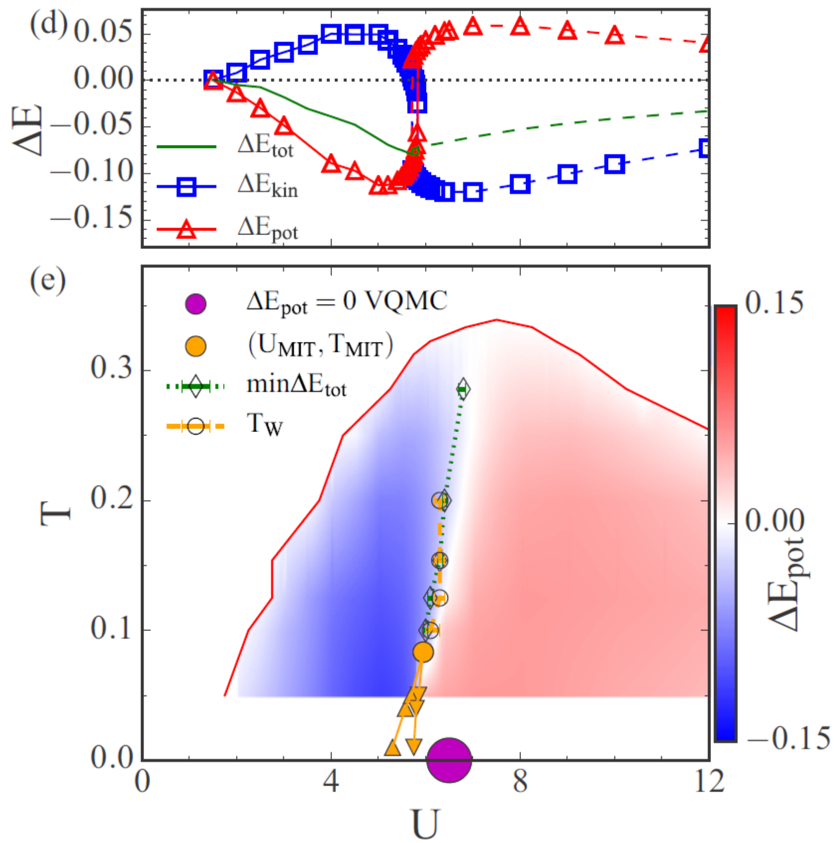
Mott transition at half-filling, CDMFT 2 x 2



Walsh, Sémon, Poulin, G. Sordi, AMST, PRB **99**, 075122 (2019)

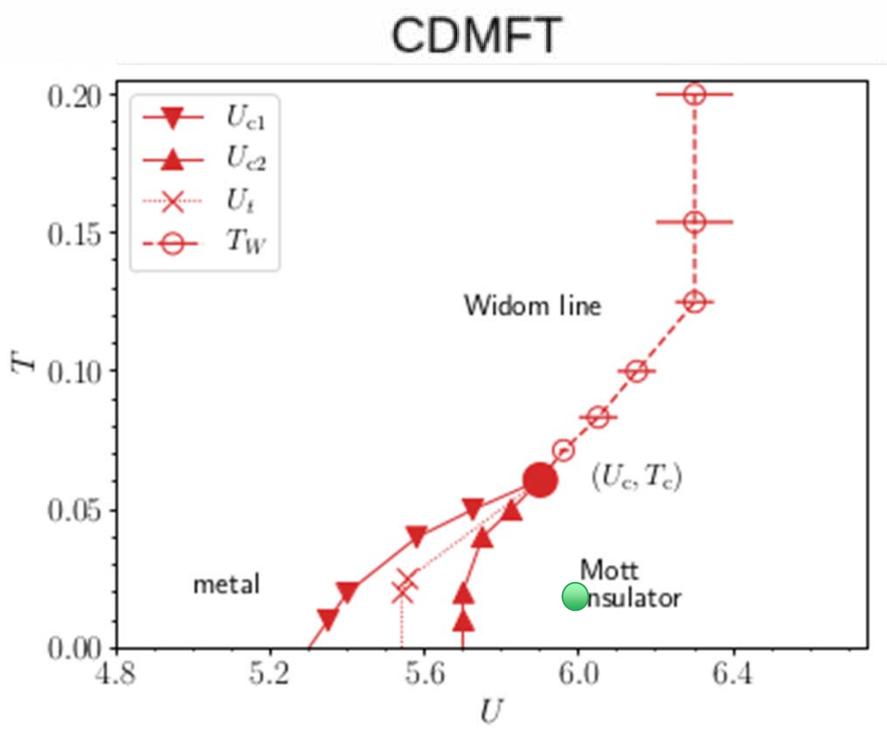
Park, Haule, Kotliar, Phys. Rev. Lett. **101**, 186403 (2008)

Change in potential energy due to large ξ

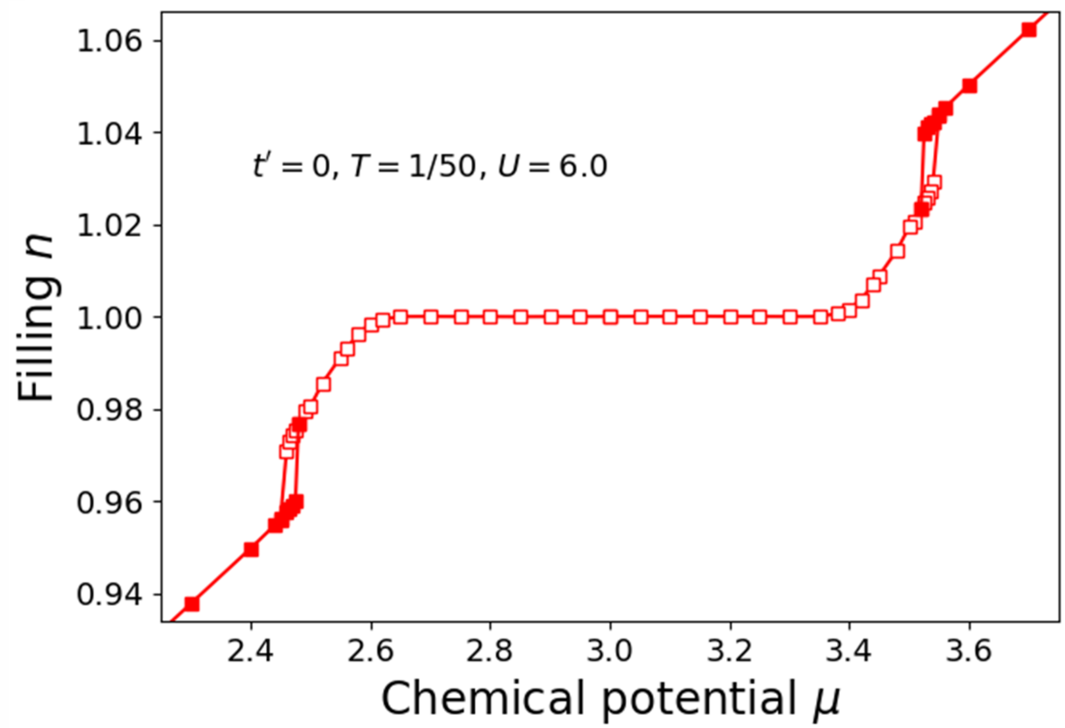


Fratino, Sémon, Charlebois, Sordi, AMST, PRB **95**, 235109 (2017)

Mott and Sordi transition: CDMFT 2 x 2



C. Walsh, Phys. Rev. Lett., 122 : 067203 – Feb 2019



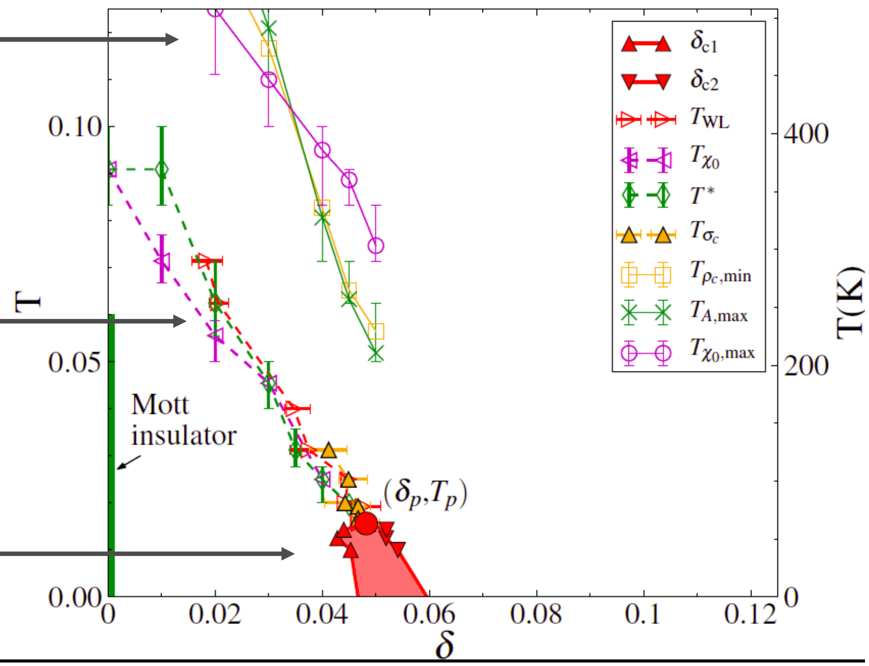
G. Sordi, PhysRevB.84.075161 – August 2011

Two crossover lines

T*

Widom line

Sordi transition



Giovanni Sordi

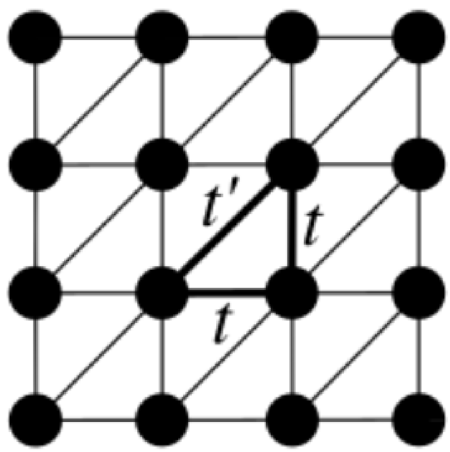
Patrick Sémon

Not in *d=1*

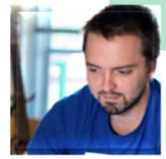
J. P. L. Faye and D. Sénéchal
Phys. Rev. B **96**, 195114

G. Sordi et al. Phys. Rev. Lett. 108, 216401/1-6 (2012)
G.Sordi et al. Phys. Rev. B 87, 041101(R)/1-5 (2013)
P. Sémon, G. Sordi, *et al.*, Phys. Rev. B **89**, 165113/1-6 (2014)

Anisotropic triangular lattice



Pierre-Olivier Downey

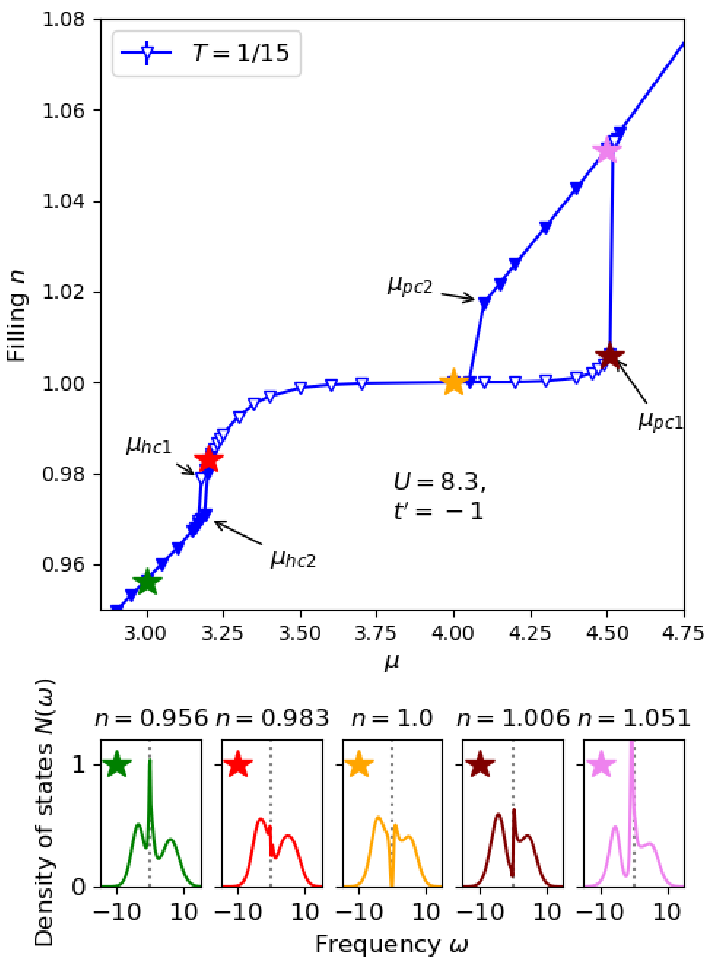


Maxime Charlebois

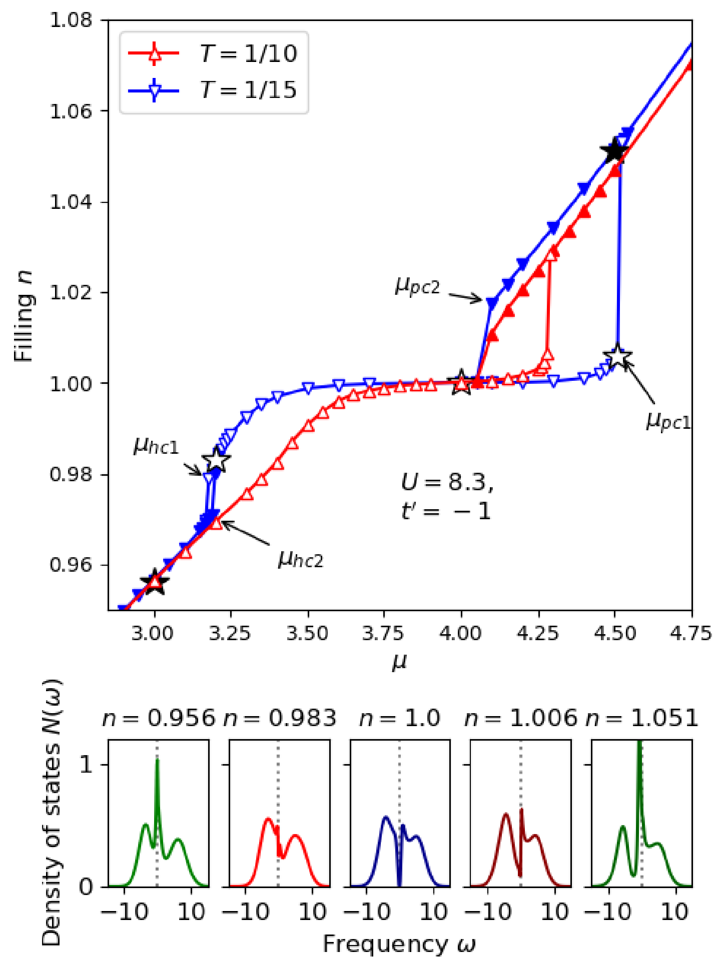
Charles-David Hébert

Olivier Gingras

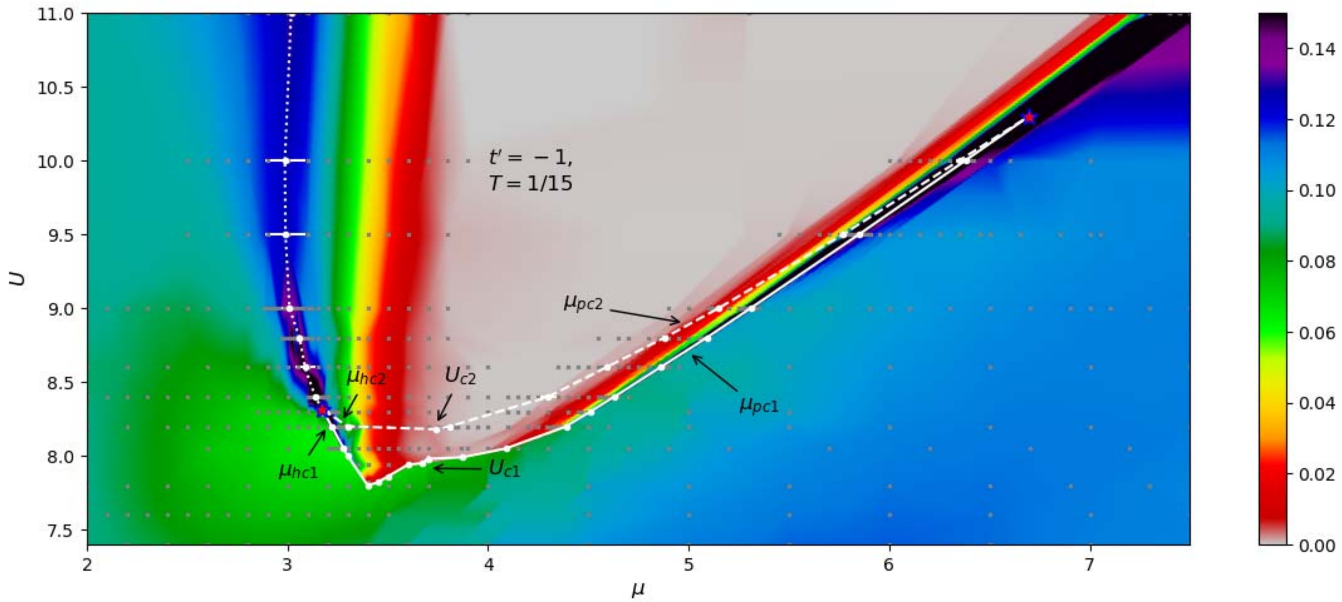
Triangular lattice with DCA, 6 patches

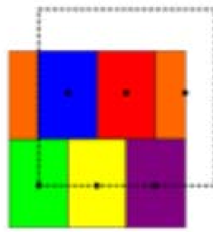


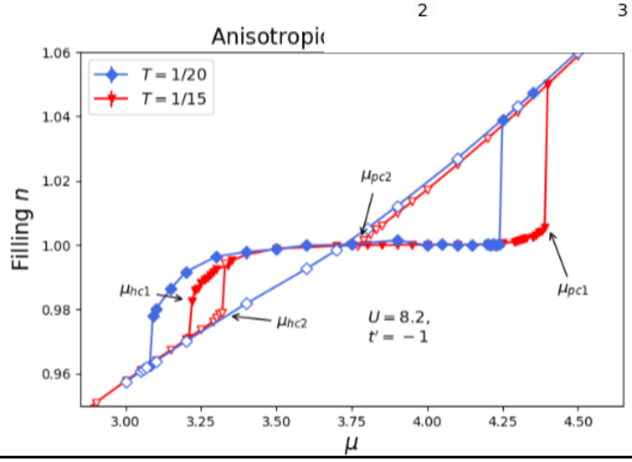
Some Physics on the triangular lattice



Mott and Sordi transition on the triangular lattice DCA, N=6

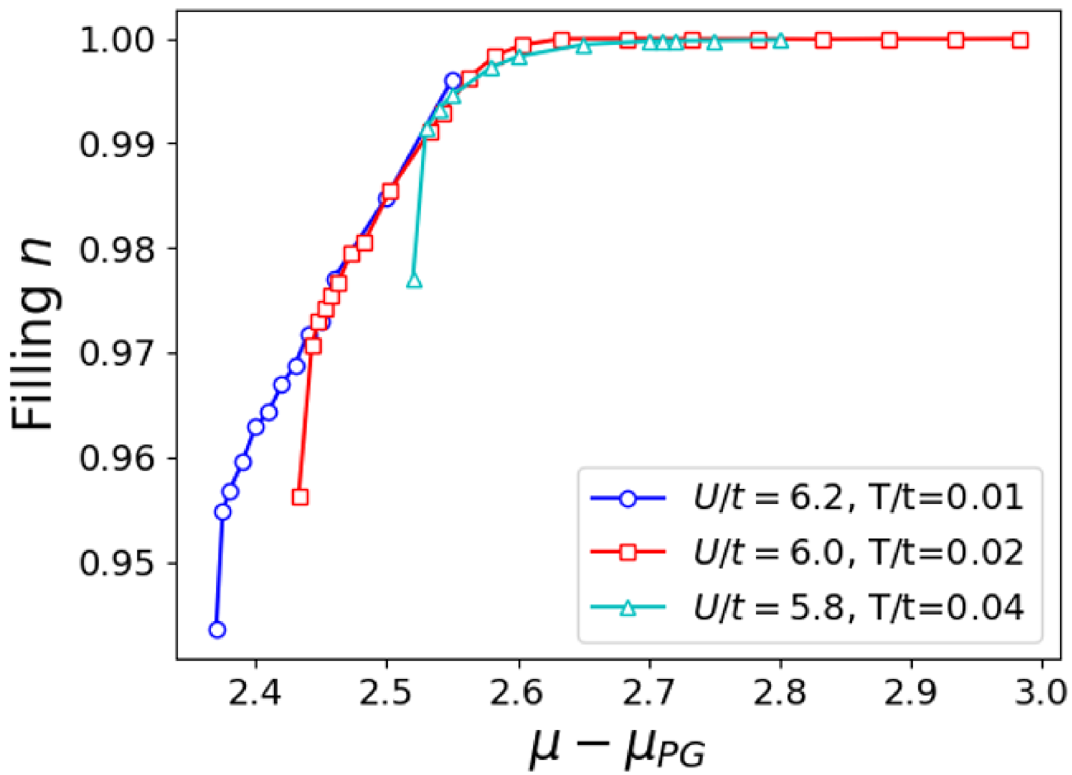






(Topological) stability

Depends on
- Cluster
- Large changes in t'



