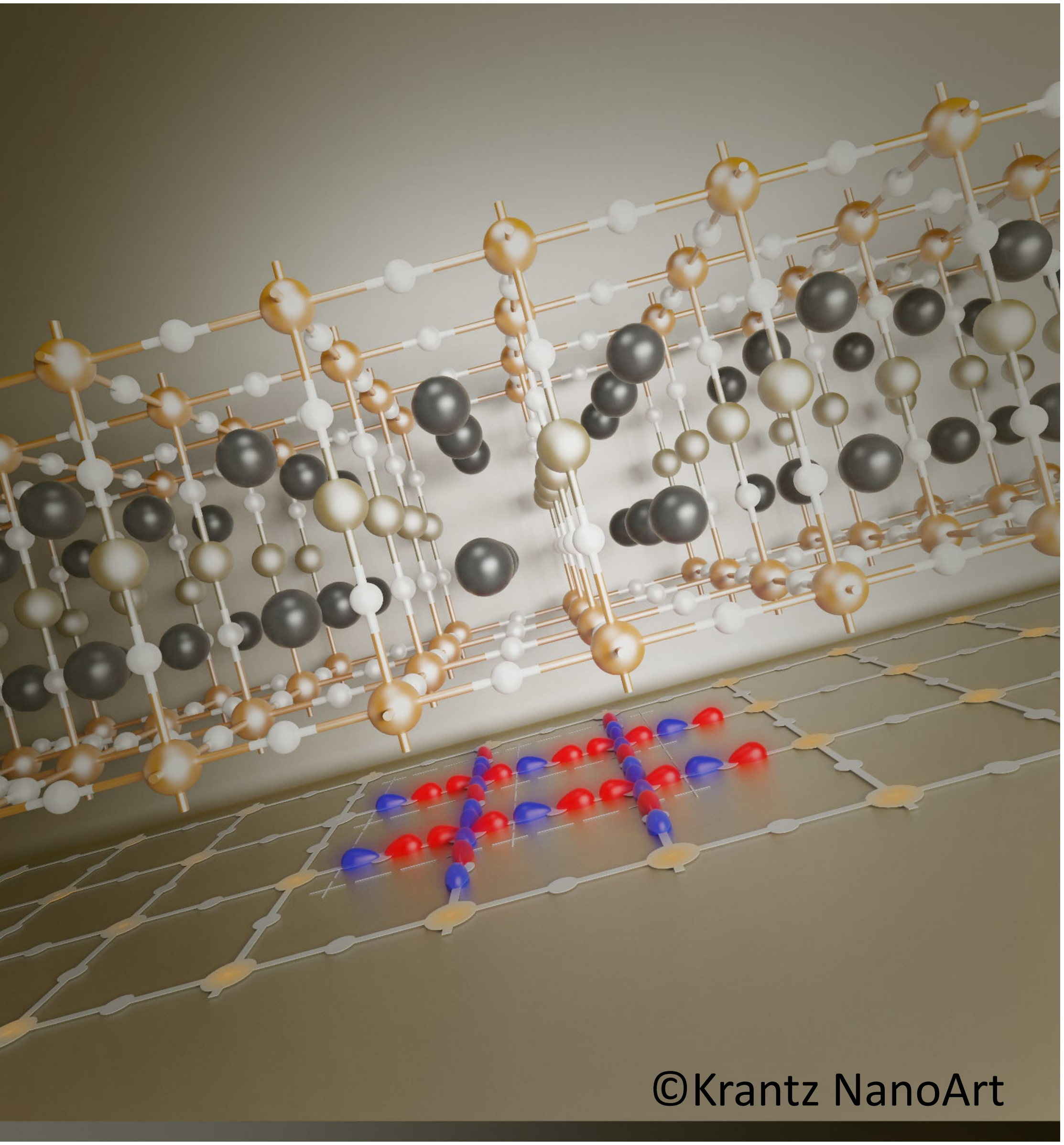

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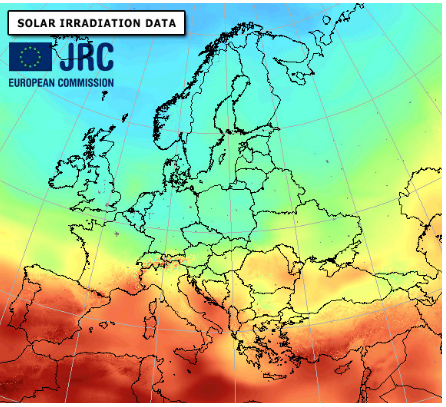
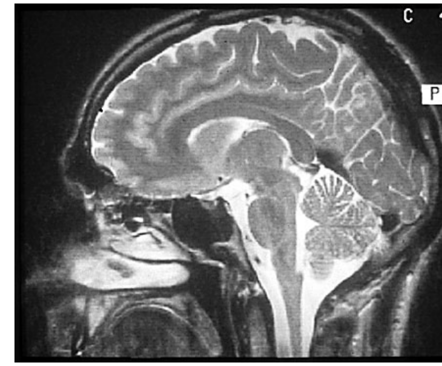
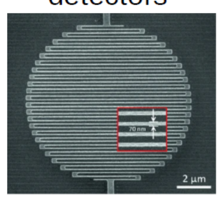
Applications



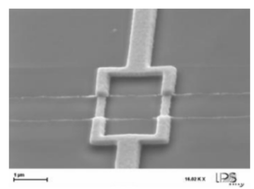


Single-photon detectors

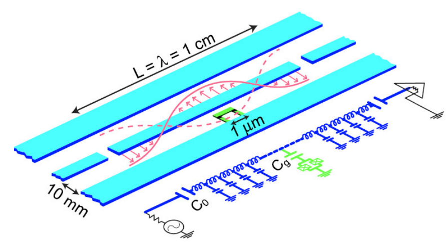


Najafi et al (2016)

Magnetometers



© : LPS



Alexandre Blais, et al. Phys. Rev. A **69**, 062320 (2004)

Photo IBM

A highly quantum mechanical problem

Université de Sherbrooke

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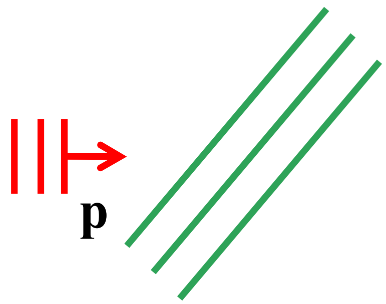
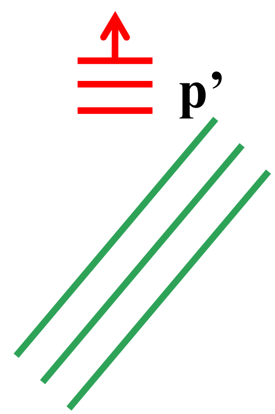
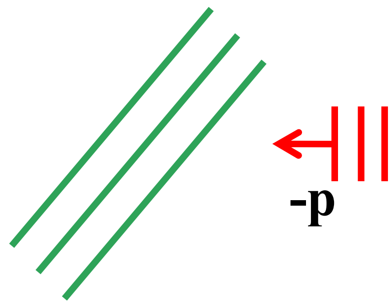
Attraction mechanism in the metallic state