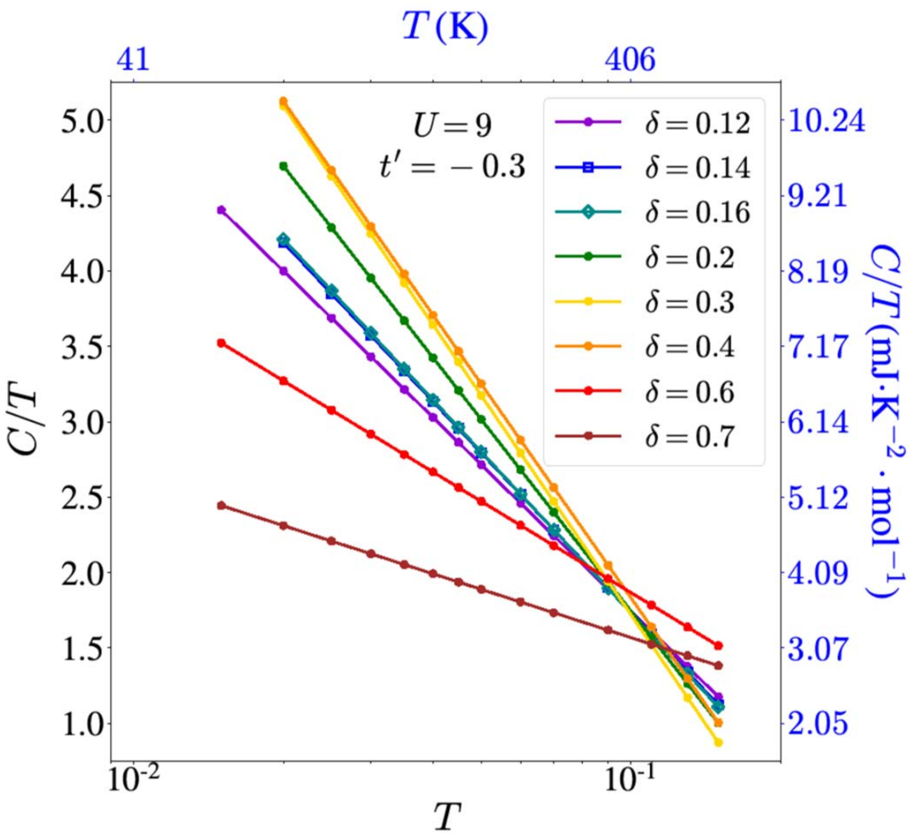
Another *Fermi Surface Reconstruction without Symmetry Breaking*

- Gazit, Assaad, Sachdev Phys. Rev. X 10, 041057

Quantum Critical point
Back to square lattice

Yang, … Zaanen, and Jarrell PRL **106**, 047004 (2011)

Specific heat in the strange metal phase



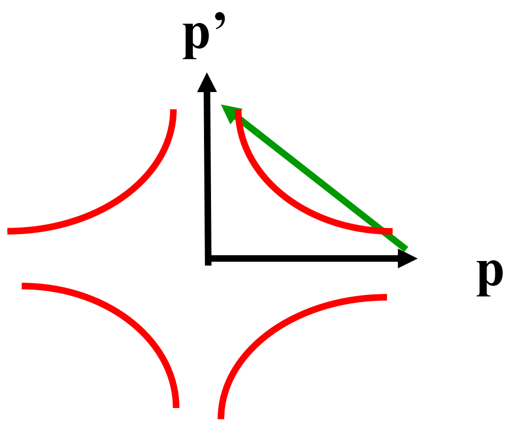
A.Reymbaut, *et al.* Phys. Rev. Research **1**, 023015 (2019)

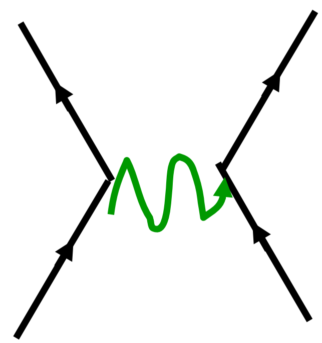
See also for C_v Maximum: Sordi, Walsh, Sémon, and A.-M.S.T, PRB **100**, 121105(R) (2019)

d-wave superconductivity

Cartoon « BCS » weak-coupling picture

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



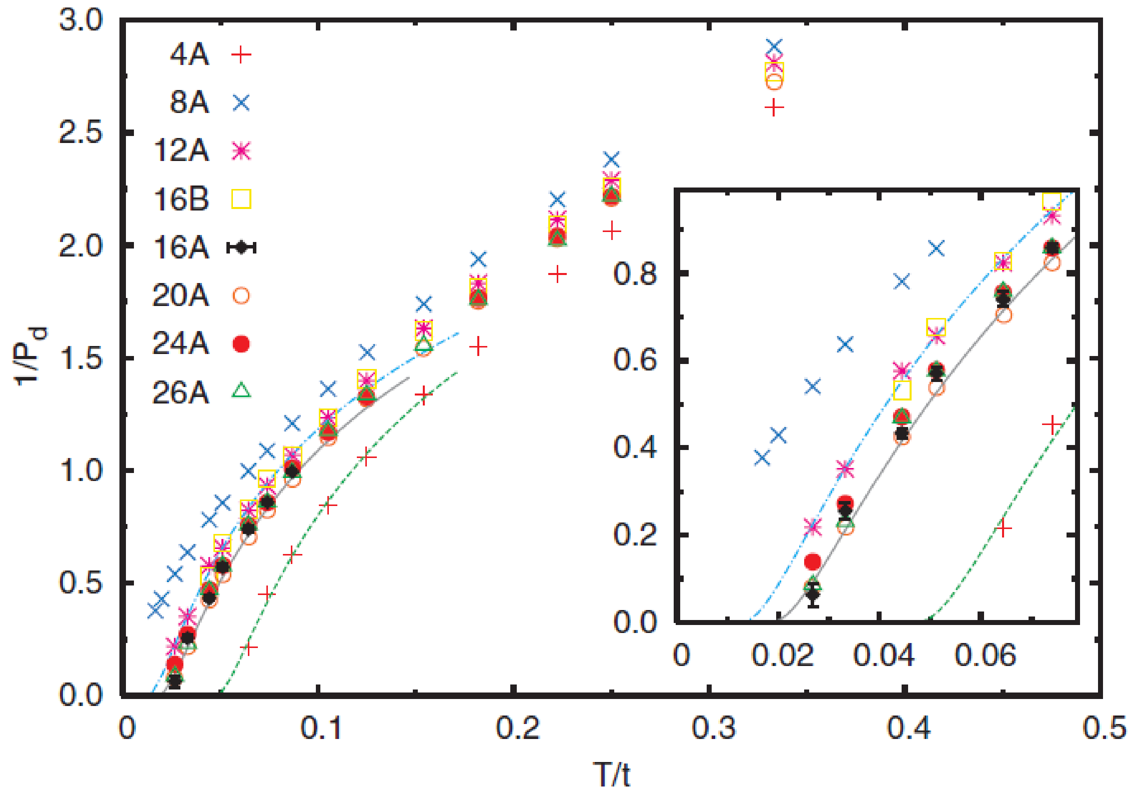


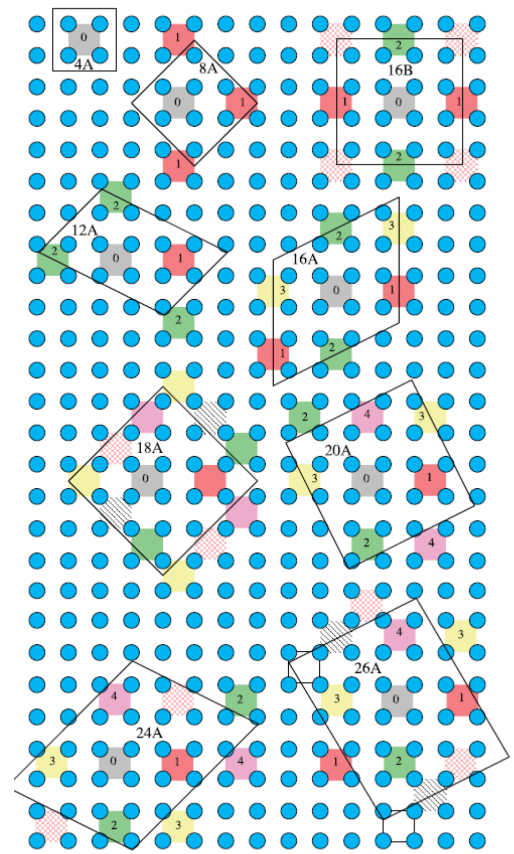
Exchange of spin waves?
Kohn-Luttinger
T_c with pressure

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

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

Exchange of spin waves, *U = 4t doping 10%*





Maier, Jarrell, Schulthess, Kent, White PRL **95,** 237001 (2005)

A cartoon strong correlation picture

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

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

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

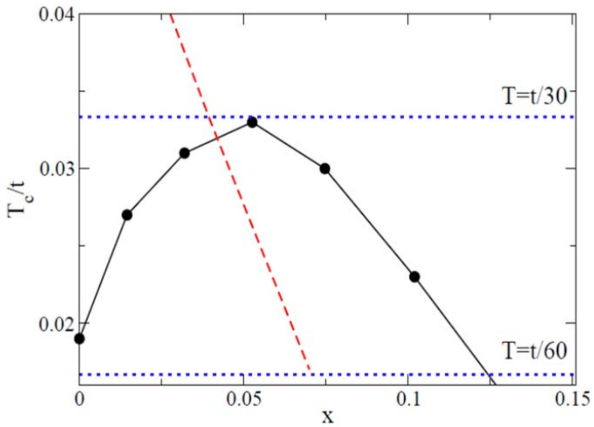
Pitaevskii Brückner:
Pair state orthogonal to repulsive core of Coulomb interaction

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

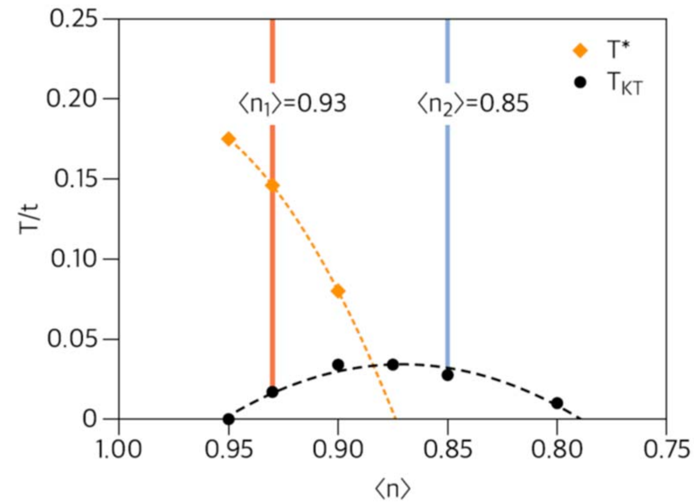
Miyake, Schmitt–Rink, and Varma P.R. B **34**, 6554-6556 (1986)

More sophisticated Slave Boson: Kotliar Liu PRB 1988

Superconducting transition temperature



E. Gull and A. J. Millis
Phys. Rev. B 88, 075127

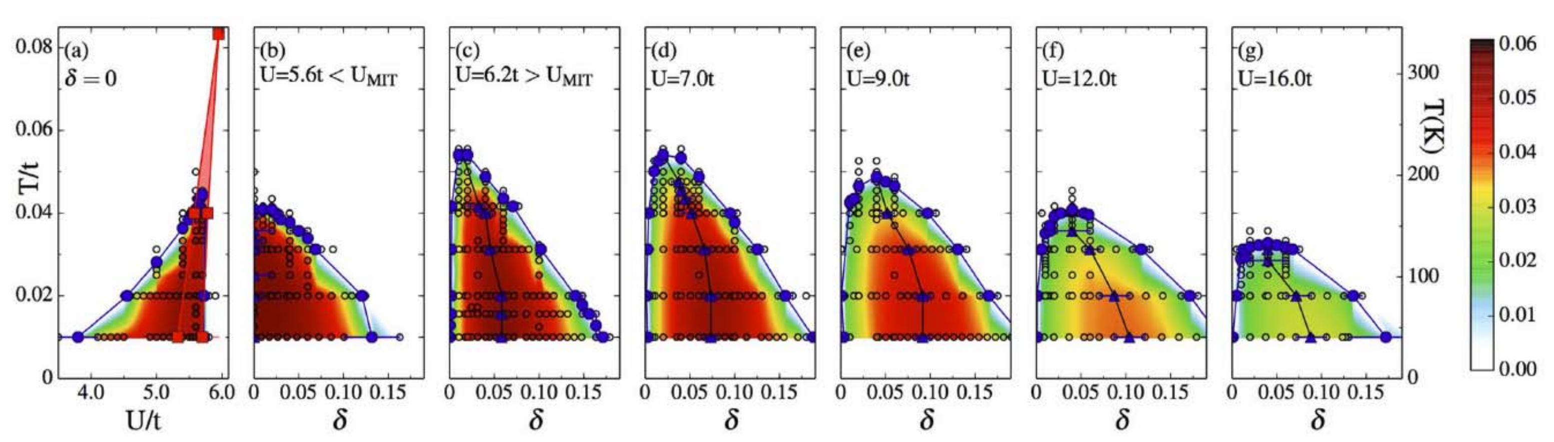


T.A. Maier, D.J. Scalapino, npj Quantum Materials (2019)

DCA, 8 sites, U/t = 6 and t′=0

DCA, 12 sites, U/t = 7 and t′/t = −0.15

T_c controlled by *J*, CDMFT *2x2*



Fratino et al.
Sci. Rep. **6**, 22715

Some experiments that suggest $T_c < T_{pair} < T^*$

T. Kondo *et al*. PRL **111** (2013)

Kondo, Takeshi, et al. Kaminski Nature Physics 2011, ***7***, 21-25

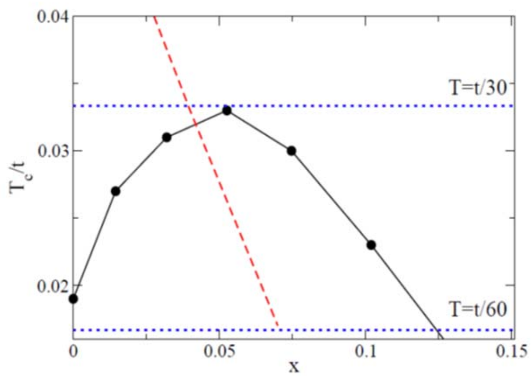
A. Pushp, Parker, … A. Yazdani, Science **364**, 1689 (2009)

Lee …Tajima (Osaka) https://arxiv.org/pdf/1612.08830

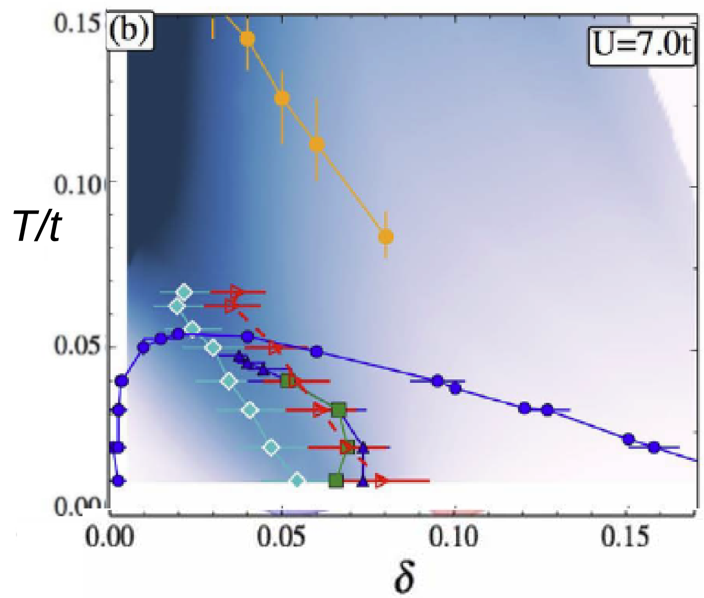
Patrick M. Rourke, et al. Hussey Nature Physics **7,** 455–458 (2011)

Lee et al. J. Phys. Soc. Jpn. 86, 023701 (2017)

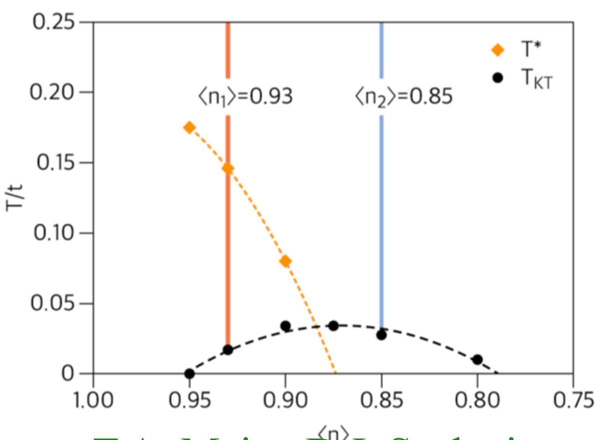
Phase diagram



E. Gull and A. J. Millis
Phys. Rev. B 88, 075127

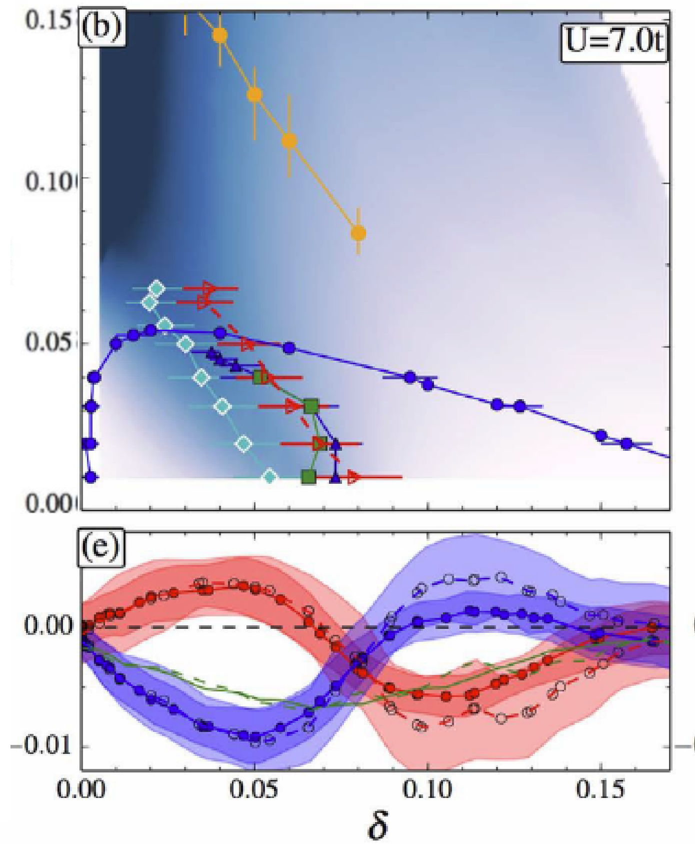


Fratino et al.
Sci. Rep. **6**, 22715



T.A. Maier, D.J. Scalapino, npj Quantum Materials (2019)

Condensation energy

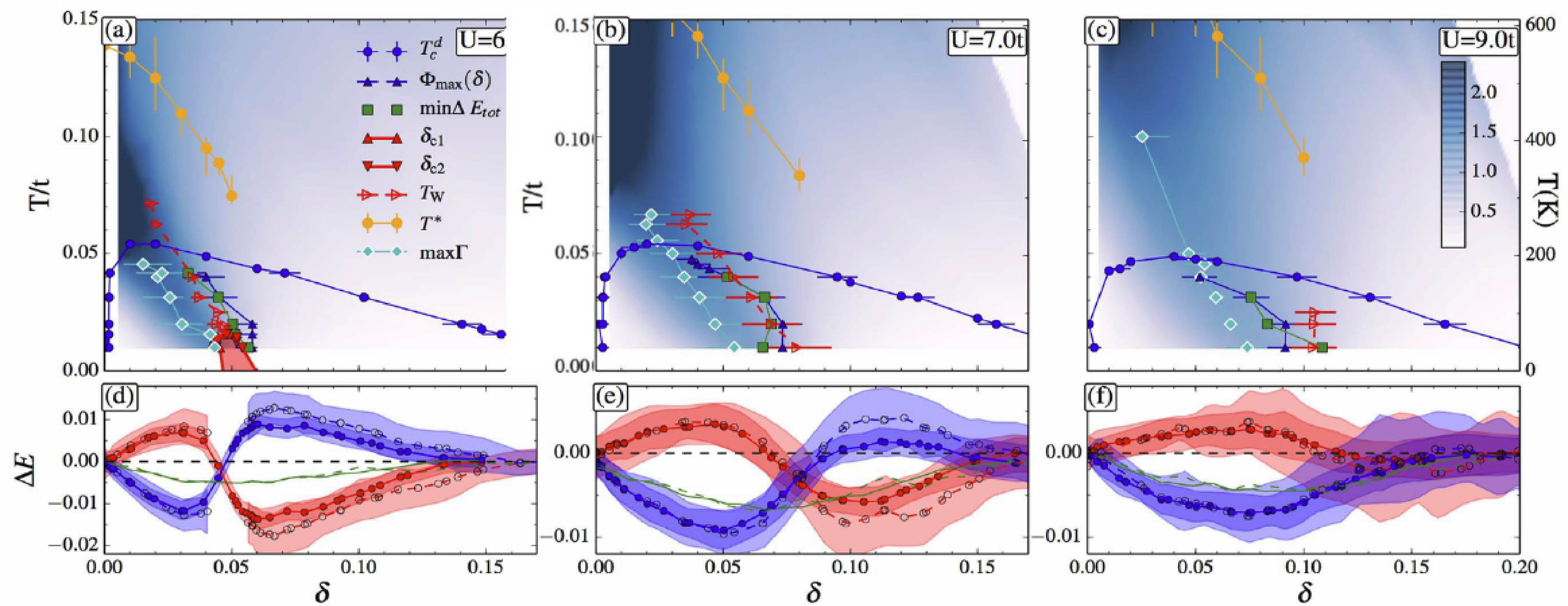


Fratino et al.
Sci. Rep. **6**, 22715

Theory, see also Jarrel PRL (2004), Gull Millis PRB (2014)
Experiments: Bontemps, Santander-Syro Van der Marel …

Condensation energy

Fratino et al.
Sci. Rep. **6**, 22715



Theory, see also Jarrel PRL (2004), Gull Millis PRB (2014)
Experiments: Bontemps, Santander-Syro Van der Marel …

D. Sénéchal

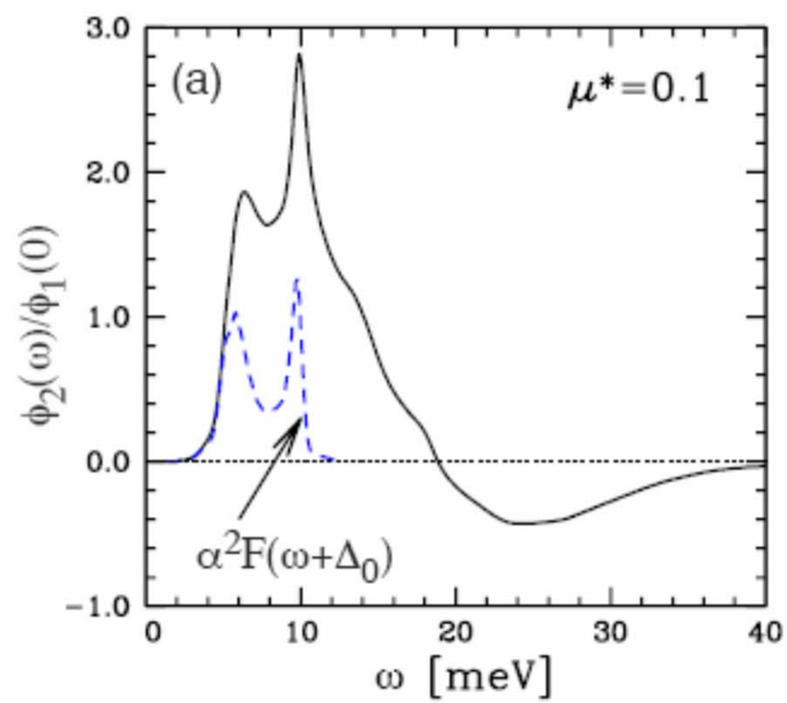
Bumsoo Kyung

The glue

Kyung, Sénéchal, Tremblay, Phys. Rev. B **80,** 205109 (2009)
Sénéchal, Day, Bouliane, AMST, Phys. Rev. B **87**, 075123 (2013)
A. Reymbaut *et al*. PRB **94** 155146 (2016)

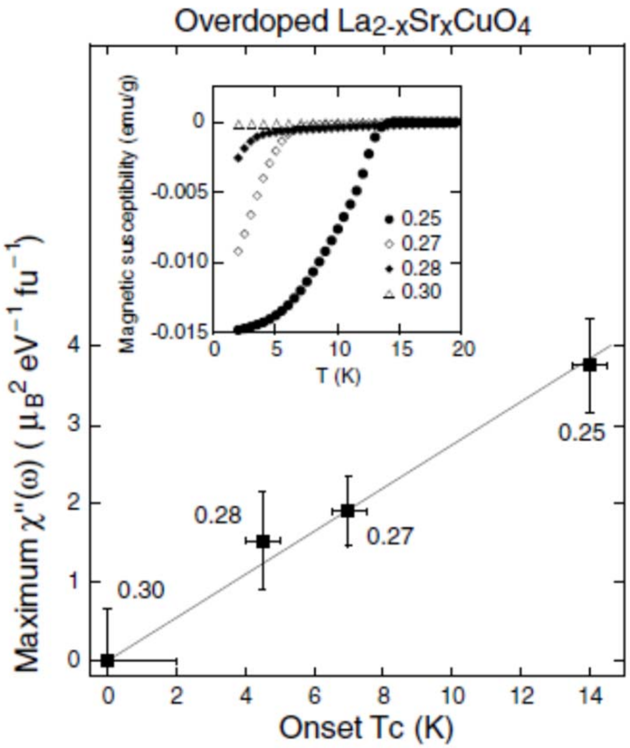
Im Σ_{an} and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)

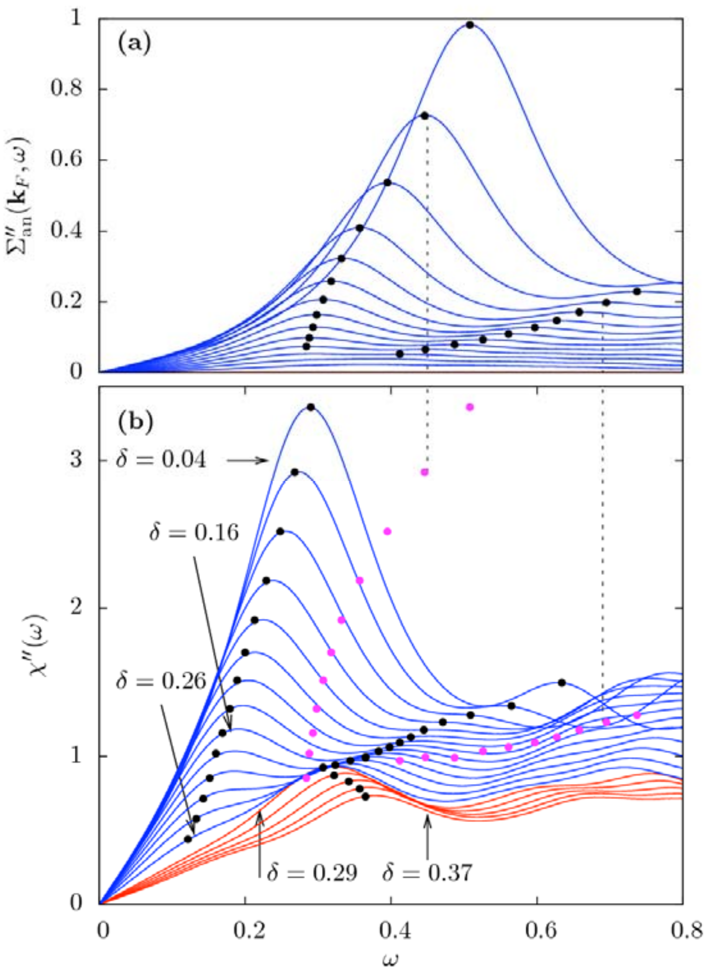


The glue CDMFT 2x2, T=0

Kyung, Sénéchal, Tremblay, Phys. Rev. B **80,** 205109 (2009)



Wakimoto … Birgeneau PRL (2004)



The glue and neutrons

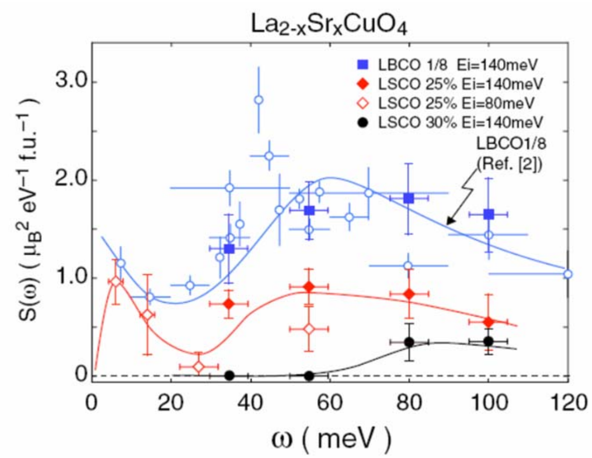
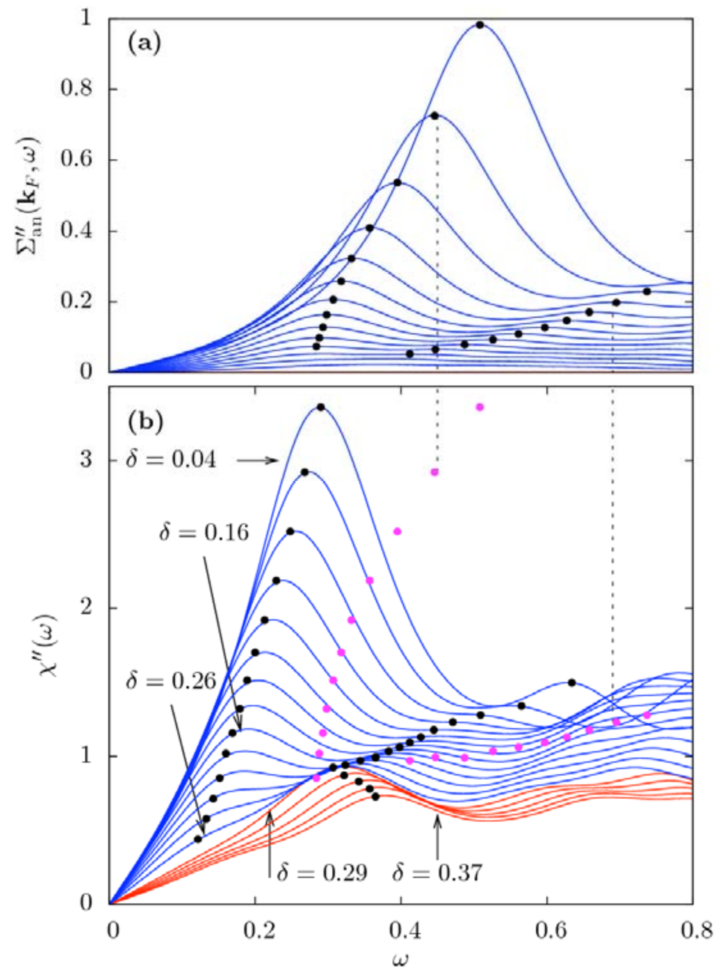


FIG. 3 (color online). **Q**-integrated dynamic structure factor $S(\omega)$ which is derived from the wide-H integrated profiles for LBCO 1/8 (squares), LSCO $x = 0.25$ (diamonds; filled for $E_i = 140$ meV, open for $E_i = 80$ meV), and $x = 0.30$ (filled circles) plotted over $S(\omega)$ for LBCO 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)



Three-band (Emery VSA) Hubbard model

V. J. Emery, Phys. Rev. Lett. **58**, 2794 (1987)

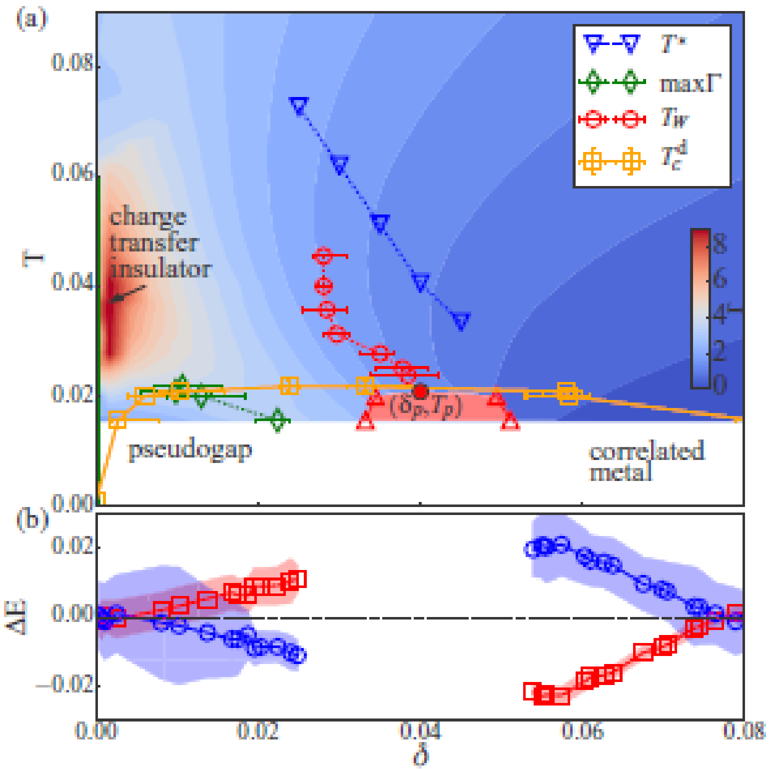
C. M. Varma, S. Schmitt-Rink, and E. Abrahams, Solid State Communications **62**, 681–685 (1987), ISSN 0038-1098,

Nicolas Kowalski

Sidhartha Dash

David Sénéchal

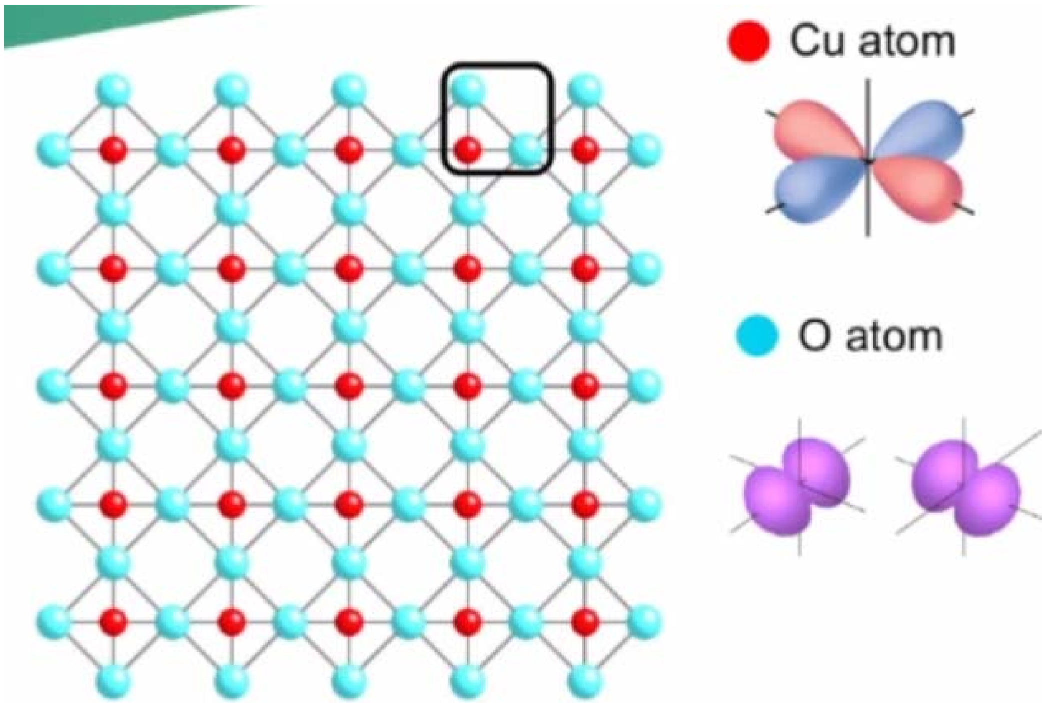
Sordi transition linked to the Mott transition

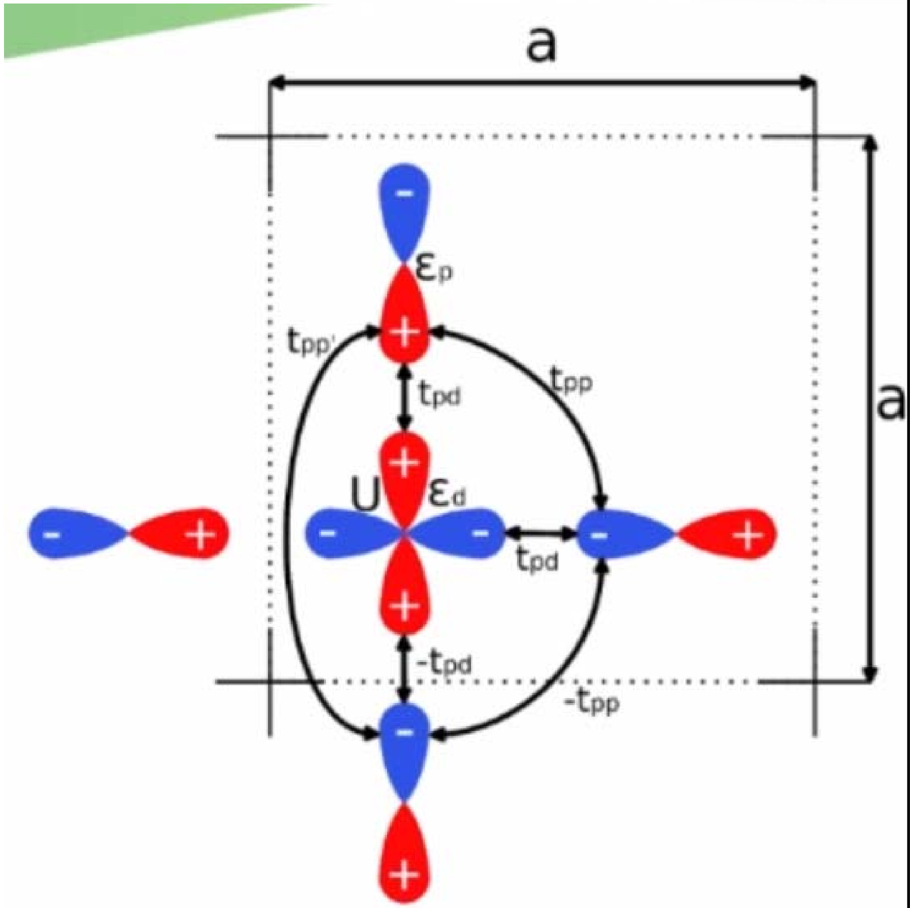


Fratino, Sémon, Sordi, A.-M.S. T. PRB **93**, 245147 (2016)

Superconductivity

Copper and oxygen planes





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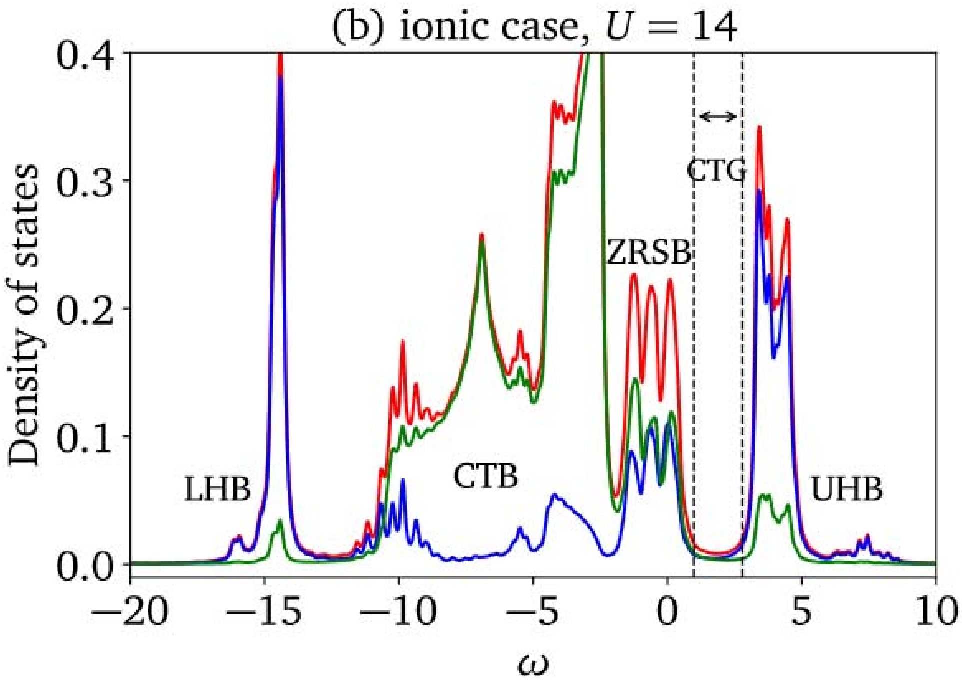
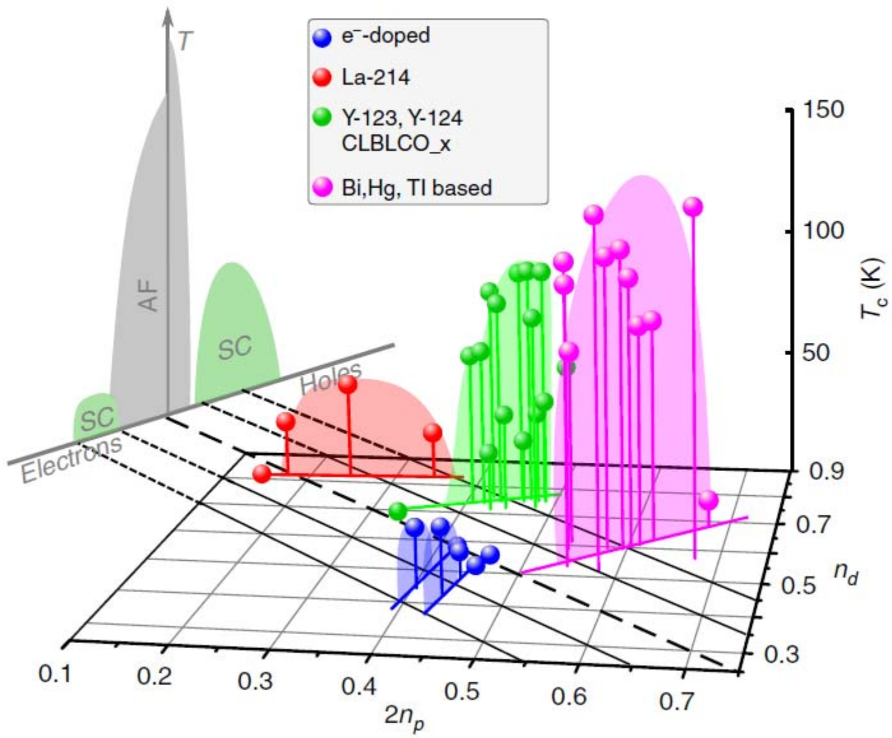
"Ionic" limiting cases with manageable sign problem