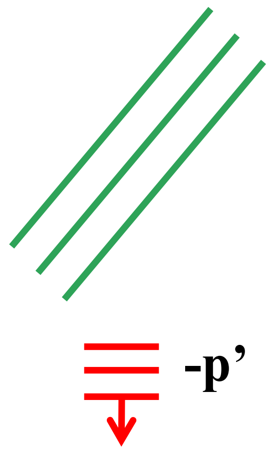
Attraction mechanism in the metallic state



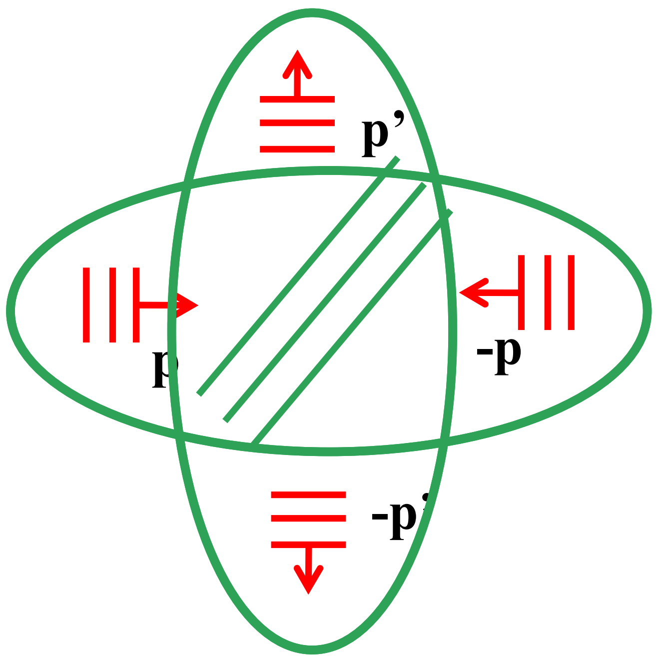
Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



Attraction mechanism in the metallic state

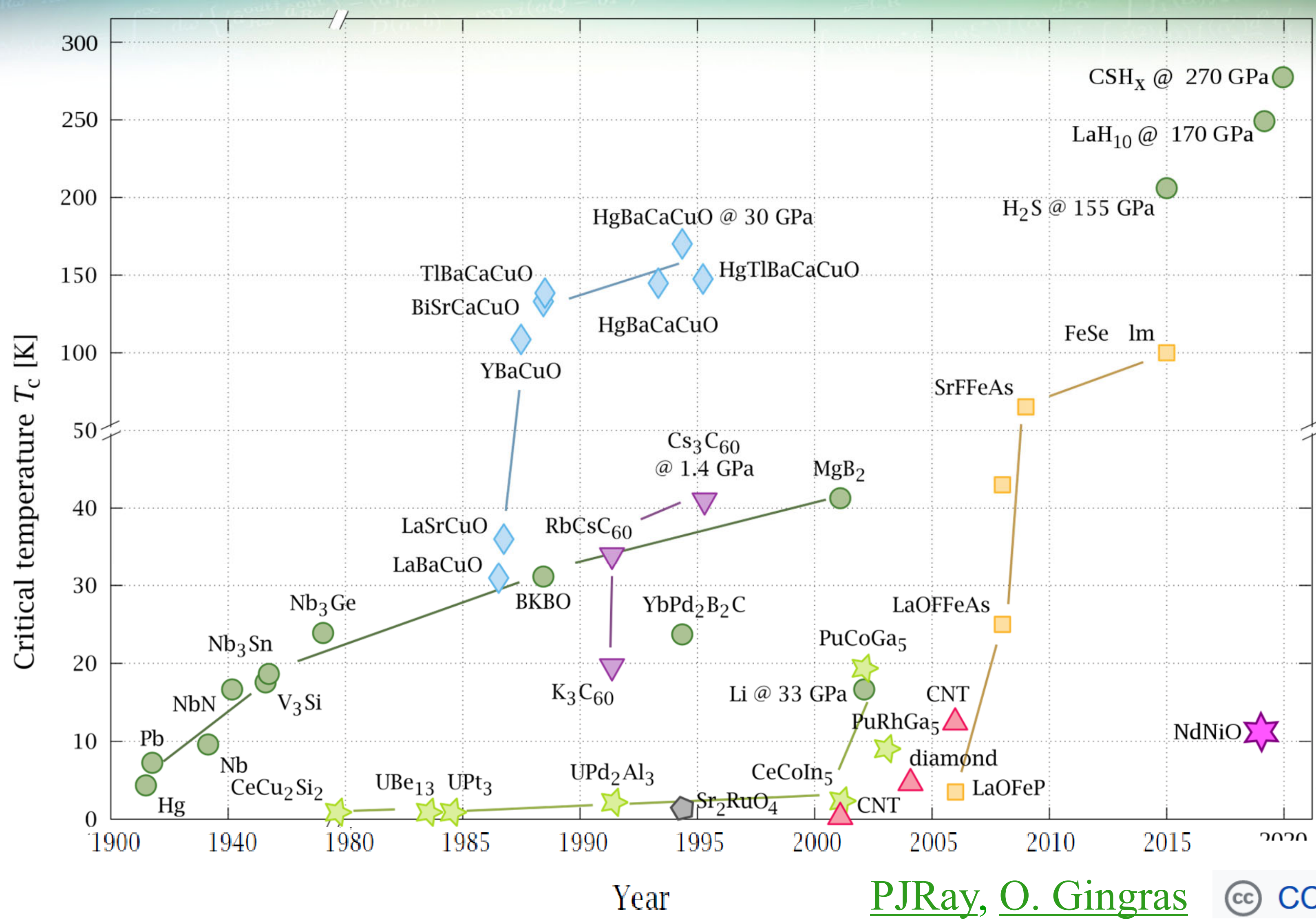


#1 Cooper pair, #2 Phase coherence

$$E_P = \sum_{\mathbf{p},\mathbf{p}'} U_{\mathbf{p}-\mathbf{p}'} \psi^*_{\mathbf{p}'\uparrow,-\mathbf{p}'\downarrow} \psi_{\mathbf{p}\uparrow,-\mathbf{p}\downarrow}$$

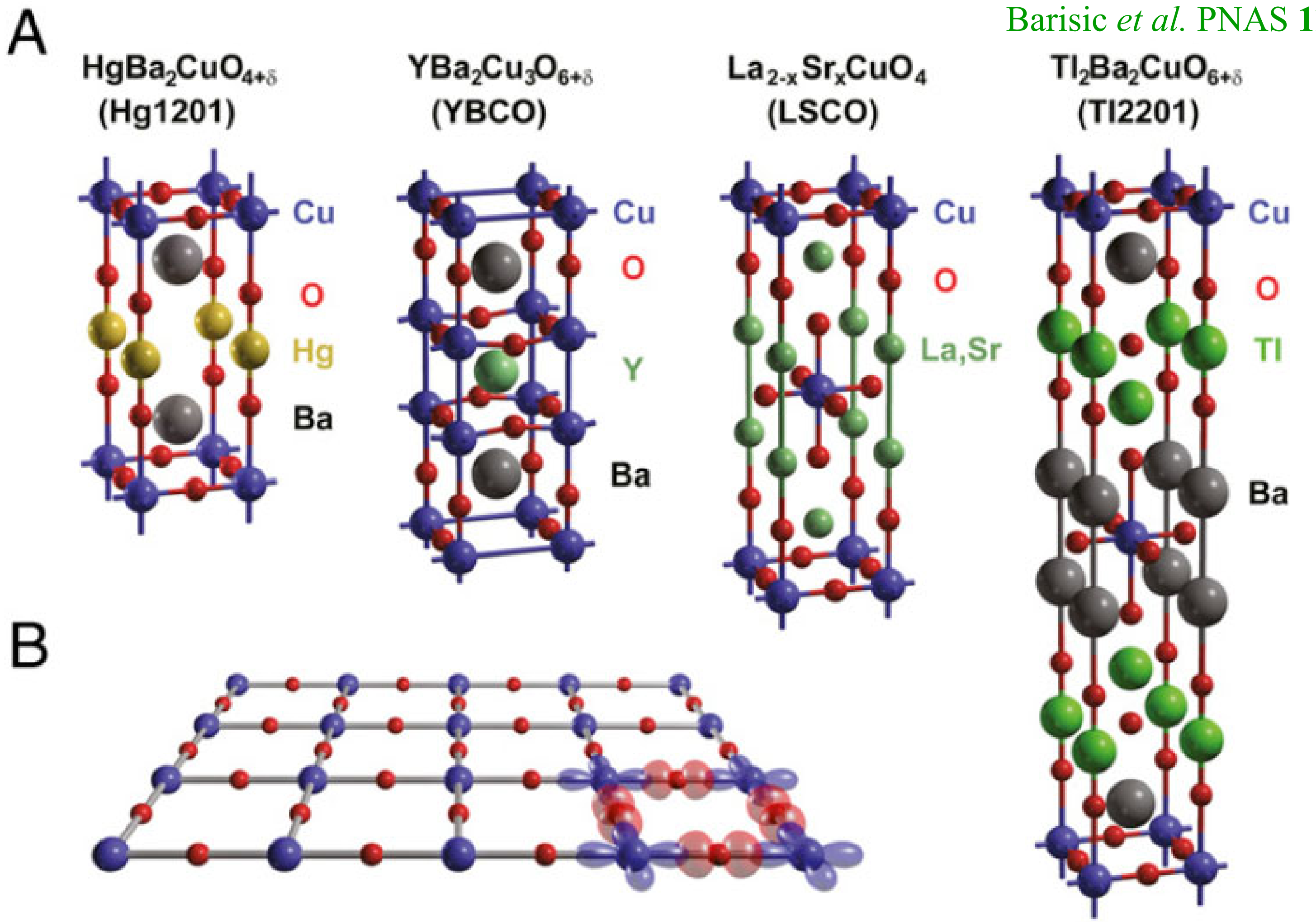
$$E_P = \sum_{\mathbf{p},\mathbf{p}'} U_{\mathbf{p}-\mathbf{p}'} \left\langle \psi^*_{\mathbf{p}'\uparrow,-\mathbf{p}'\downarrow} \right\rangle \left\langle \psi_{\mathbf{p}\uparrow,-\mathbf{p}\downarrow} \quad \right\rangle$$

$$|\mathrm{BCS}(\theta)\rangle = \ldots + e^{iN\theta}|N\rangle + e^{i(N+2)\theta}|N+2\rangle + \ldots.$$

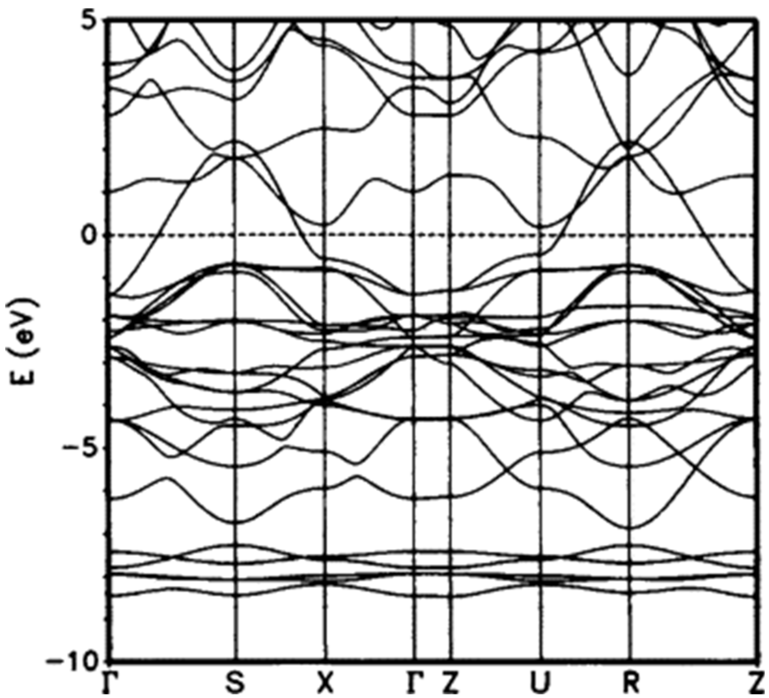

Critical temperature T_c [K]
Year
300
250
200
150
100
50
40
30
20
10
0
1900
1940
1980
1985
1990
1995
2000
2005
2010
2015
2020
CSH$_x$ @ 270 GPa
LaH$_{10}$ @ 170 GPa
H$_2$S @ 155 GPa
HgBaCaCuO @ 30 GPa
TlBaCaCuO
HgTlBaCaCuO
BiSrCaCuO
HgBaCaCuO
YBaCuO
FeSe lm
SrFFeAs
Cs$_3$C$_{60}$
@ 1.4 GPa
MgB$_2$
LaSrCuO
RbCsC$_{60}$
LaBaCuO
BKBO
Nb$_3$Ge
YbPd$_2$B$_2$C
LaOFFeAs
Nb$_3$Sn
PuCoGa$_5$
NbN
V$_3$Si
K$_3$C$_{60}$
Li @ 33 GPa
CNT
PuRhGa$_5$
NdNiO
Pb
Nb
diamond
CeCu$_2$Si$_2$
UBe$_{13}$
UPt$_3$
UPd$_2$Al$_3$
CeCoIn$_5$
LaOFeP
Hg
Sr$_2$RuO$_4$
CNT

There are different kinds of cuprates : All with CuO_2 planes

Barisic *et al.* PNAS **110**, 12235 (2013)