- $\varepsilon_p - \varepsilon_d = 7.0$, $t_{pd} = 1.5$, $t_{pp} = 1.0$, $t'_{pp} = 1.0$

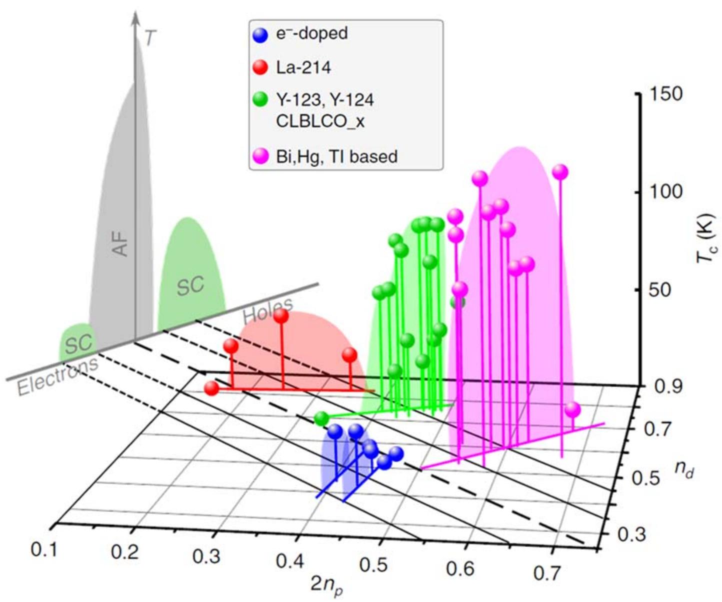
Experimental puzzle #1 with oxygen



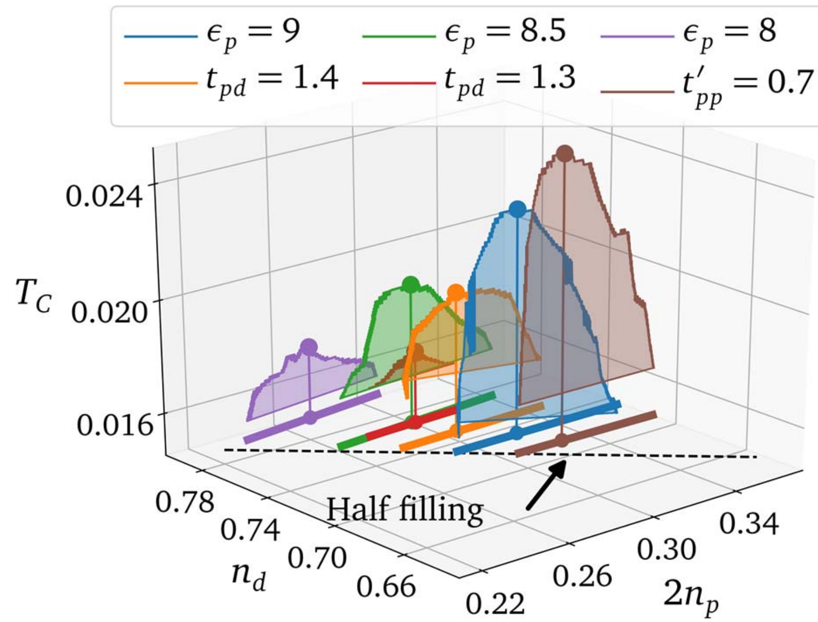
Rybicki,,, Haase, Nat. Comm. 7, 11413 (2016)

Results

Critical Temperature



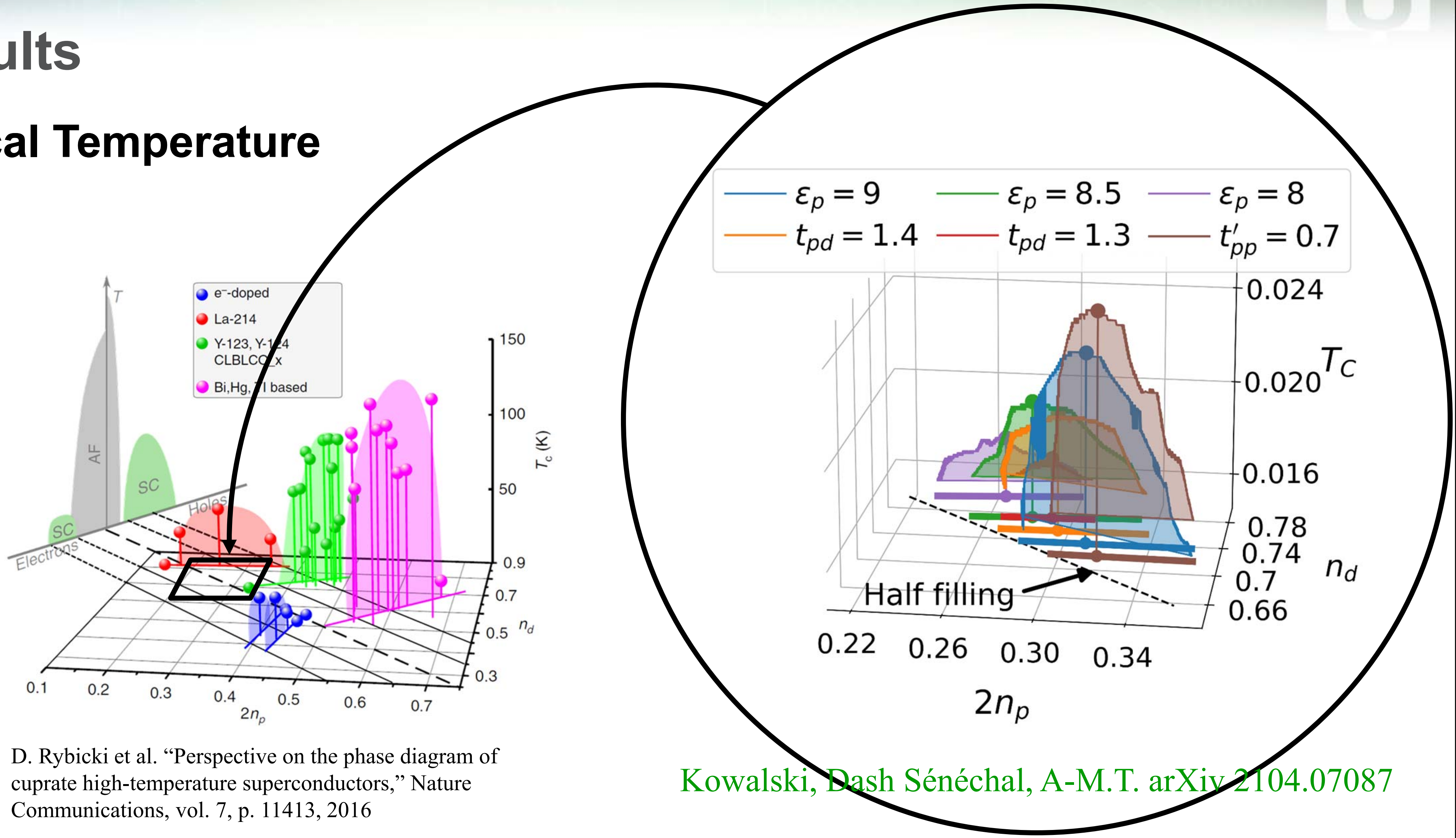
D. Rybicki et al. “Perspective on the phase diagram of cuprate high-temperature superconductors,” Nature Communications, vol. 7, p. 11413, 2016



Kowalski, Dash Sénéchal, A-M.T. arXiv 2104.07087

Results

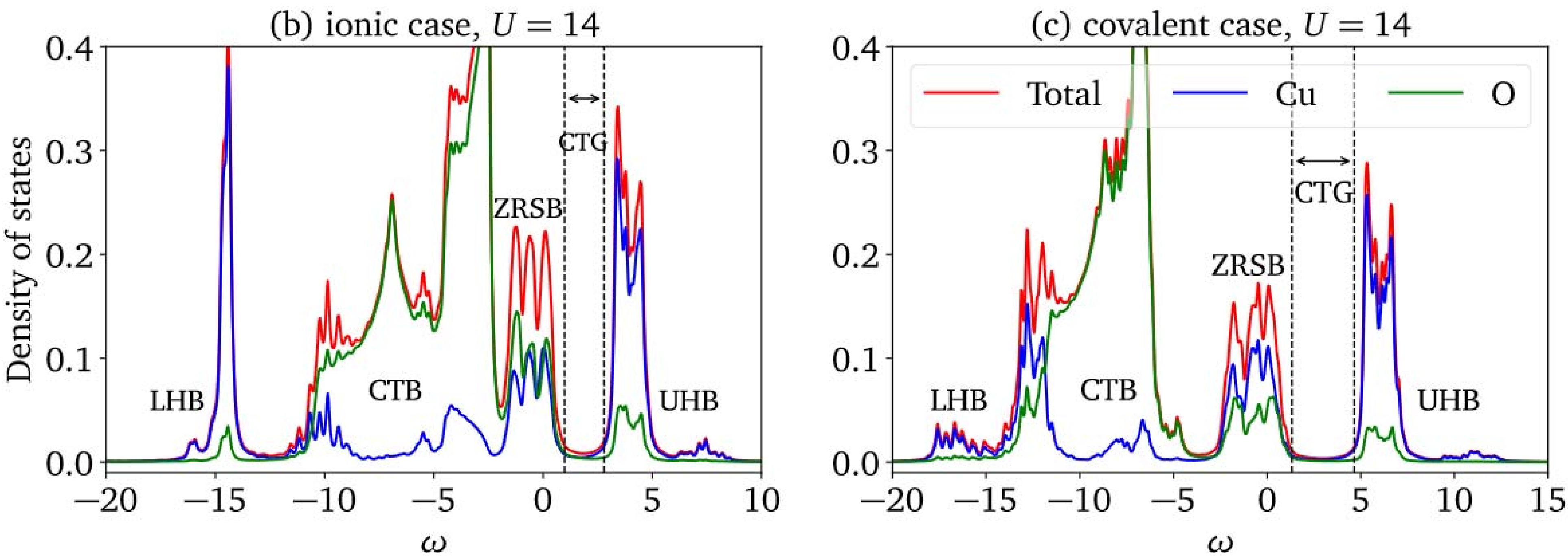
Critical Temperature



D. Rybicki et al. "Perspective on the phase diagram of cuprate high-temperature superconductors," Nature Communications, vol. 7, p. 11413, 2016

Kowalski, Dash Sénéchal, A-M.T. arXiv 2104.07087

Two limiting cases

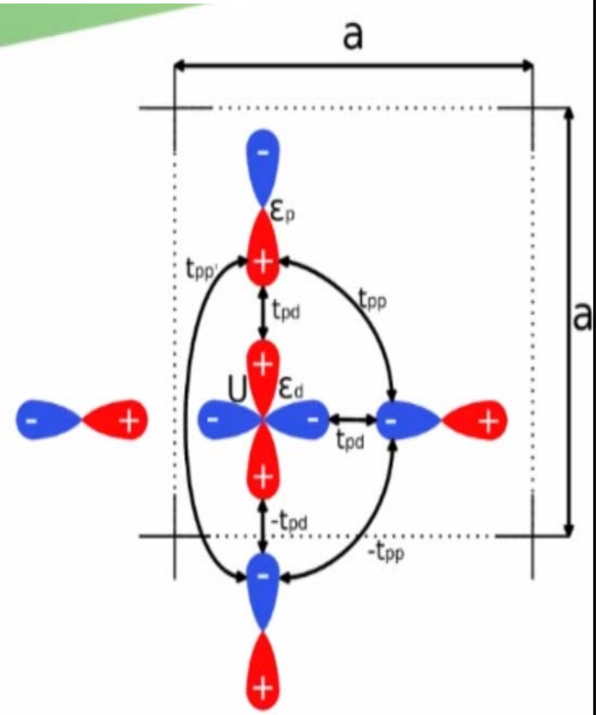


● $\varepsilon_p - \varepsilon_d = 7.0$, $t_{pd} = 1.5$, $t_{pp} = 1.0$, $t'_{pp} = 1.0$

○ $\varepsilon_p - \varepsilon_d = 2.3$, $t_{pd} = 2.1$, $t_{pp} = 1.0$, $t'_{pp} = 0.2$

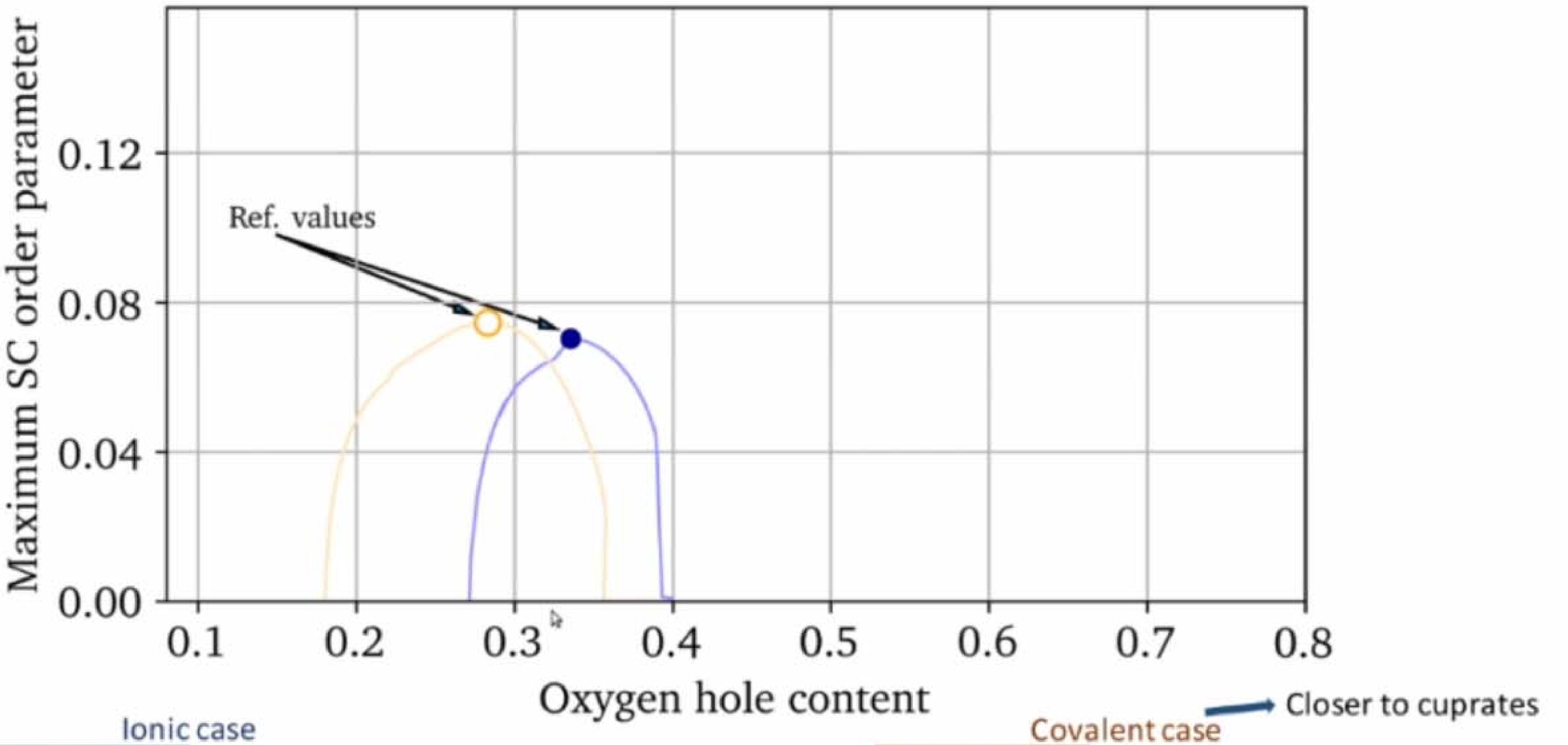
Electronic structure

	Compound	$\epsilon_d - \epsilon_p$ (eV)	t_{pd} (eV)	t_{pp} (eV)	$t_{pp'}$ (eV)	t'/t	layers	d_{Cu-O}^{apical} (Å)	T_c (K)
(1)	La_2CuO_4	2.61	1.39	0.640	0.103	0.070	1	2.3932	38
(2)	$Pb_2Sr_2YCu_3O_8$	2.32	1.30	0.673	0.160	0.108	2	2.3104	70
(3)	$Ca_2CuO_2Cl_2$	2.21	1.27	0.623	0.132	0.085	1	2.7539	26
(4)	$La_2CaCu_2O_6$	2.20	1.31	0.644	0.152	0.120	2	2.2402	45
(5)	$Sr_2Nd_2NbCu_2O_{10}$	2.10	1.25	0.612	0.144	0.110	2	2.0450	28
(6)	$Bi_2Sr_2CuO_6$	2.06	1.36	0.677	0.153	0.105	1	2.5885	24
(7)	$YBa_2Cu_3O_7$	2.05	1.28	0.673	0.150	0.110	2	2.0936	93
(8)	$HgBa_2CaCu_2O_6$	1.93	1.28	0.663	0.187	0.133	2	2.8053	127
(9)	$HgBa_2CuO_4$	1.93	1.25	0.649	0.161	0.122	1	2.7891	90
(10)	$Sr_2CuO_2Cl_2$	1.87	1.15	0.590	0.140	0.108	1	2.8585	30
(11a)	$HgBa_2Ca_2Cu_3O_8$ (outer)	1.87	1.29	0.674	0.184	0.141	3	2.7477	135
(11b)	$HgBa_2Ca_2Cu_3O_8$ (inner)	1.94	1.29	0.656	0.167	0.124	3	2.7477	135
(12)	$Tl_2Ba_2CuO_6$	1.79	1.27	0.630	0.150	0.121	1	2.7143	90
(13)	$LaBa_2Cu_3O_7$	1.77	1.13	0.620	0.188	0.144	2	2.2278	79
(14)	$Bi_2Sr_2CaCu_2O_8$	1.64	1.34	0.647	0.133	0.106	2	2.0033	95
(15)	$Tl_2Ba_2CaCu_2O_8$	1.27	1.29	0.638	0.140	0.131	2	2.0601	110
(16a)	$Bi_2Sr_2Ca_2Cu_3O_{10}$ (outer)	1.24	1.32	0.617	0.159	0.138	3	1.7721	108
(16a)	$Bi_2Sr_2Ca_2Cu_3O_{10}$ (inner)	2.24	1.32	0.678	0.198	0.121	3	1.7721	108



Weber, Yee, Haule, Kotliar, EPL 100, 2012

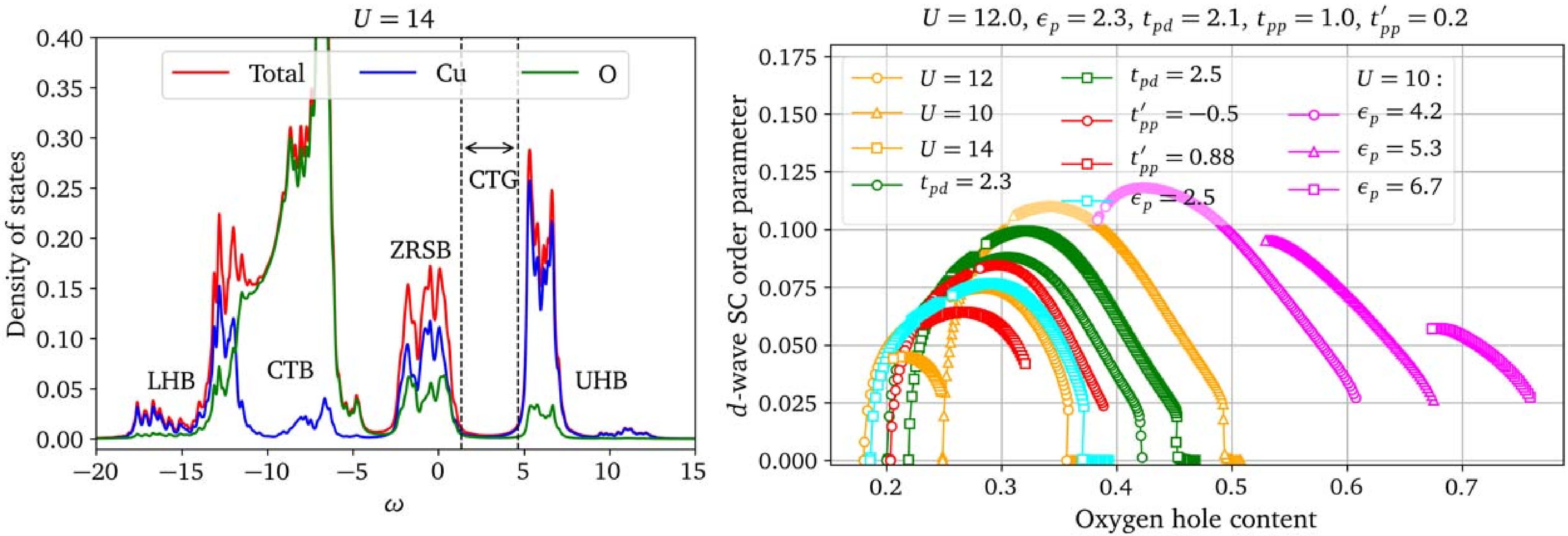
$T = 0$ superconducting domes for the reference models