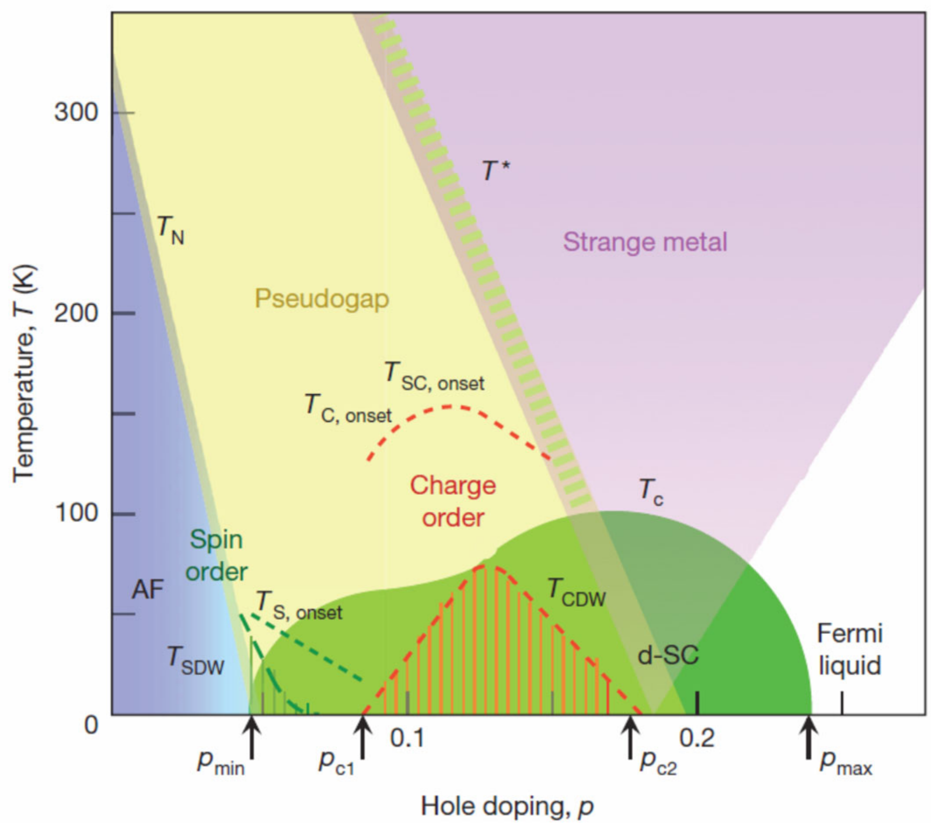


Electronic structure (band) Hg1201



Charles P. PooleJr., ... Ruslan Prozorov, in Superconductivity (Second Edition), 2007

Phase diagram $YBa_2Cu_3O_{7-x}$



p or δ

Keimer et al., Nature 518, 179 (2015)

Model

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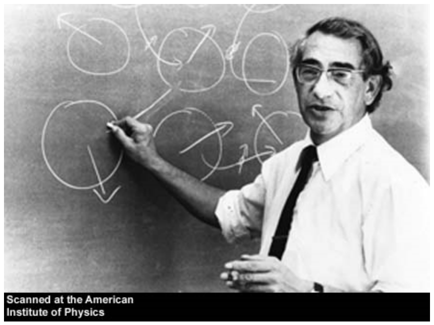
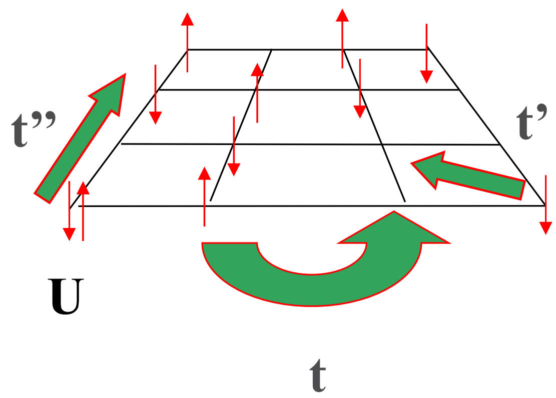
Hubbard Model



1931-1980

μ

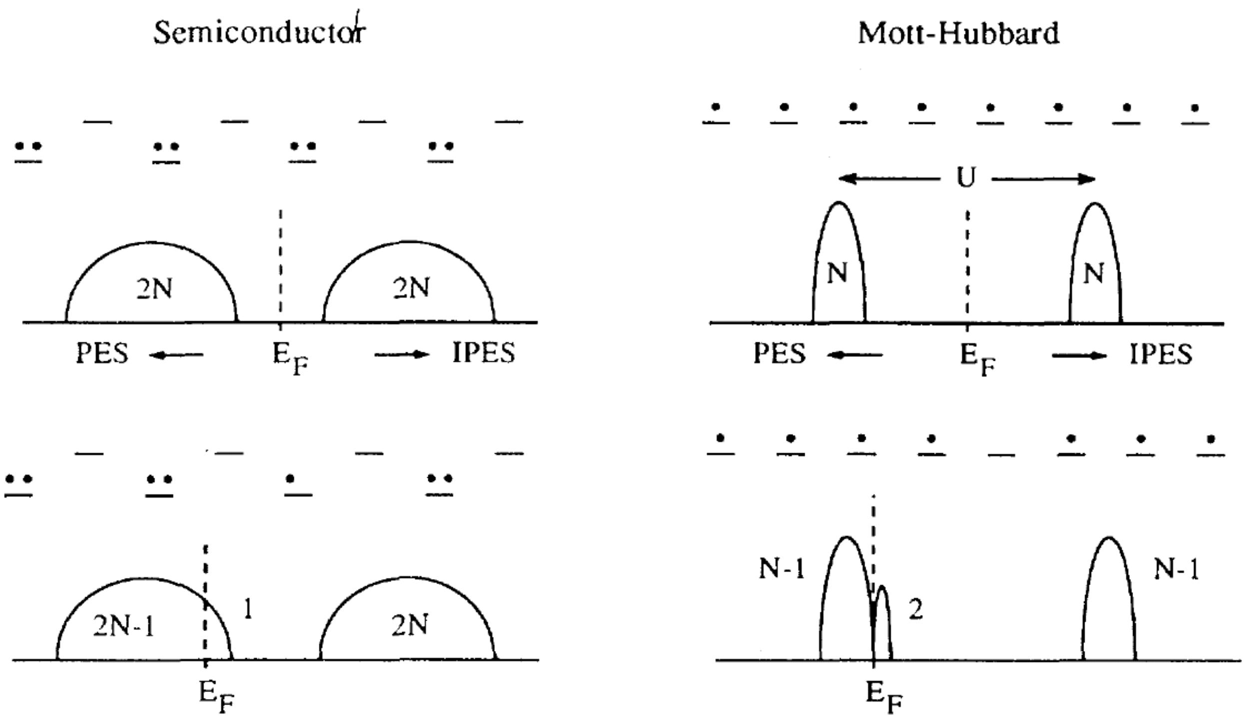


$$H = -\sum_{<ij>\sigma} t_{i,j} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$$t = 1, \; k_B = 1, \; \hbar = 1$$

Attn: Charge transfer insulator

Mott insulator vs band insulator : Spectral weight transfer



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

Method
Solving the models

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

Method

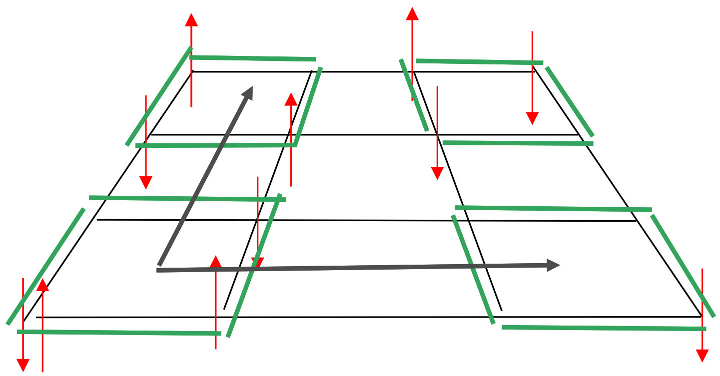
Cluster generalization of
Dynamical Mean-Field Theory : DMFT