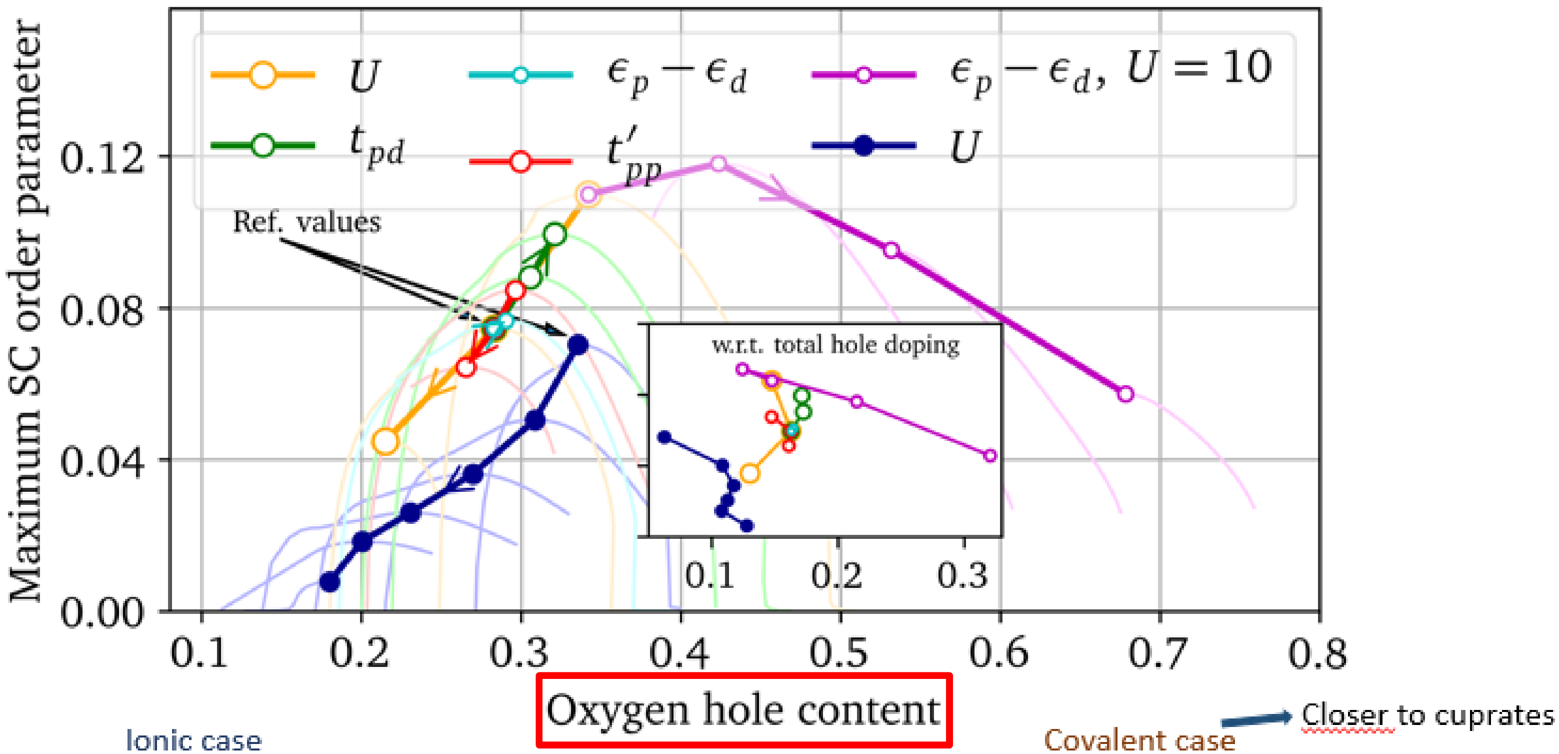
● $U = 12, \boxed{\epsilon_p - \epsilon_d = 7.0}, \; t_{pd} = 1.5, \; t_{pp} = 1.0, \; t'_{pp} = 1.0$ ○ $U = 12, \boxed{\epsilon_p - \epsilon_d = 2.3}, \; t_{pd} = 2.1, \; t_{pp} = 1.0, \; t'_{pp} = 0.2$

Kowalski, Dash Sénéchal, A-M.T. arXiv 2104.07087

T = 0 superconducting domes for the covalent model



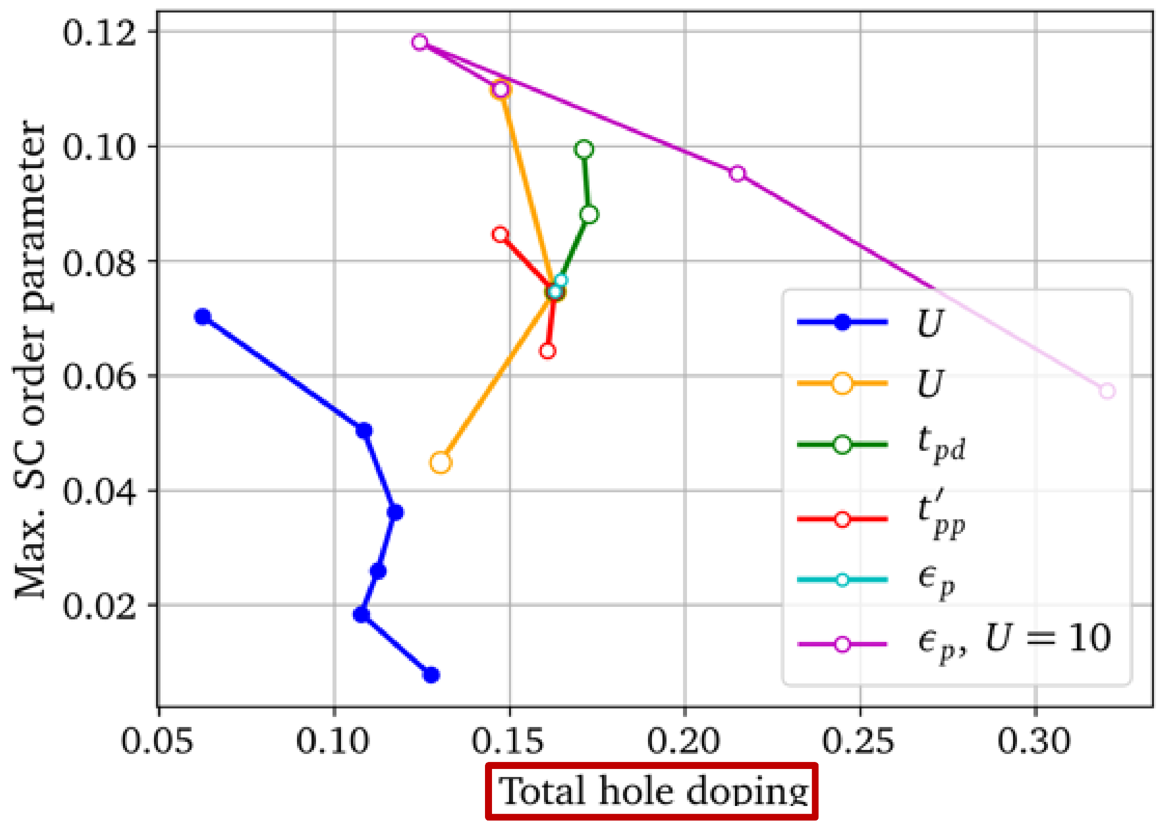
$T = 0$ max order parameter for the two models



● $U = 12,\ \epsilon_p - \epsilon_d = 7.0,\ t_{pd} = 1.5,\ t_{pp} = 1.0,\ t'_{pp} = 1.0$ ○ $U = 12,\ \epsilon_p - \epsilon_d = 2.3,\ t_{pd} = 2.1,\ t_{pp} = 1.0,\ t'_{pp} = 0.2$

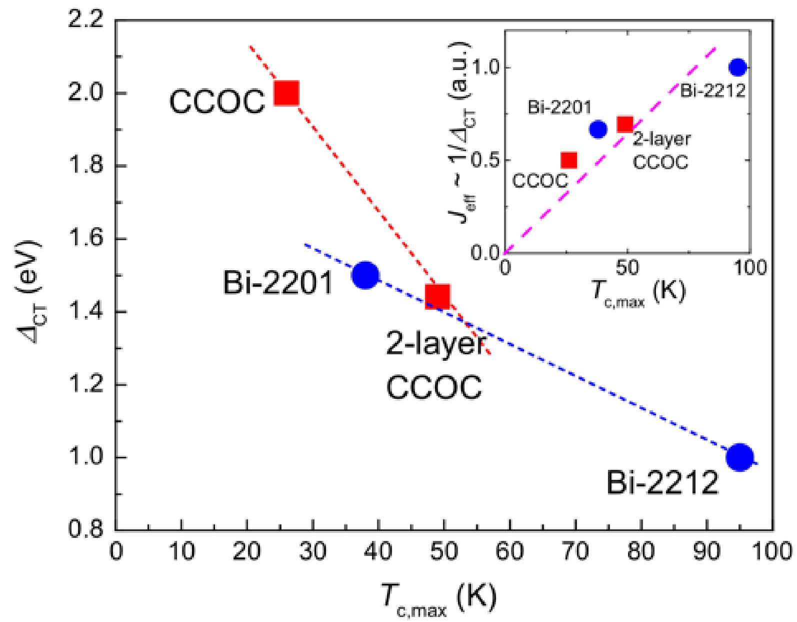
Kowalski, Dash Sénéchal, A-M.T. arXiv 2104.07087

$T = 0$ max order parameter for the two models

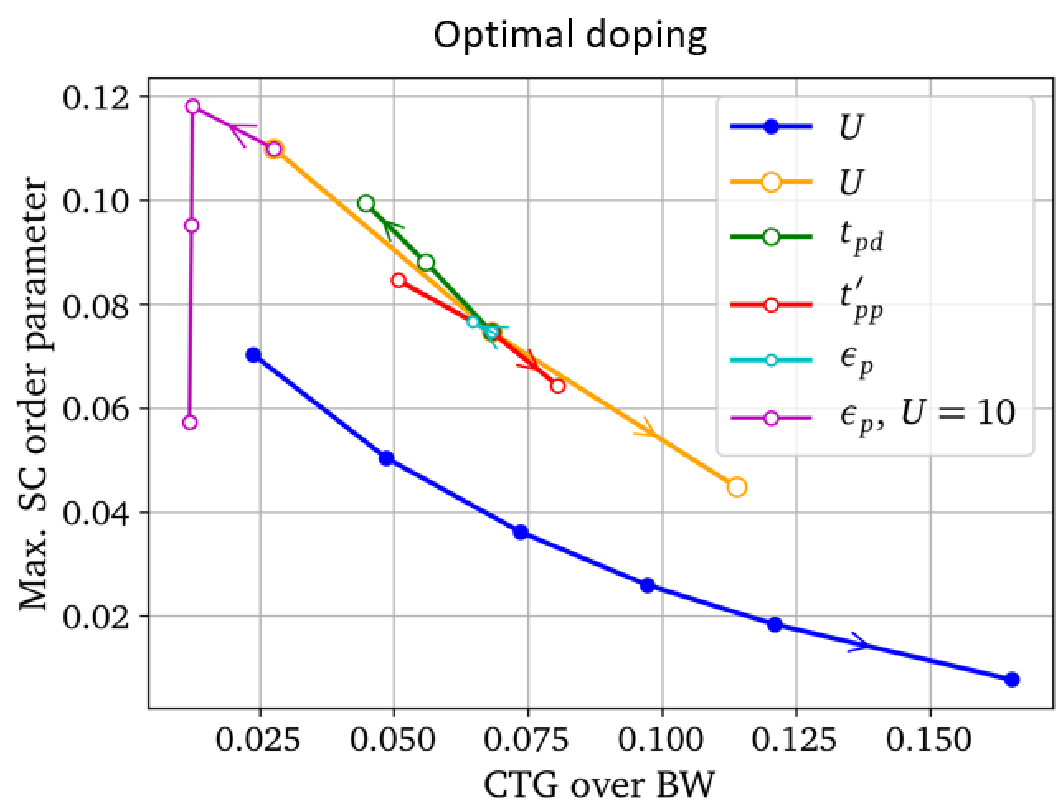


Kowalski, Dash Sénéchal, A-M.T. arXiv 2104.07087

Experimental puzzle #2 with Charge Transfer Gap

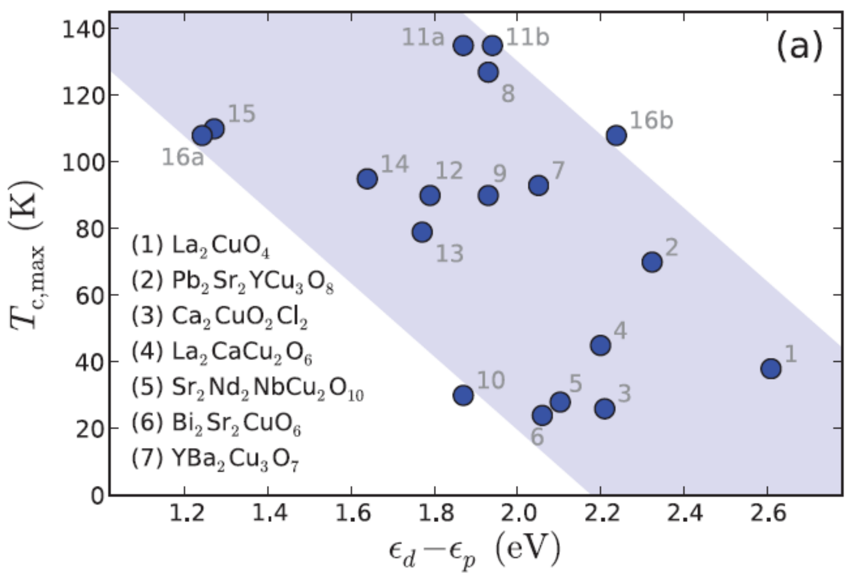


Ruan *et al.* Sci. Bull. **61** (2016)

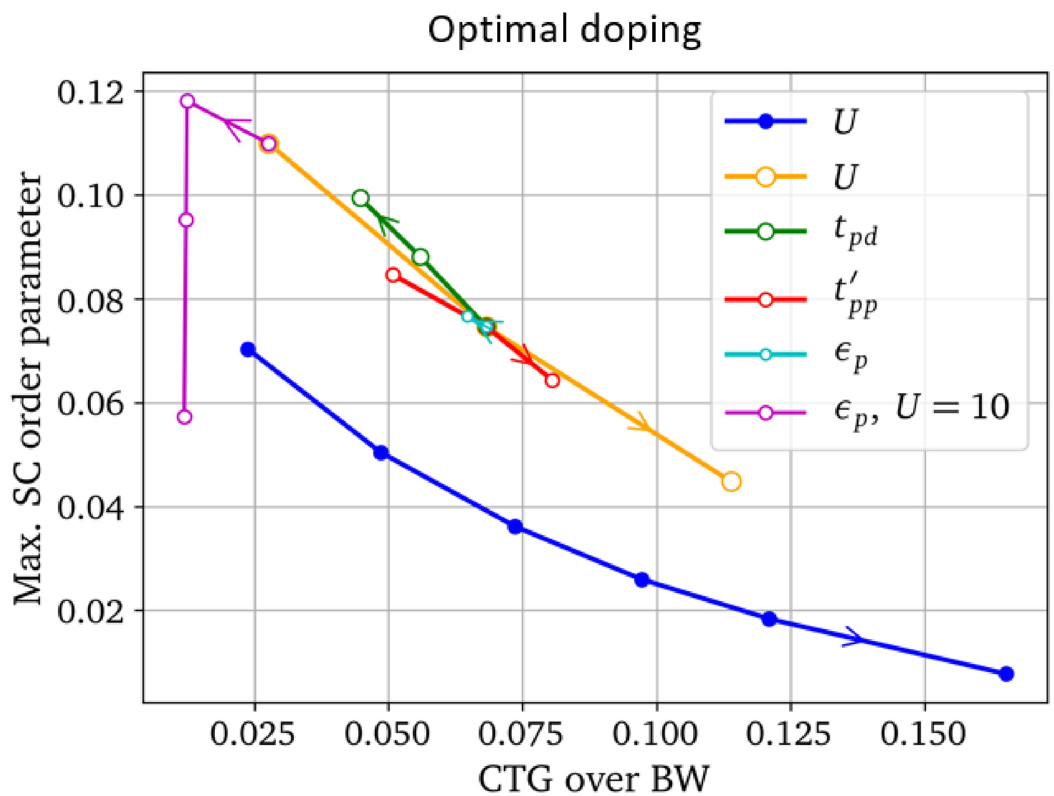


Kowalski, Dash Sénéchal, A-M.T. arXiv 2104.07087

Experimental puzzle #2 with Charge Transfer Gap

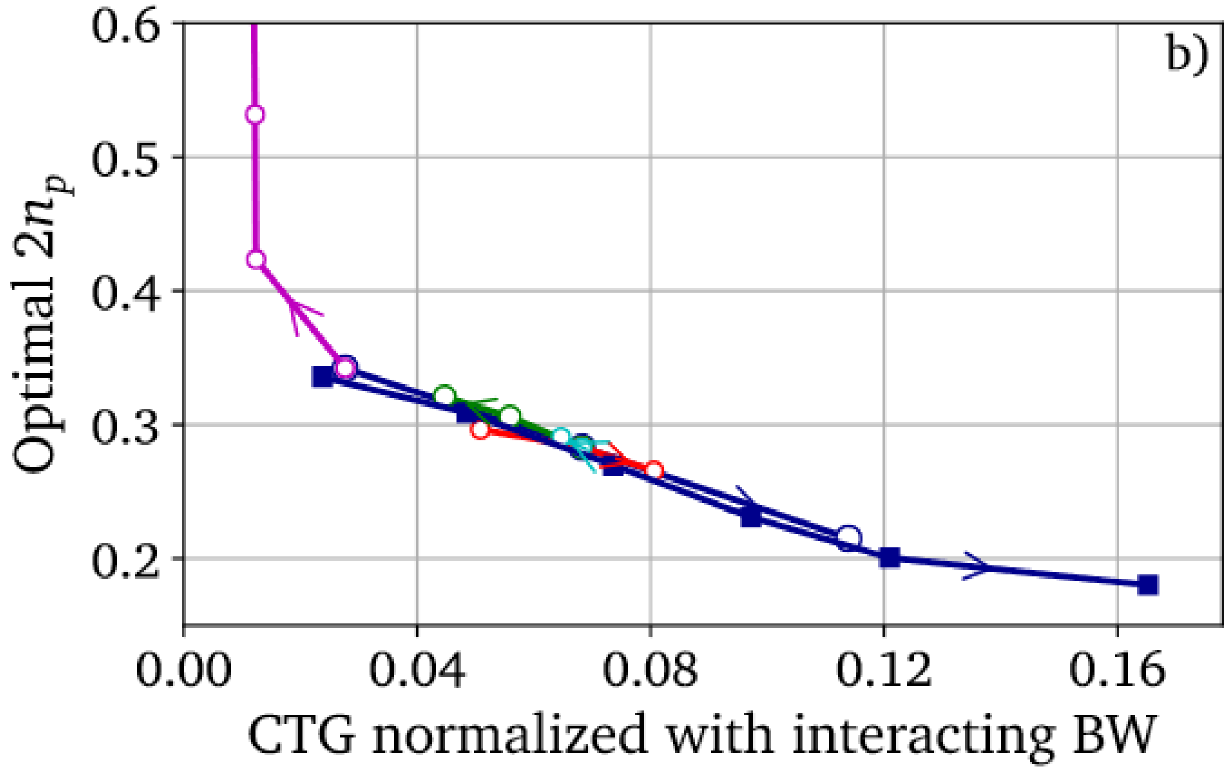


Weber, Yee, Haule, Kotliar, EPL 100, 2012



Kowalski, Dash Sénéchal, A-M.T. arXiv 2104.07087

Charge-transfer gap, oxygen hole content



Kowalski, Dash Sénéchal, A-M.T. arXiv 2104.07087

Importance of each parameter

Optimal CTG (Δ_{opt}) : $\left|\frac{\partial \Delta_{opt}}{\partial t_{pd}}\right| > \left|\frac{\partial \Delta_{opt}}{\partial U}\right| > \left|\frac{\partial \Delta_{opt}}{\partial t'_{pp}}\right| > \left|\frac{\partial \Delta_{opt}}{\partial \epsilon_p}\right|$

- + + -

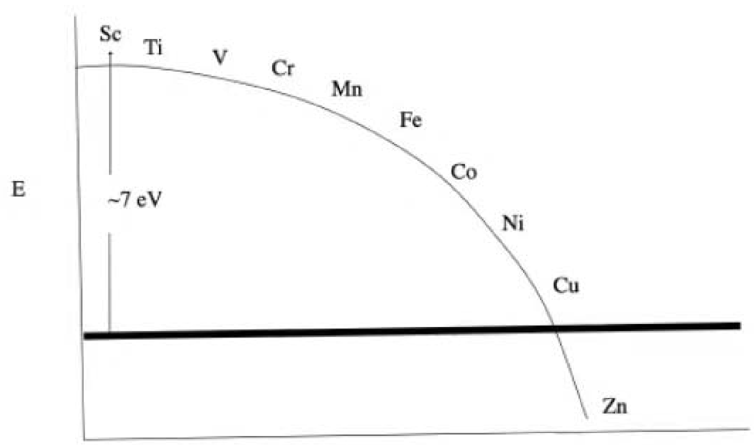
Optimal SC order parameter (ψ_{opt}) : $\left|\frac{\partial \psi_{opt}}{\partial t_{pd}}\right| > \left|\frac{\partial \psi_{opt}}{\partial U}\right| > \left|\frac{\partial \psi_{opt}}{\partial t'_{pp}}\right| > \left|\frac{\partial \psi_{opt}}{\partial \epsilon_p}\right|$

+ - - +

Order of importance of parameters: $t_{pd} > U > t'_{pp} > \epsilon_p$

Covalency (talk by Chandra Varma)

Affinity Energy ($E(M^{2+}) - E(M^{1+})$) of first row Trans. Metals in relation to Ionization Energy of Oxygen ($E(O^{2-}) - E(O^{1-})$)

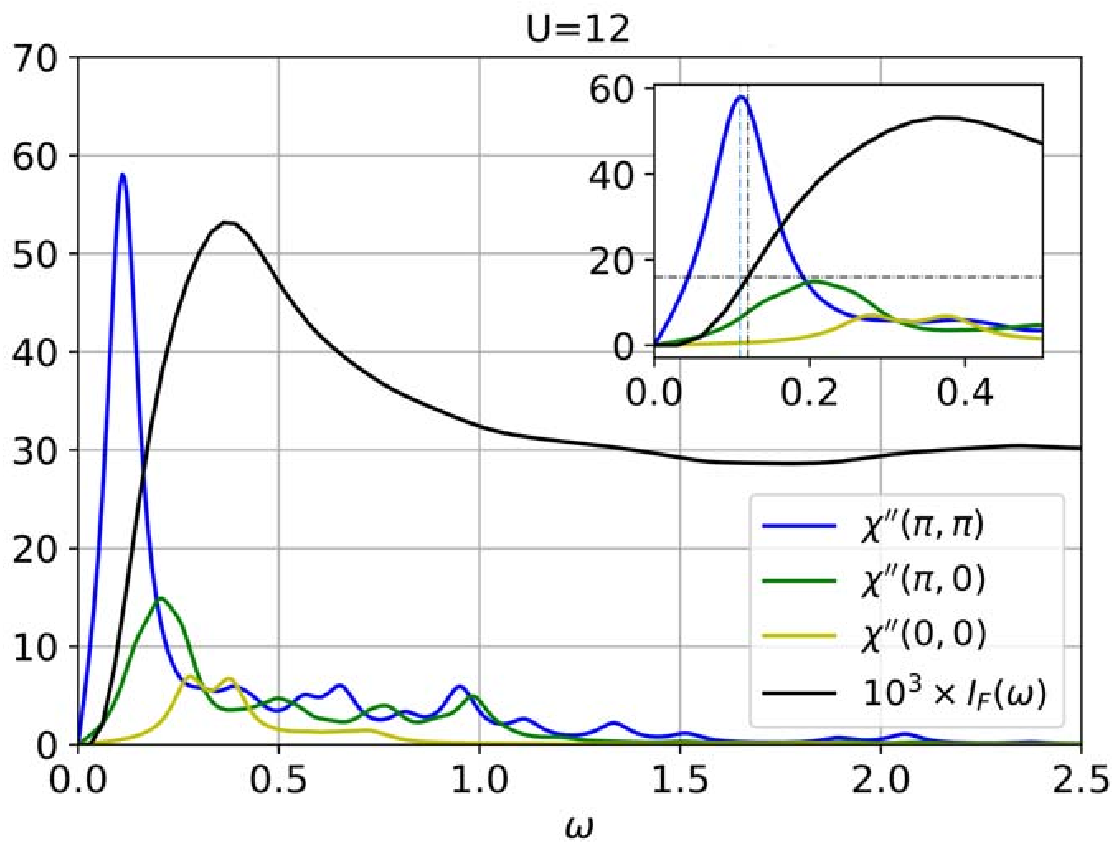


Also, Zaanen, Sawatzky, Allen (prl 1985).

C. M. Varma and T. Giamarchi, *Model for copper oxide metals and superconductors* (Elsevier Science B.V., 1995).

Copper pairing mechanism

Spin fluctuations on copper



$$I_F(\omega) \equiv -\int_0^{\omega} \frac{d\omega'}{\pi} \mathrm{Im}\, F_{ij}^R(\omega')$$

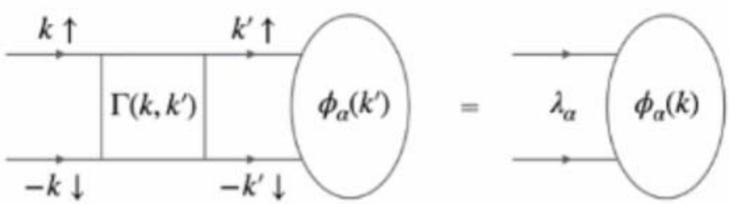
$$F_{ij} \equiv -\langle T c_{i\uparrow}(\tau) c_{j\downarrow}(0) \rangle$$

Kowalski, Dash Sénéchal, A-M.T. in preparation

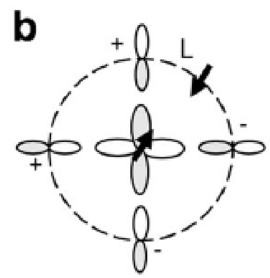
Bethe-Salpeter point of view

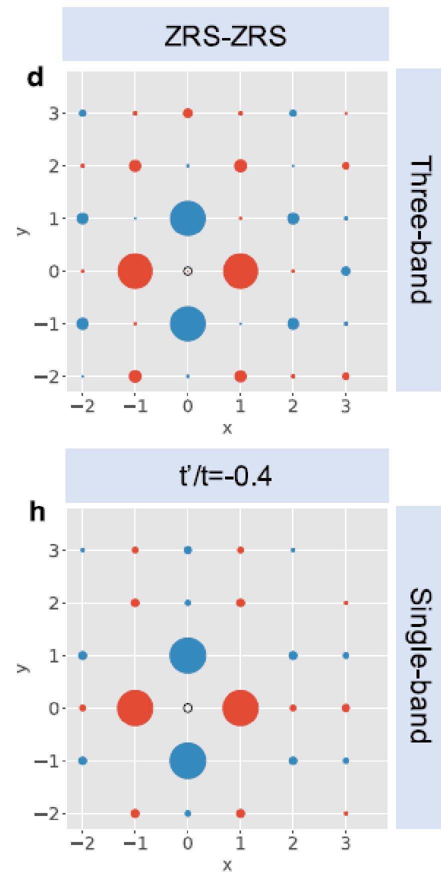
Mai, Balduzzi, Johnston, Maier npj Quantum Materials **6,** 26 (2021)

Particle-particle Bethe-Salpeter equation relates gap function $\phi(k)$ to pairing interaction $\Gamma(k, k')$



$$-\frac{T}{N}\sum_{k'}\Gamma(k,k')G(k')G(-k')\phi_\alpha(k') = \lambda_\alpha\phi_\alpha(k)$$





$U = 19\ t_{pp}$
$t_{pd} = 2.5\ t_{pp}$
$\varepsilon_p - \varepsilon_d = 7.2\ t_{pp}$
$t_{pp}' = 0$
$T = 0{,}22\ t_{pp}$

$U = 6t$
$T = 0.2t$

Summary Conclusion

Summary

- Intrinsic to the doped Mott insulator
  - Pseudogap
  - First-order transition – QCP
  - d-wave superconductivity
    - Short-range spin fluctuations (J)
    - Role of charge-transfer gap and of oxygen-hole doping

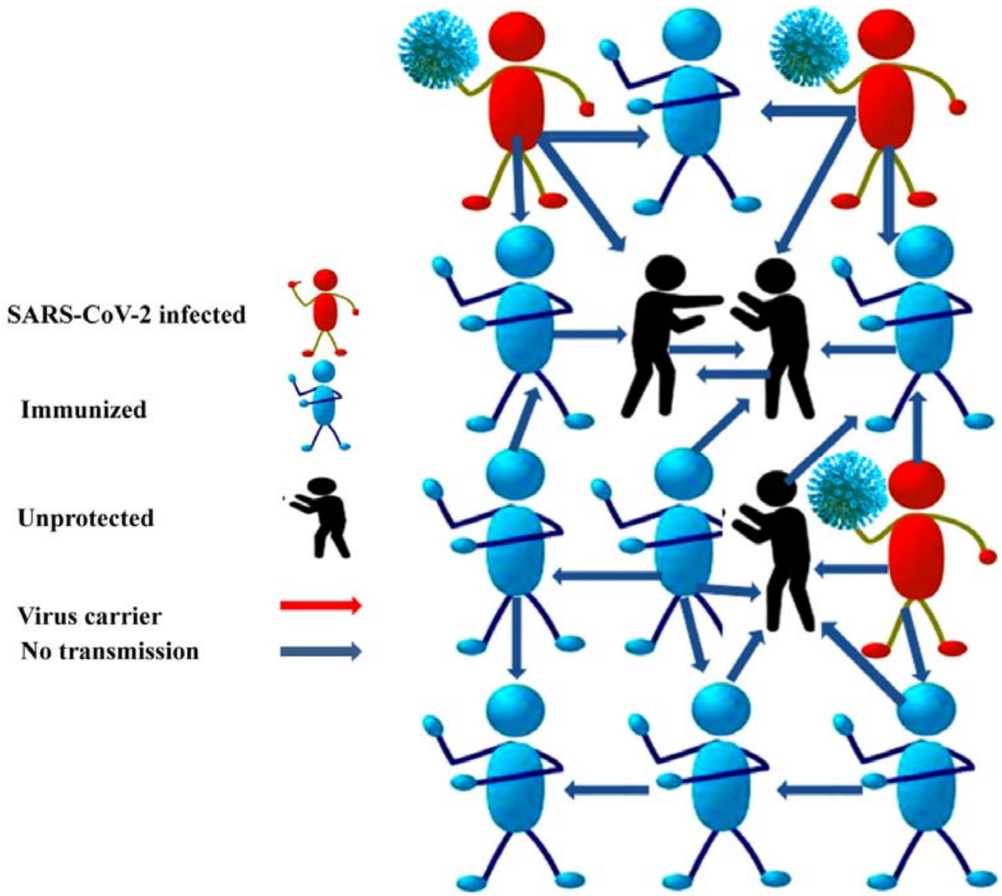
- Other effects that have not been discussed ***V >> J***
  - Reymbaut, Charlebois, Fellous Asiani, Fratino, Sémon, Sordi A.-M.S.T. PRB **94**, 155146 (2016)
- Other experiment consistent with doped Mott picture
  - Frachet, … Leboeuf, Julien Nat. Phys. 10.1038/s41567-020-0950-5

Entanglement properties

- Sharp variation in the entanglement-related properties and not broken symmetry phases characterizes the onset of the pseudogap phase at finite temperature.
  - Walsh, Sémon, Poulin, Sordi, A.-M.S.T. PRX QUANTUM **1**, 020310 (2020)

What is the most important problem from your point of view? Smoking gun calculation

Lone genius



Herd immunity

Herd genius

Merci
Thank you

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Entanglement entropy and mutual information near the Mott transition

Caitlin Walsh

Patrick Sémon

David Poulin

Giovanni Sordi

C. Walsh, *et al.*
Phys. Rev. Lett. **122**, 067203 (2019)
Phys. Rev. B **99**, 075122 (2019)

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Single-site entanglement entropy

Schrödinger: I would not call [entanglement] *one* but rather *the* characteristic trait of quantum mechanics, the one that enforces its entire departure from classical lines of thought.

Proceedings of the Cambridge Philosophical Society **31**, 555 (1935); **32**, 446 (1936).

Motivation

PHYSICAL REVIEW X **7**, 031025 (2017)

Measuring Entropy and Short-Range Correlations in the Two-Dimensional Hubbard Model

E. Cocchi,[1,2] L. A. Miller,[1,2] J. H. Drewes,[1] C. F. Chan,[1] D. Pertot,[1] F. Brennecke,[1] and M. Köhl[1]

First-order nature of the transition,
universality class of the end point,
crossovers emanating from the end point.

For quantum critical or finite temperature critical points

A. Anfossi *et al*. Phys. Rev. Lett. **95**, 056402 (2005).
L. Amico *et al*. Europhys. Lett. **77**, 17001 (2007).
L. Amico *et al*. Rev. Mod. Phys. **80**, 517 (2008).
D. Larsson *et al*. Phys. Rev. A **73**,042320 (2006).
D. Larsson *et al*. Phys. Rev. Lett. **95**, 196406 (2005).

What is measured (Using CDMFT CT-HYB on plaquette)

- Single site entanglement entropy for fermions [1]

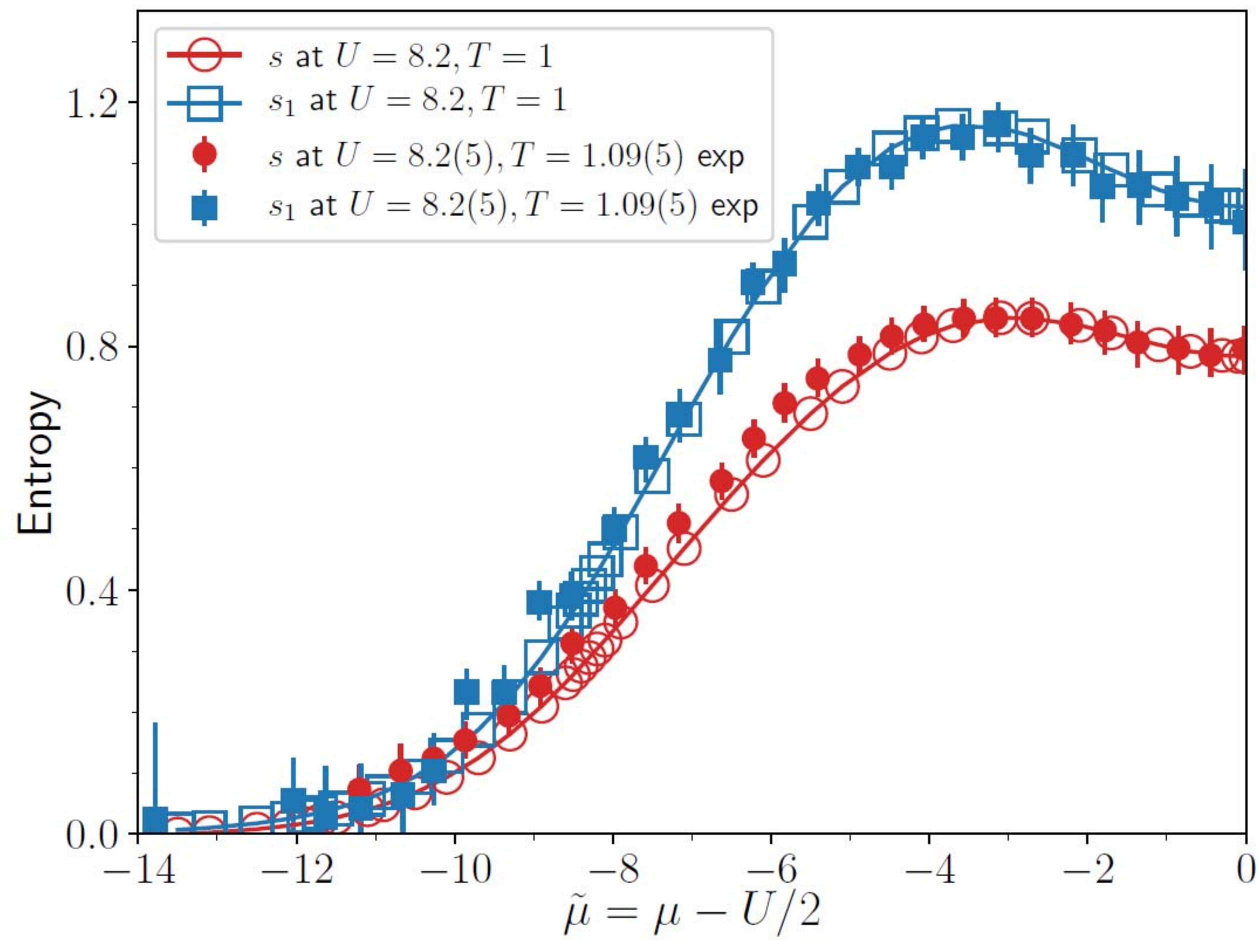
$$\rho_A = \mathrm{Tr}_B[\rho_{AB}] \qquad s_A = -\mathrm{Tr}_A[\rho_A \ln \rho_A]$$

$$\rho = \mathrm{diag}(p_0, p_\uparrow, p_\downarrow, p_{\uparrow\downarrow}) \qquad s_1 = -\sum_i p_i \ln(p_i)$$

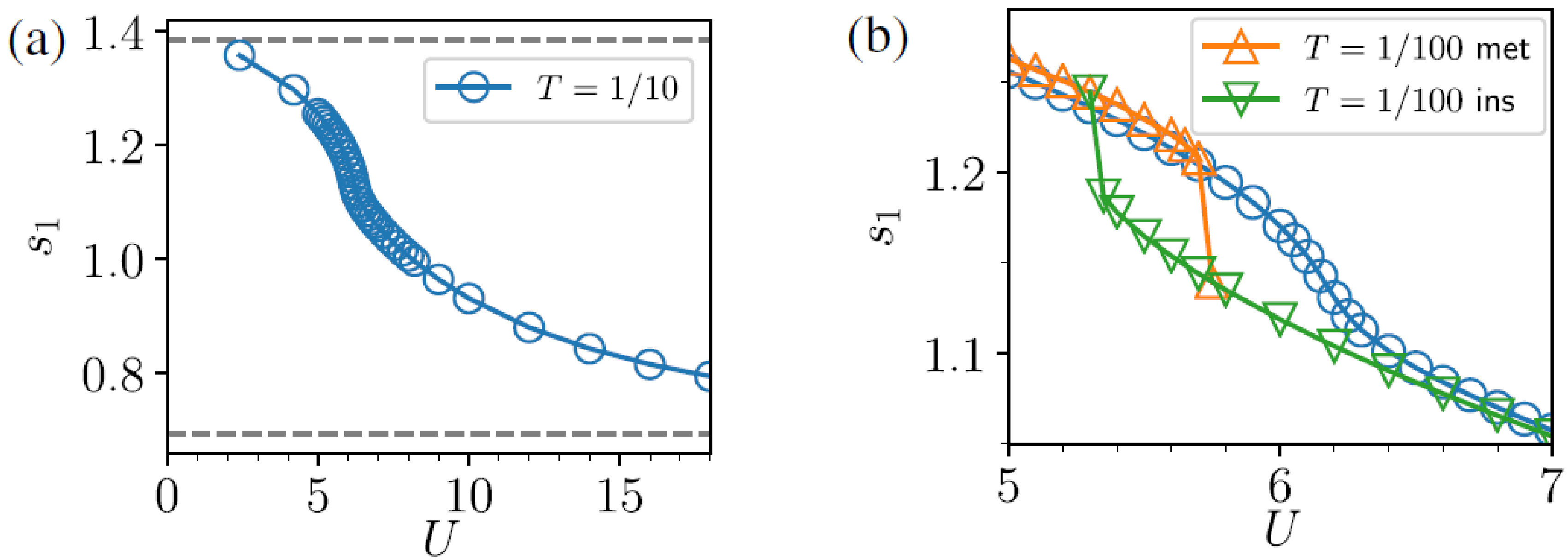
$$p_{\uparrow\downarrow} = \langle n_{i\uparrow} n_{i\downarrow} \rangle \qquad p_\uparrow = p_\downarrow = \langle n_{i\uparrow} - n_{i\uparrow} n_{i\downarrow} \rangle \qquad p_0 = 1–2p_\uparrow - p_{\uparrow\downarrow}$$

[1] P. Zanardi *et al.* Phys. Rev. A **65**, 042101 (2002).