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

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

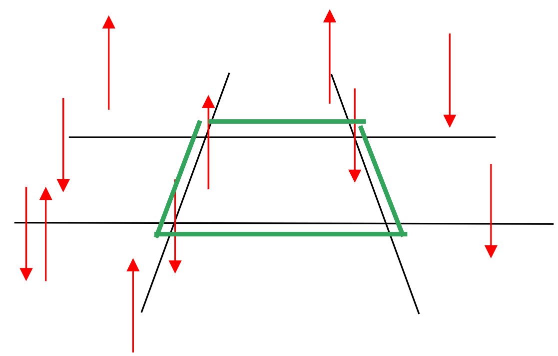
Localized and delocalized pictures C-DMFT

Delocalized



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

Localized



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

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

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

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

Impurity solvers

Impurity solver : continuous-time quantum Monte Carlo

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

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**

Two messages:

1. Condensation energy for large interaction U

2. Quantum-information measure of the superconducting state

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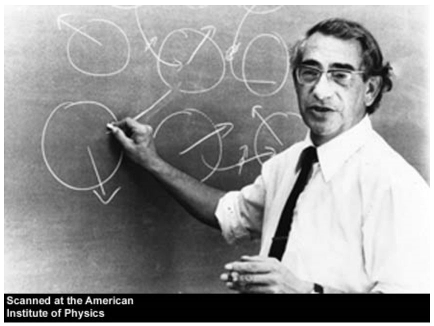
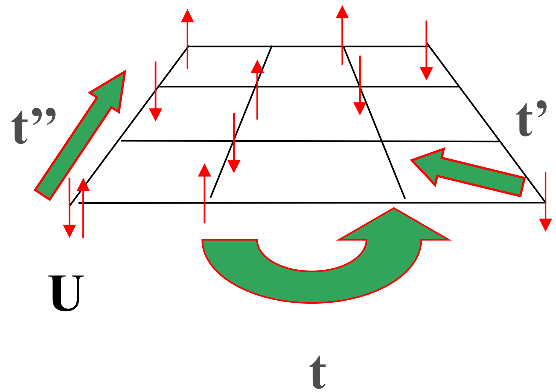
Superconductivity in cuprates
Condensation energy

Hubbard model

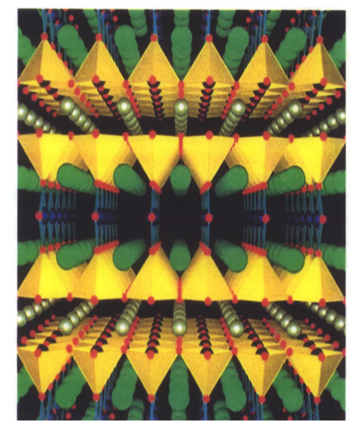


1931-1980

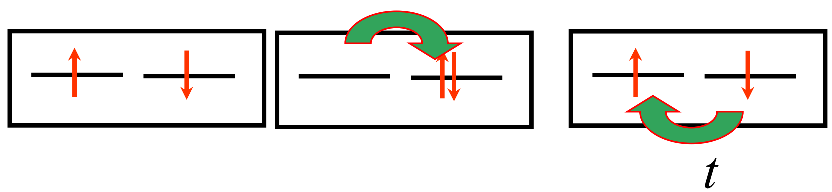
μ



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



Spin 1/2

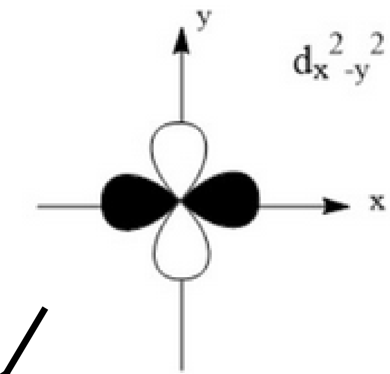


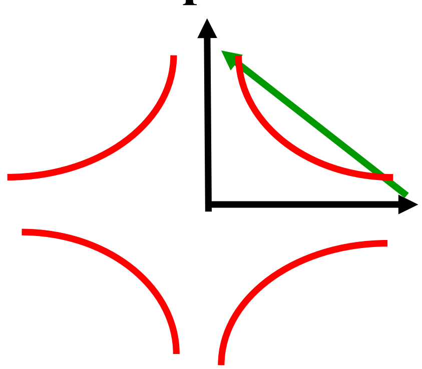
Effective model, Heisenberg: $J = 4t^2/U$

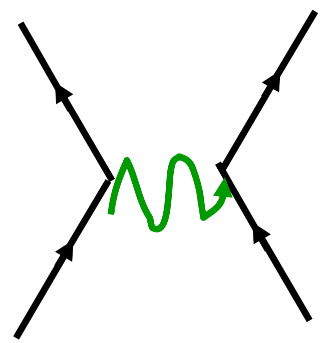
Attn: Charge transfer insulator

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)

A cartoon strong correlation picture

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

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

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

Pitaevskii Brückner:

Pair state orthogonal to repulsive core of Coulomb interaction

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

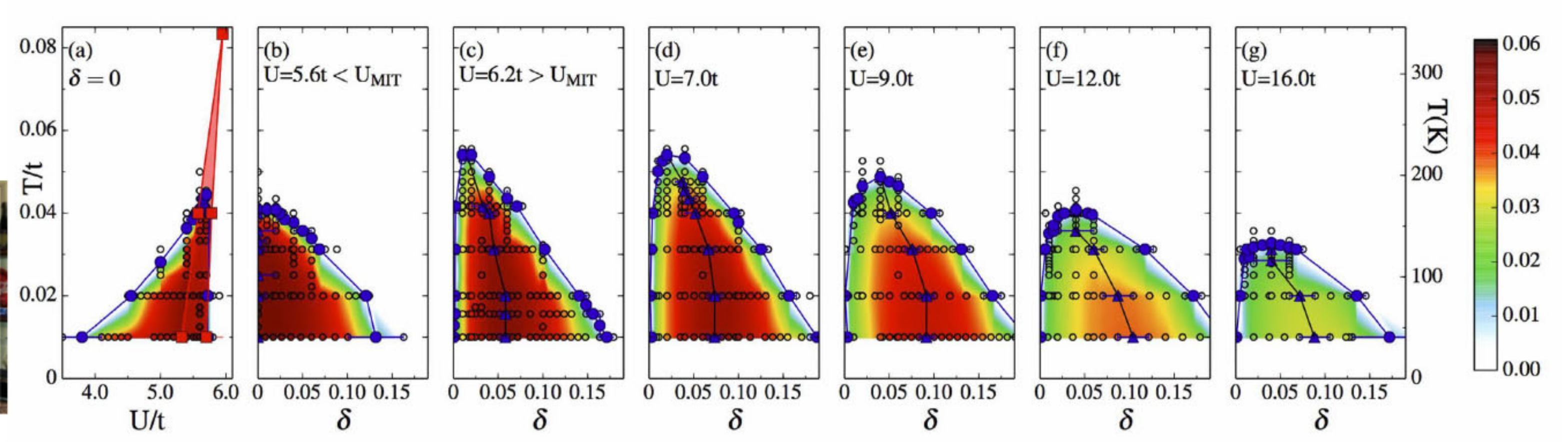
Miyake, Schmitt–Rink, and Varma P.R. B **34**, 6554-6556 (1986)

More sophisticated Slave Boson: Kotliar Liu PRB 1988

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

Fratino et al. Sci. Rep., 6, 22715 (2016)

$J = 4t^2 / U$



Lorenzo Fratino

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

Patrick Sémon

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

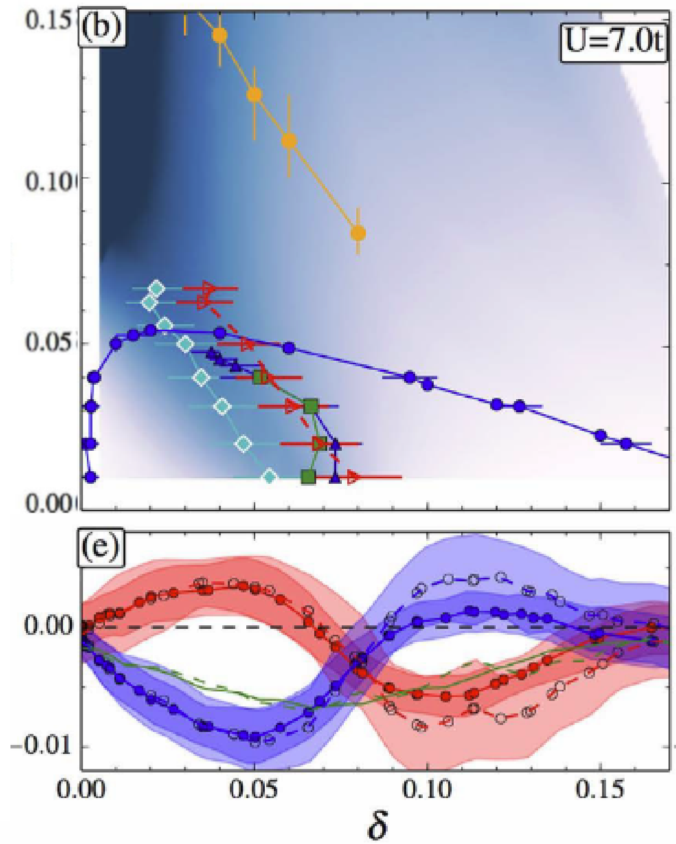
Patrick M. Rourke, et al. Hussey Nature Physics **7,** 455–458 (2011)

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

Giovanni Sordi

Condensation energy

Fratino et al. Sci. Rep. 6, 22715 (2016)



Theory, see also Jarrel PRL (2004), Gull Millis PRB (2014)

Experiments: Bontemps, Santander-Syro Van der Marel …

Message from part I

- Tc for Cooper pair formation is controled by J in the doped Mott insulator.

- Kinetic energy can favor pairing near half-filling (Anderson)

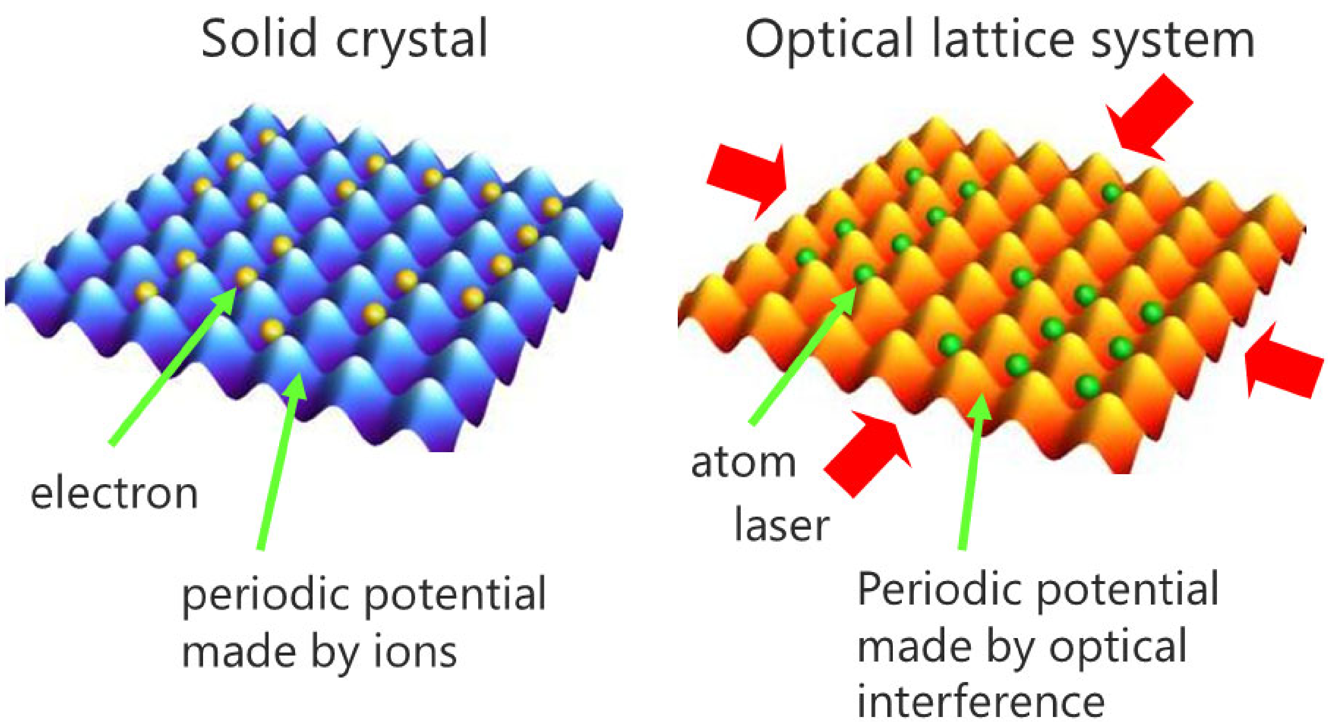
Part II
Quantum Information perspective

PRL 122, 067203 (2019)

PRX Quantum 1, 020310 1/17 (2020)

PNAS, 118 (25), e2104114118, (2021).