Agreement with experiment

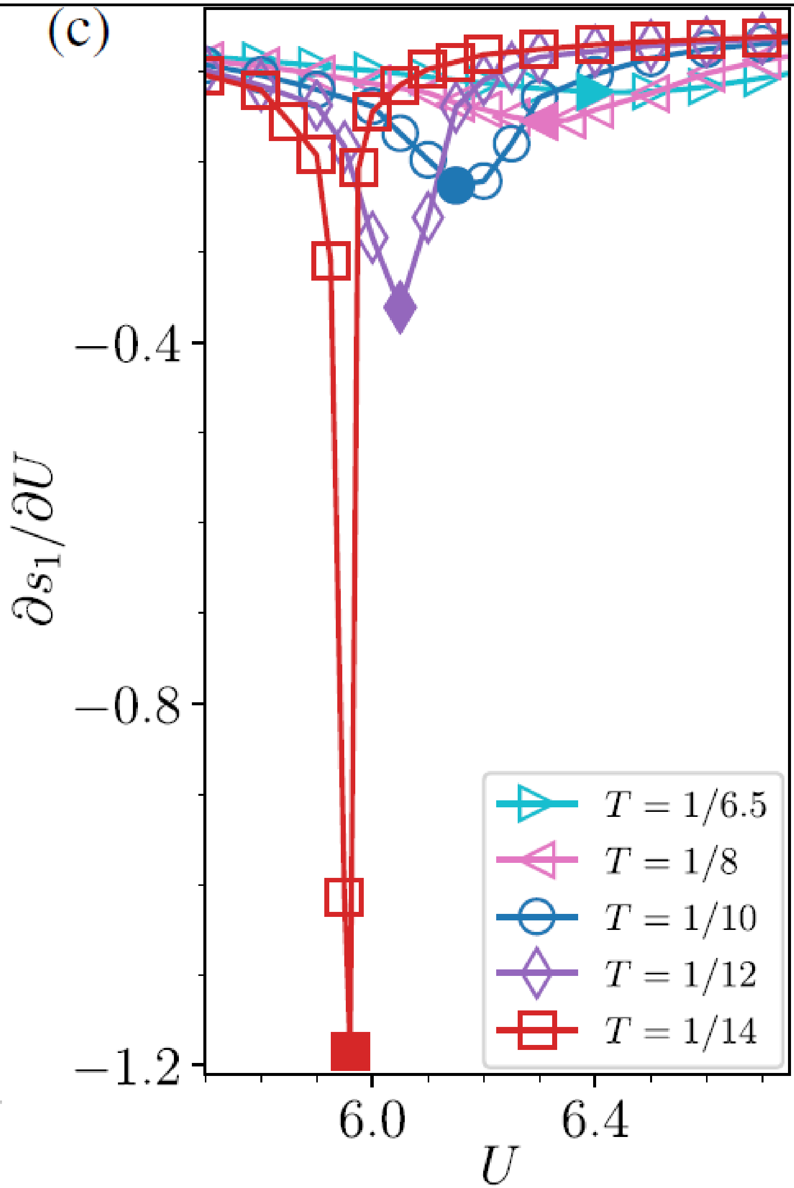


Results



$$\partial s_1 / \partial T < 0$$

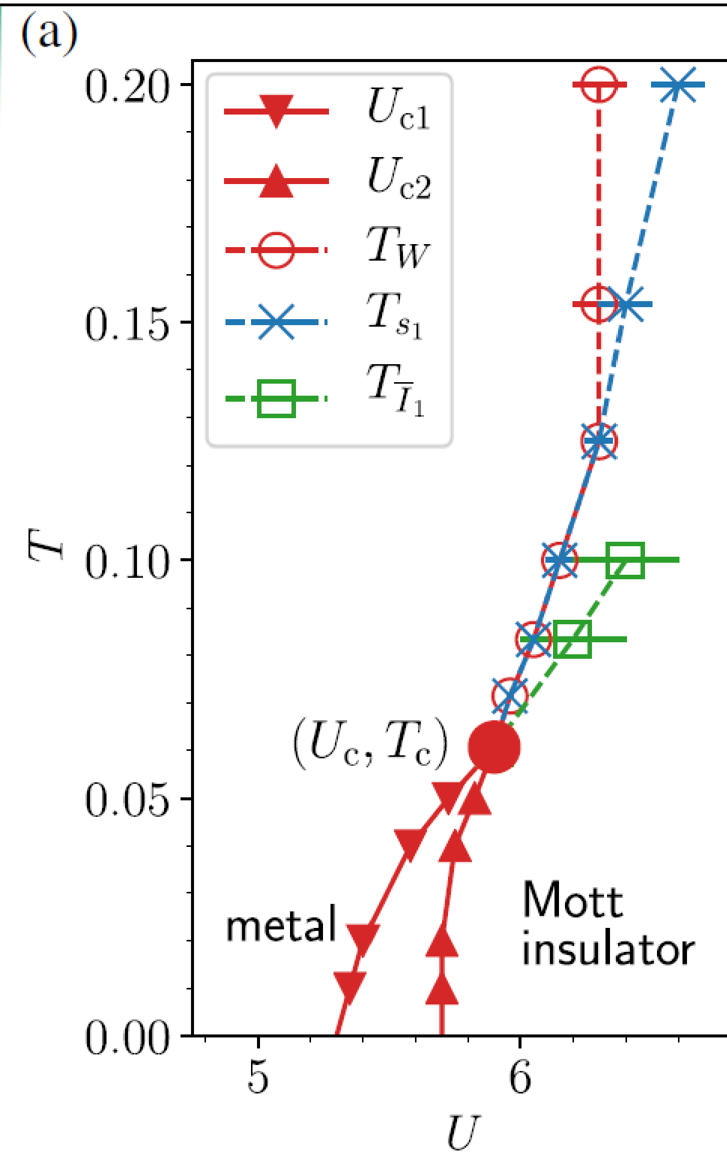
Results



$$(\partial s_1/\partial D)(\partial D/\partial U)$$

$$\partial D/\partial U \sim -|U - U_c|^{-1+1/\delta}$$

Transition and crossovers



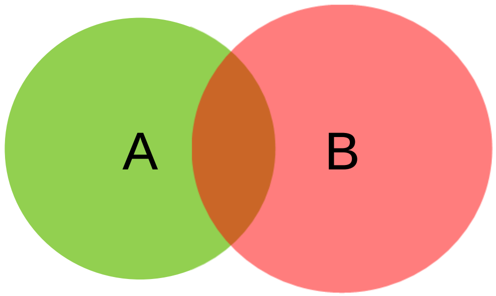
From single-site entanglement entropy

- The Mott transition,
- Critical exponent (not usually the case)
- Associated high-temperature crossovers,
  - Without knowledge of the order parameter of the transition

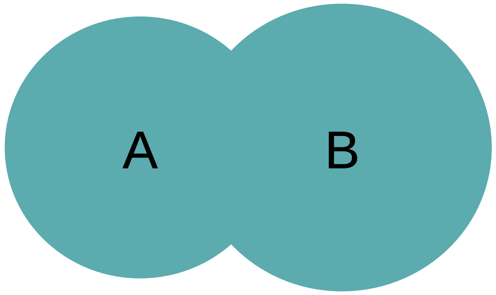
Mutual information

Mutual information

$$I(A:B) = s_A + s_B - s_{AB}$$



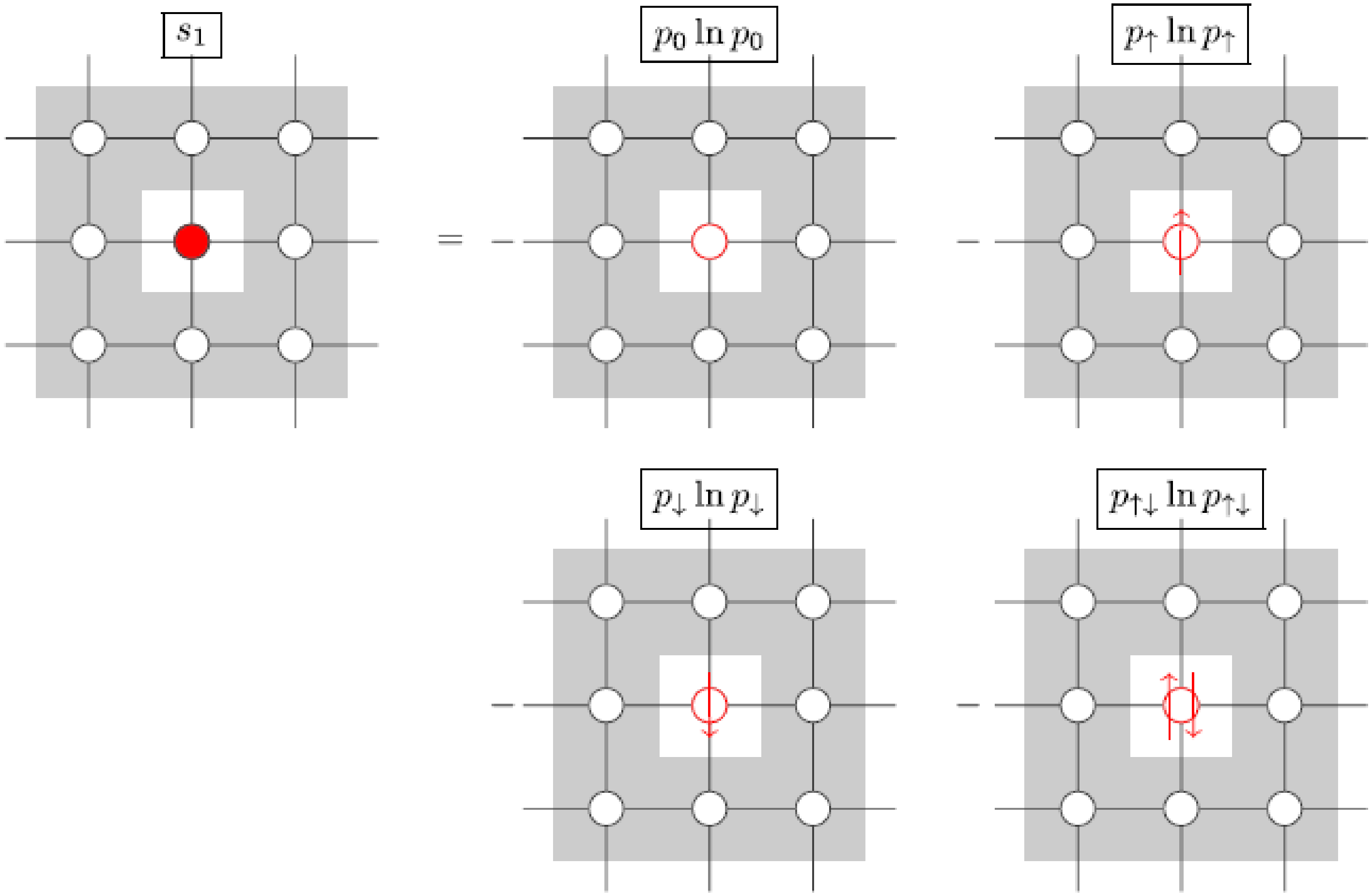
Here we are *not* looking at the area law

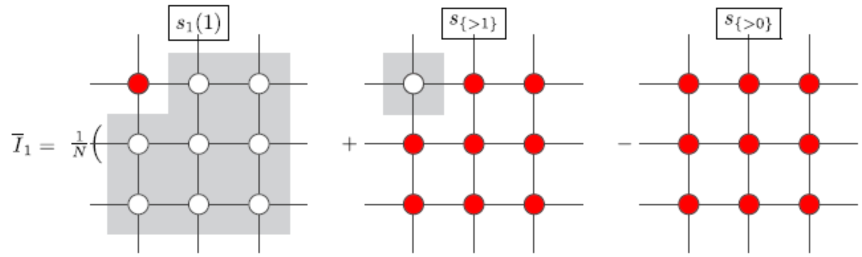


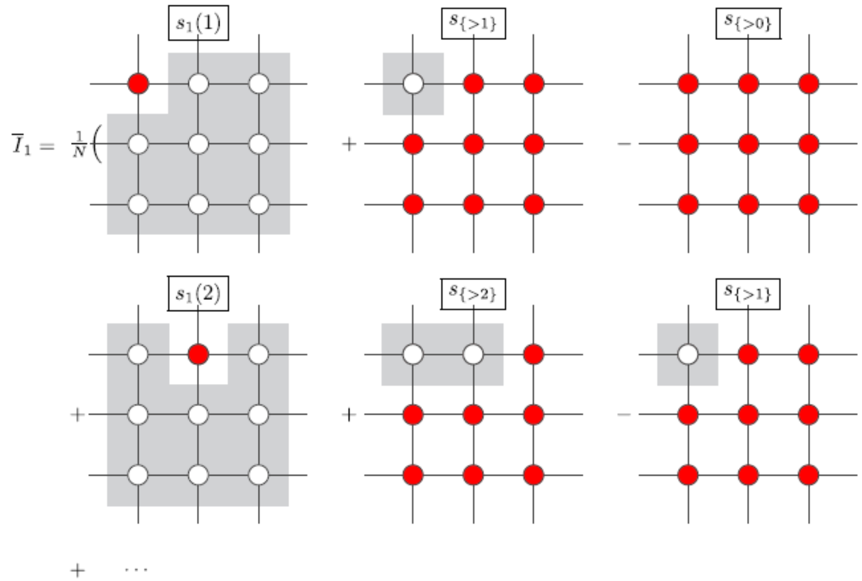
What is measured experimentally

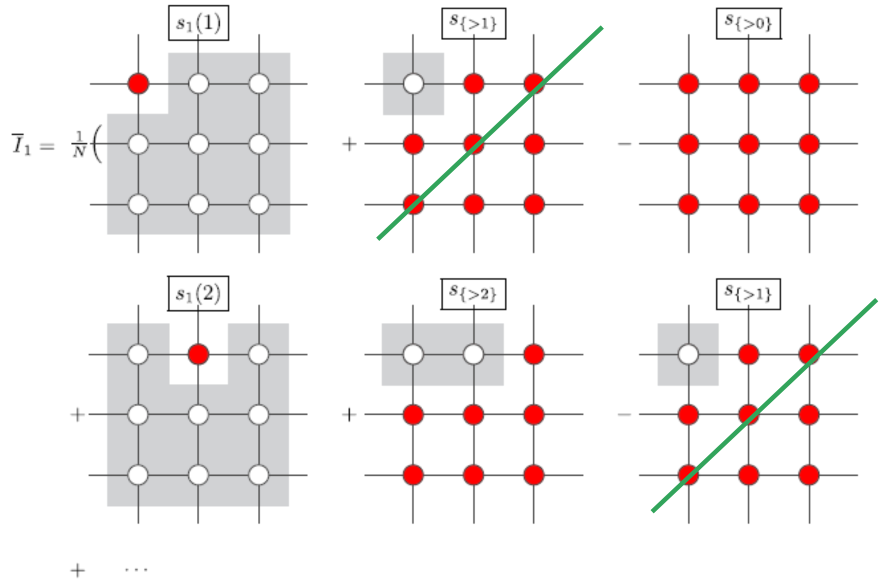
$$\bar{I}_1 = s_1 - s.$$

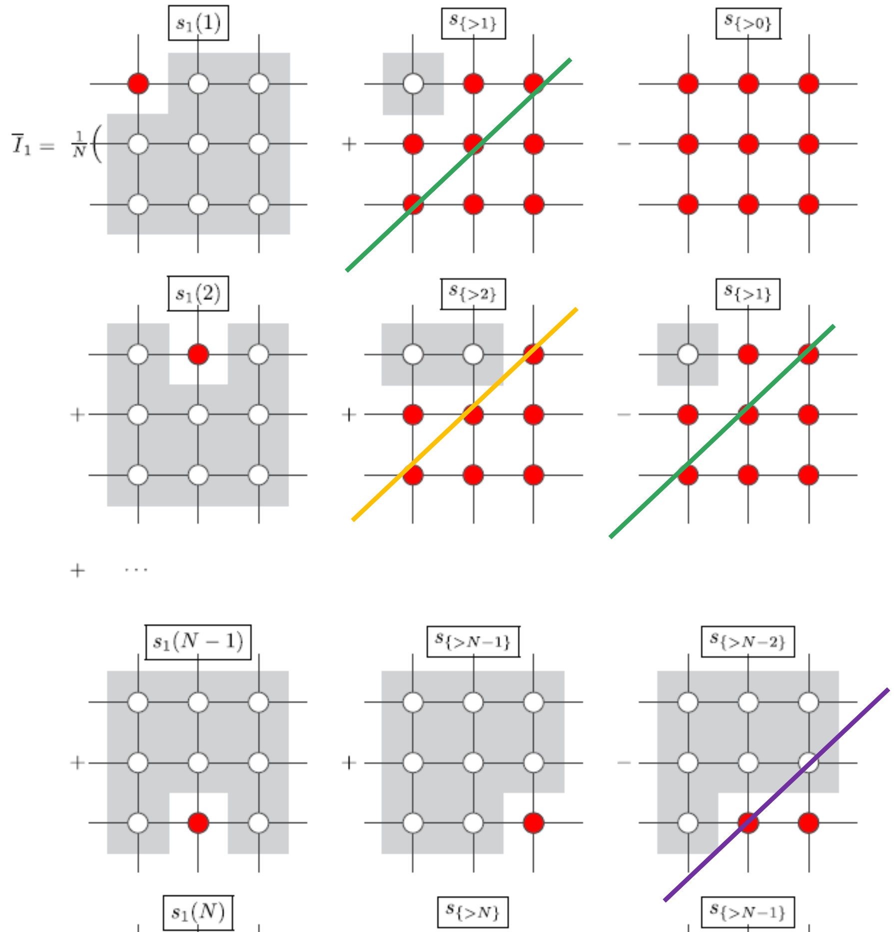
Total mutual information

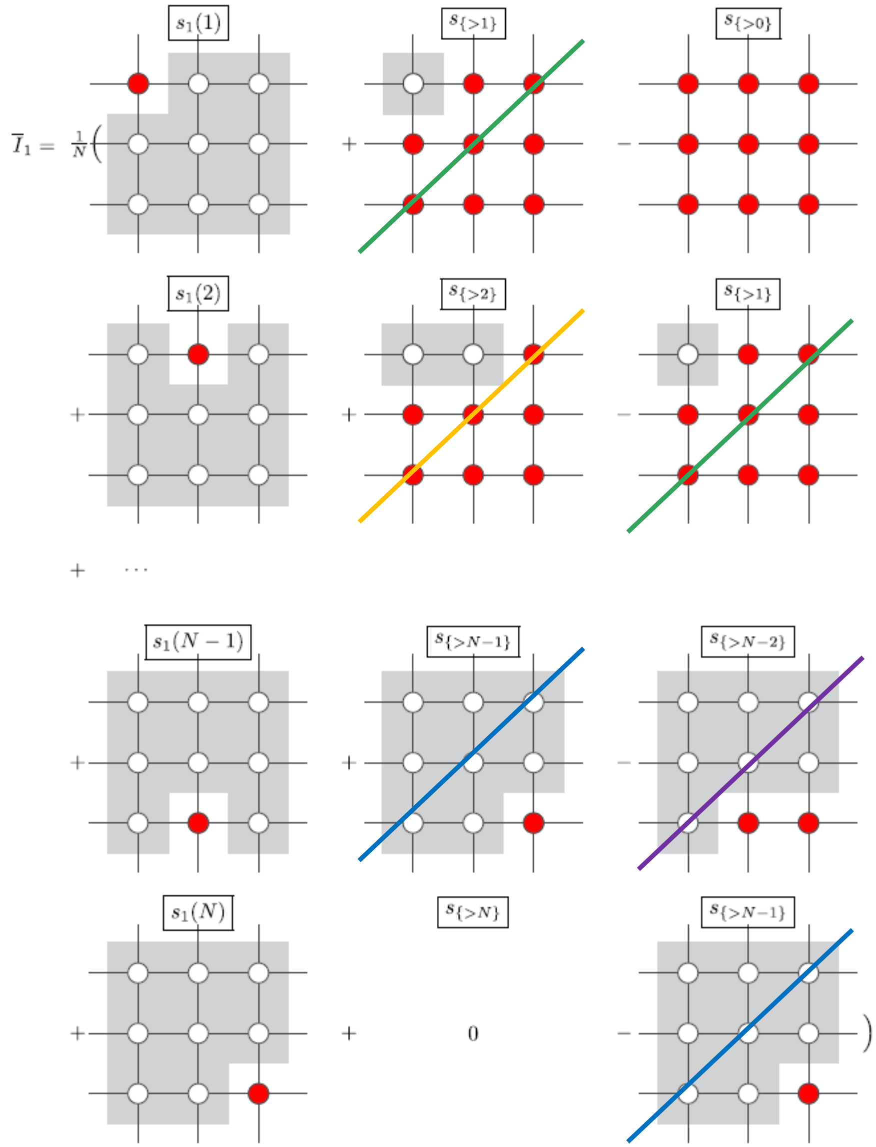

s_1
$=$
$-$
$p_0 \ln p_0$
$-$
$p_\uparrow \ln p_\uparrow$
$-$
$p_\downarrow \ln p_\downarrow$
$-$
$p_{\uparrow\downarrow} \ln p_{\uparrow\downarrow}$


$\overline{I}_1 = \frac{1}{N}\Big($
$s_1(1)$
$+$
$s_{\{>1\}}$
$-$
$s_{\{>0\}}$


$\bar{I}_1 = \frac{1}{N}\Big($
$s_1(1)$
$+$
$s_{\{>1\}}$
$-$
$s_{\{>0\}}$
$+$
$s_1(2)$
$+$
$s_{\{>2\}}$
$-$
$s_{\{>1\}}$
$+ \cdots$