The analogy

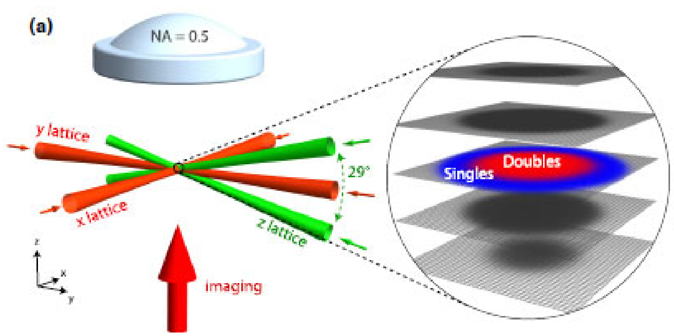


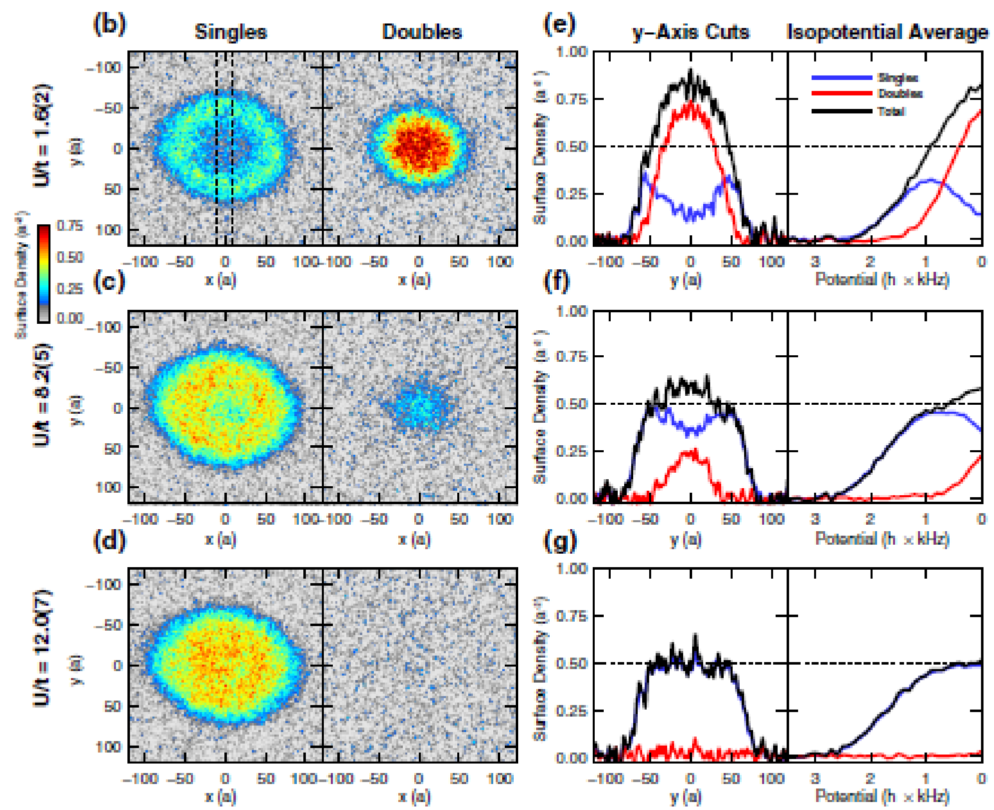
http://www.kozuma-eng.sci.titech.ac.jp/research_category/entry17.html

Selected for a Viewpoint in *Physics*
PRL **116,** 175301 (2016) PHYSICAL REVIEW LETTERS week ending 29 APRIL 2016

Equation of State of the Two-Dimensional Hubbard Model

Eugenio Cocchi,[1,2] Luke A. Miller,[1,2] Jan H. Drewes,[1] Marco Koschorreck,[1] Daniel Pertot,[1] Ferdinand Brennecke,[1] and Michael Köhl[1,*]





T = 0.3 *t*

Mutual information

PRL 122, 067203 (2019)

Caitlin Walsh

Patrick Sémon

David Poulin

Giovanni Sordi

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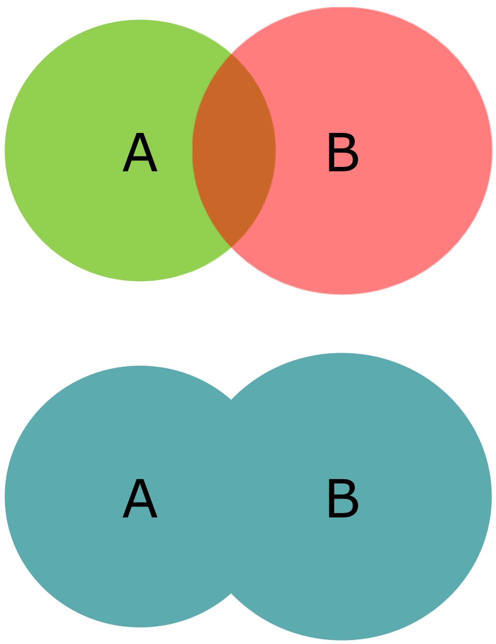
Mutual information

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

Here we are *not* looking at the area law



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).

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

- Single site entanglement entropy for fermions [1]

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

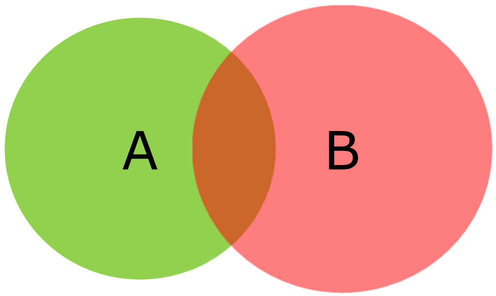
$$\rho = \mathrm{diag}(p_0, p_\uparrow, p_\downarrow, p_{\uparrow\downarrow}) \qquad s_1 = -\sum_i p_i \ln(p_i)$$

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

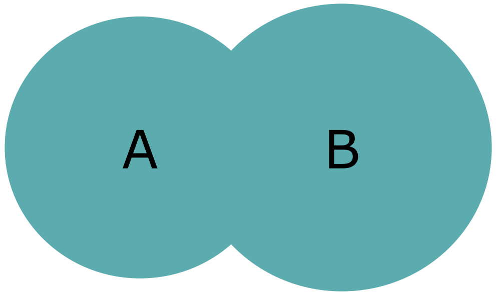
[1] P. Zanardi *et al.* Phys. Rev. A **65**, 042101 (2002).

Mutual information

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



What is measured experimentally



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

Total mutual information

What is measured

- Entropy

$$sdT - adP + nd\mu = 0$$

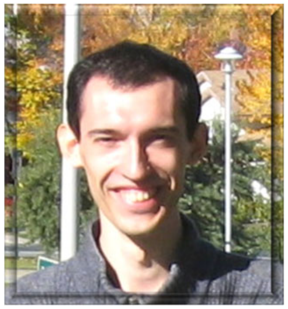
$$P(T)_U = \frac{1}{a}\int_{-\infty}^{U/2} n(\mu, T)d\mu$$