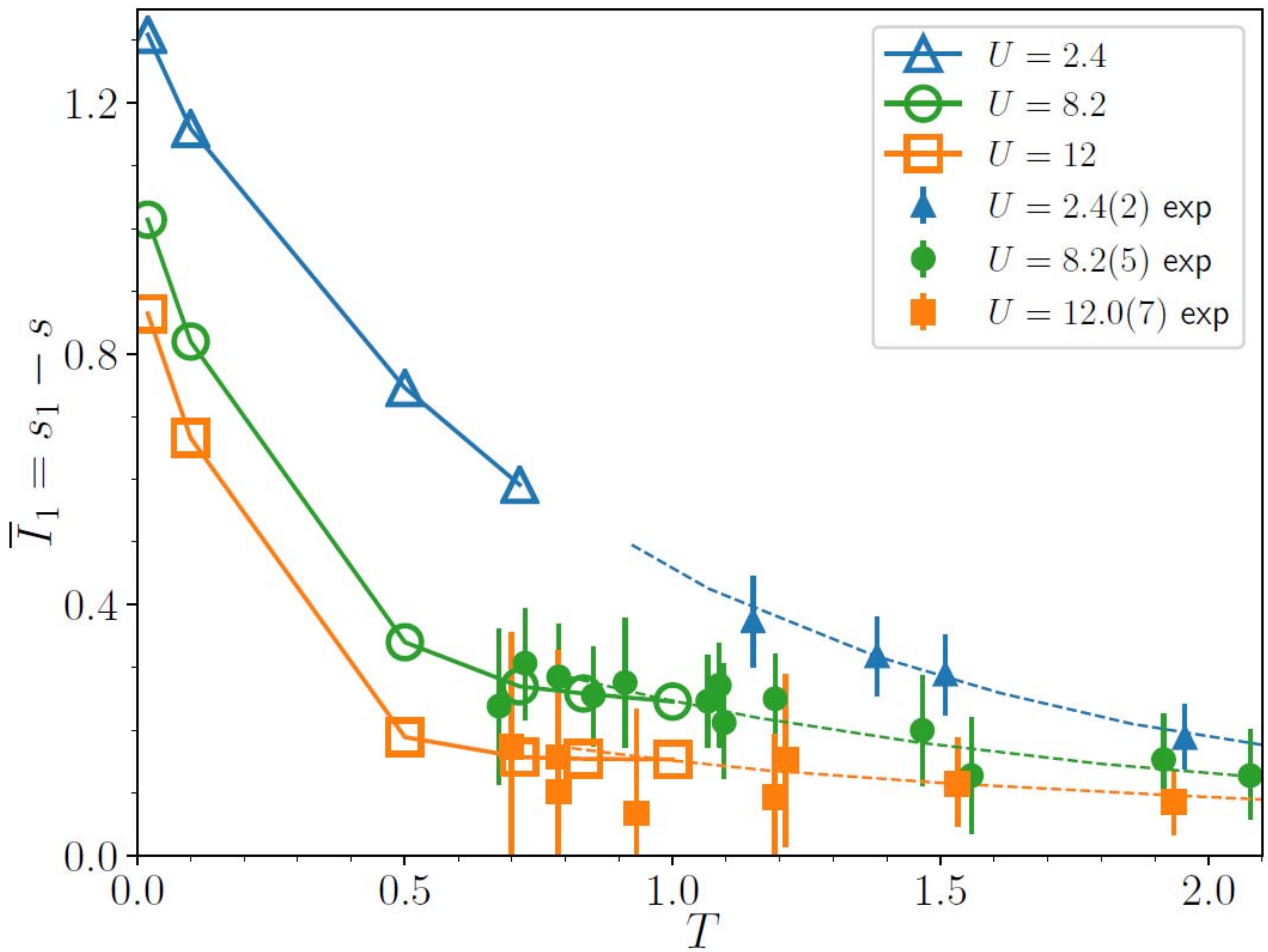

$\bar{I}_1 = \frac{1}{N}\Big($
$s_1(1)$
$+$
$s_{\{>1\}}$
$-$
$s_{\{>0\}}$
$+$
$s_1(2)$
$+$
$s_{\{>2\}}$
$-$
$s_{\{>1\}}$
$+ \cdots$


$\bar{I}_1 = \frac{1}{N}\Big($
$s_1(1)$
$+$
$s_{\{>1\}}$
$-$
$s_{\{>0\}}$
$+$
$s_1(2)$
$+$
$s_{\{>2\}}$
$-$
$s_{\{>1\}}$
$+ \cdots$
$+$
$s_1(N-1)$
$+$
$s_{\{>N-1\}}$
$-$
$s_{\{>N-2\}}$
$s_1(N)$
$s_{\{>N\}}$
$s_{\{>N-1\}}$



$\overline{I}_1 = \frac{1}{N}\Big($
$s_1(1)$
$+$
$s_{\{>1\}}$
$-$
$s_{\{>0\}}$
$s_1(2)$
$+$
$s_{\{>2\}}$
$-$
$s_{\{>1\}}$
$+ \quad \cdots$
$s_1(N-1)$
$+$
$s_{\{>N-1\}}$
$-$
$s_{\{>N-2\}}$
$s_1(N)$
$+$
$s_{\{>N\}}$
0
$-$
$s_{\{>N-1\}}$
$\Big)$

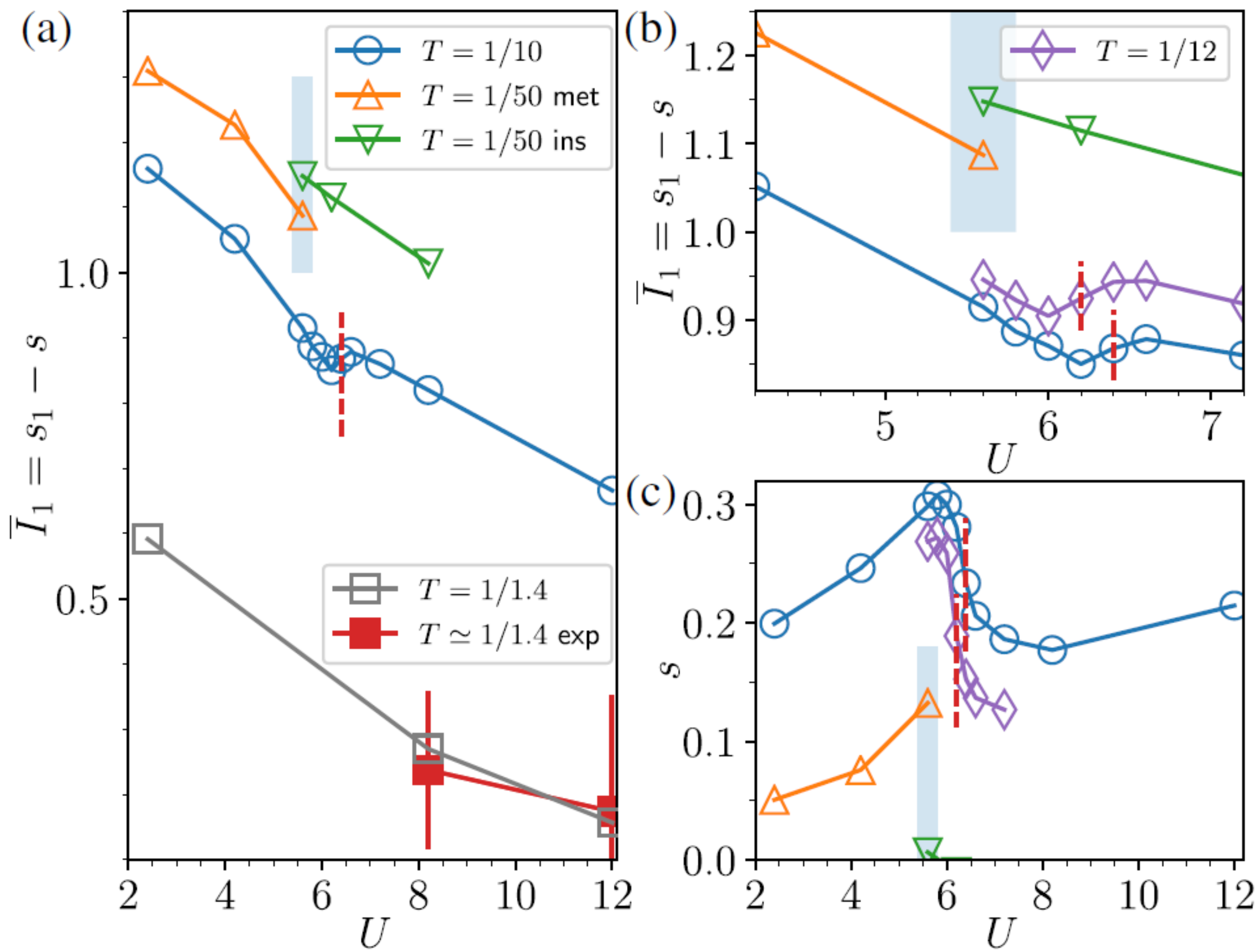
Agreement with experiment



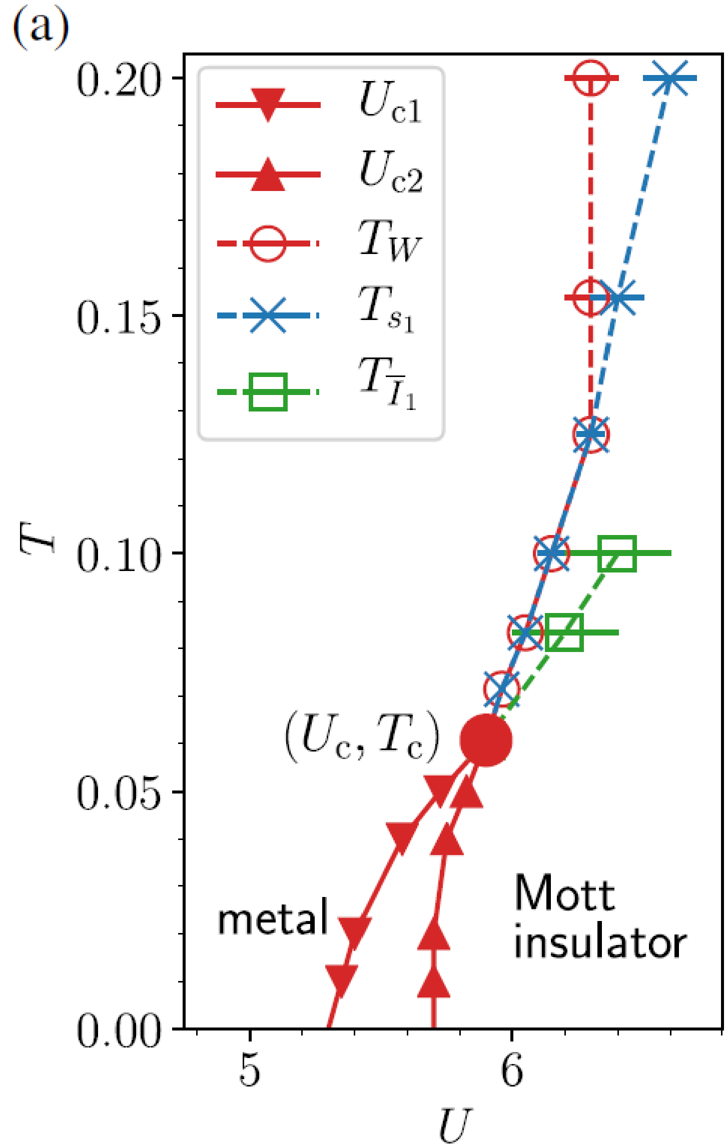
Results

$$\bar{I}_1 \sim \mathrm{sgn}(U - U_c)|U - U_c|^{1/\delta}$$

$$J = \frac{4t^2}{U}$$



Transition and crossovers



From average mutual information

- The Mott transition,
- Critical exponent (not usually the case)
- Associated high-temperature crossovers,
  - Without knowledge of the order parameter of the transition

Mutual information at the Doping-Driven Mott Transition

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PRX QUANTUM **1**, 020310 (2020)

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APOGÉE CANADA
FONDS D'EXCELLENCE EN RECHERCHE

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Total mutual information near the Widom line

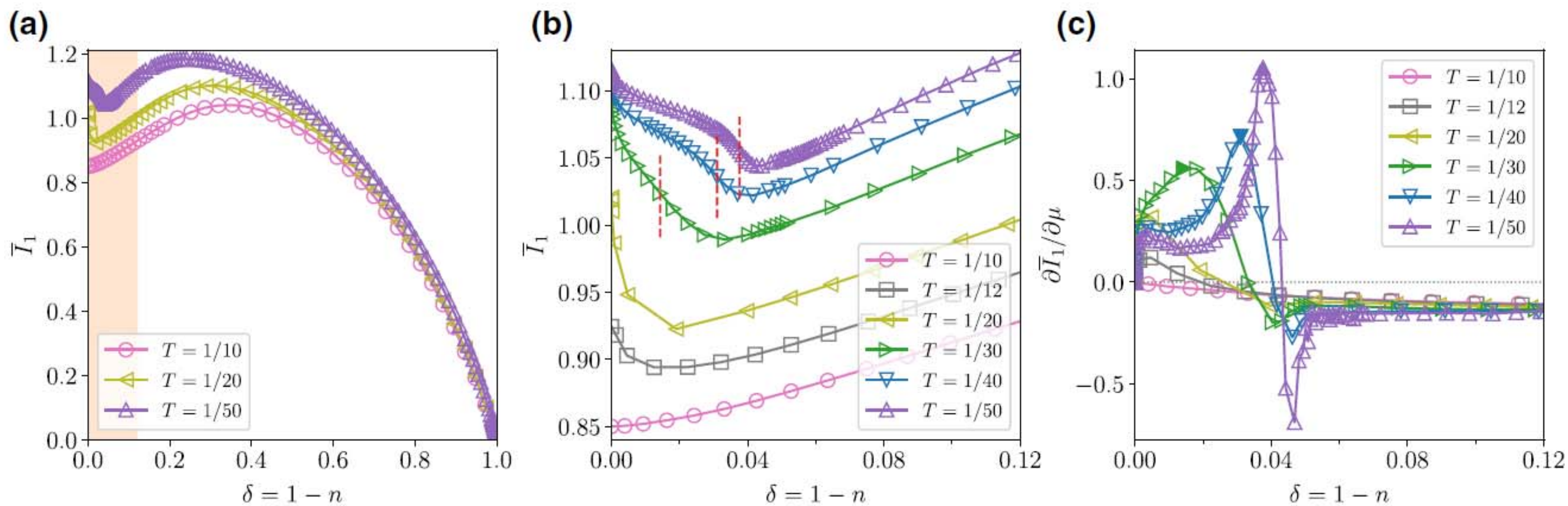
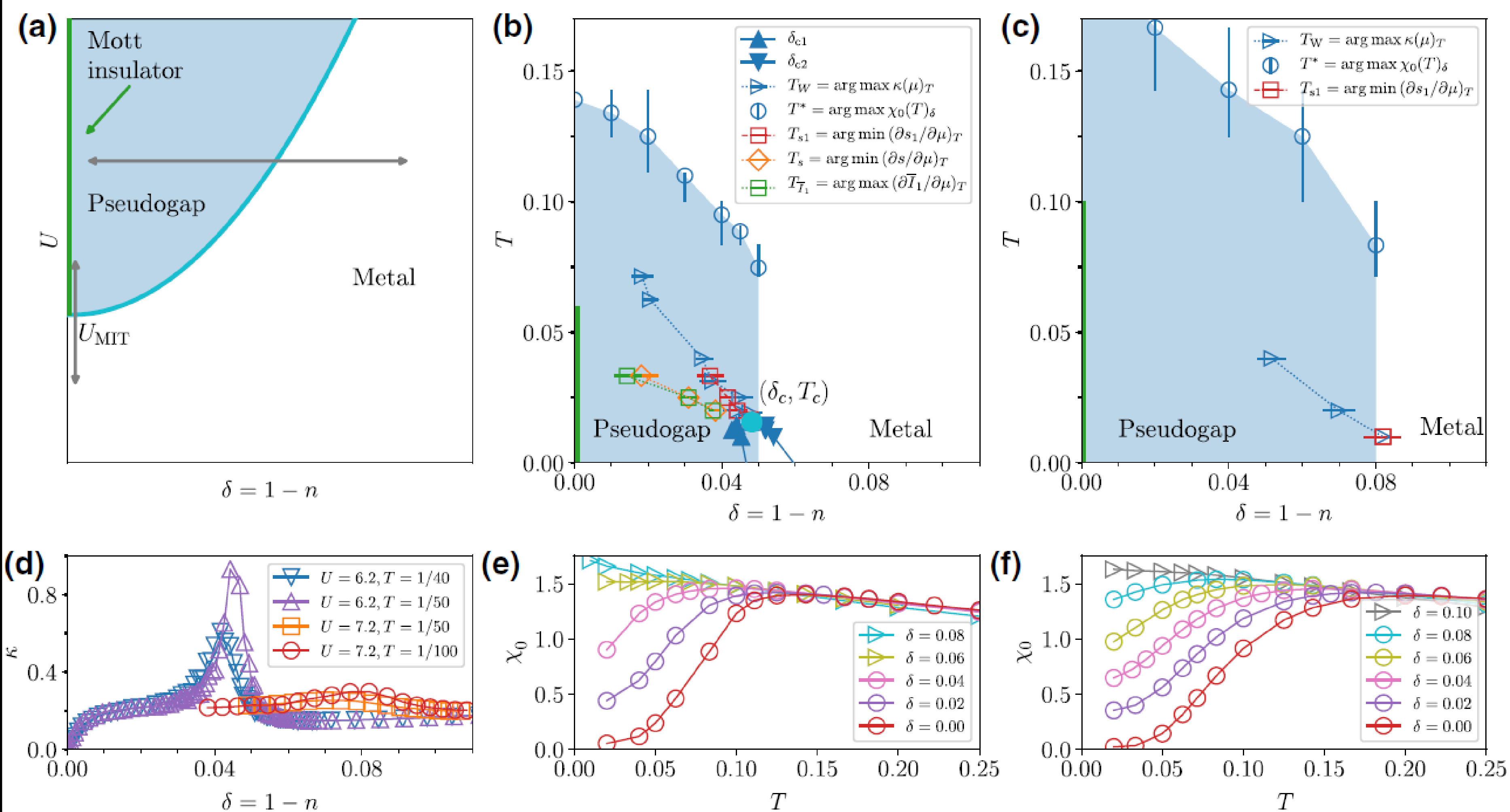


FIG. 10. (a) Total mutual information $\overline{I}_1$ versus δ for $U = 6.2 > U_{\mathrm{MIT}}$ and different temperatures. (b) The same as (a) for the doping interval shaded in (a), and highlighting the positions of the inflections that can be seen in $\overline{I}_1(\mu)_T$ (which are not visible as a function of δ) with vertical dashed lines. (c) Plot of $\partial\overline{I}_1/\partial\mu$ versus δ for different temperatures at $U = 6.2$, showing the peaks that become more pronounced on approaching T_c. We have used the loci of the inflections that show the sharpest change in $\overline{I}_1(\mu)$ to obtain the crossover line $T_{\overline{I}_1}$ in the $T - \delta$ phase diagram of Fig. 4(b).

Detecting the Sordi transition



Mutual information in the superconducting state

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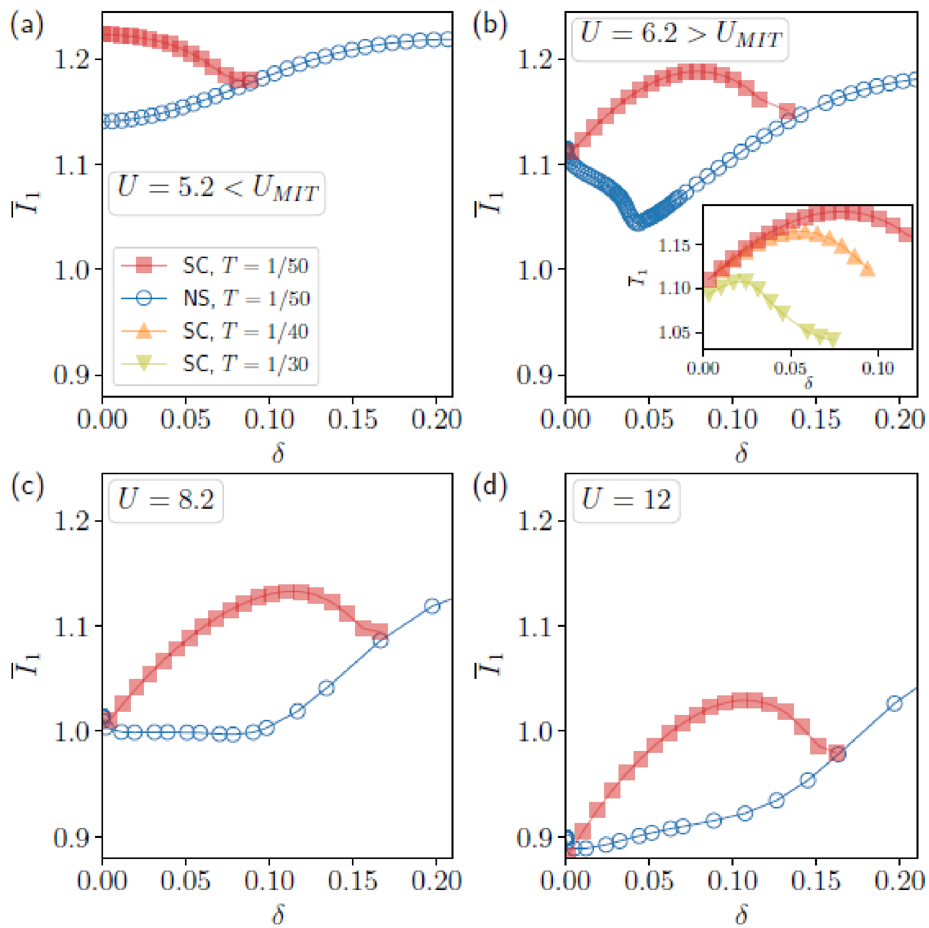
Total mutual information



Merci

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