$$s = a(dP/dT)_\mu$$

Caitlin Walsh

Patrick Sémon

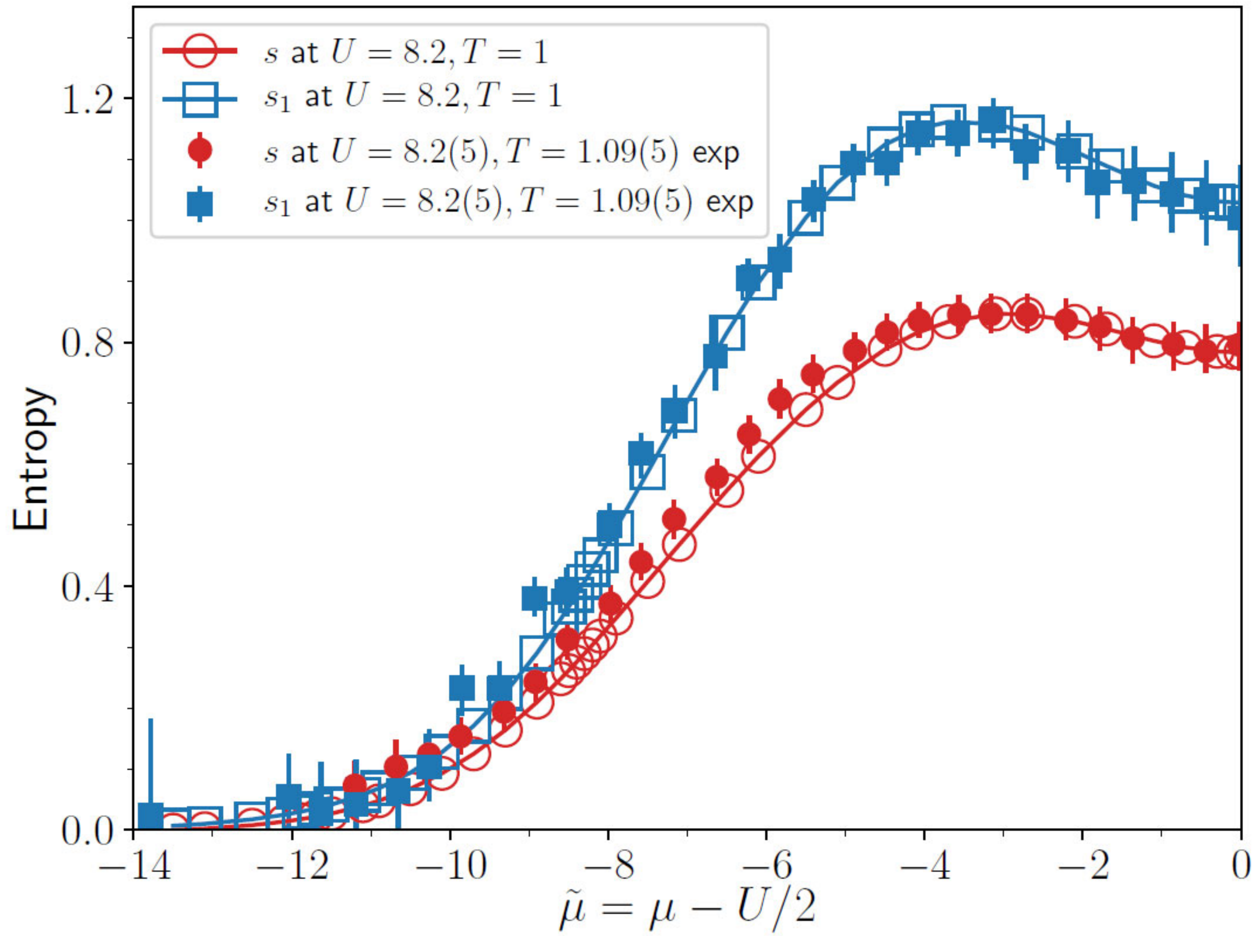
David Poulin



Giovanni Sordi

PRL 122, 067203 (2019)

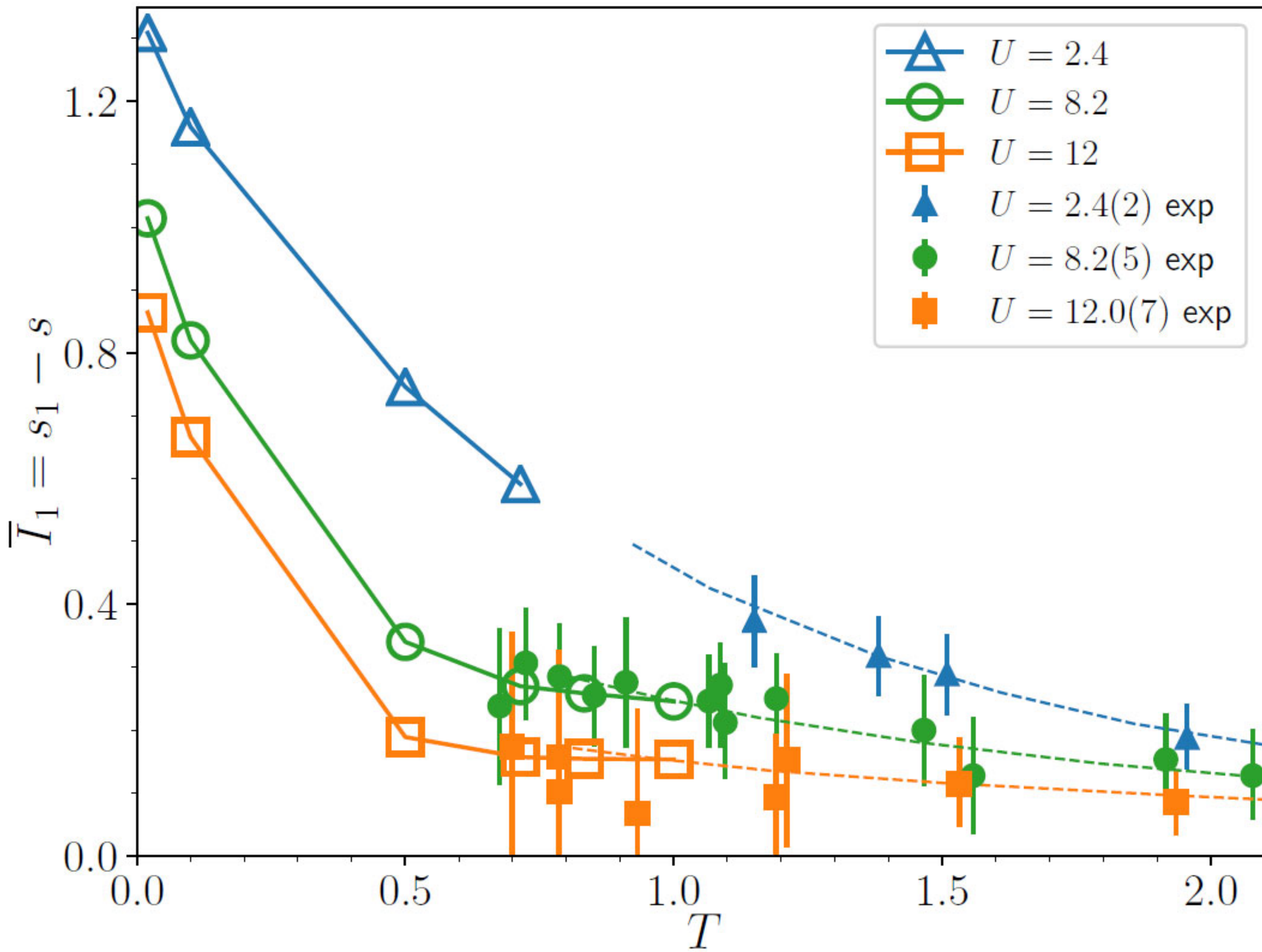
Agreement with experiment



PRL 122, 067203 (2019)

EXP: E. Cocchi et al., Phys. Rev. X 7, 031025 (2017)

Agreement with experiment for the total mutual information



PRL 122, 067203 (2019)

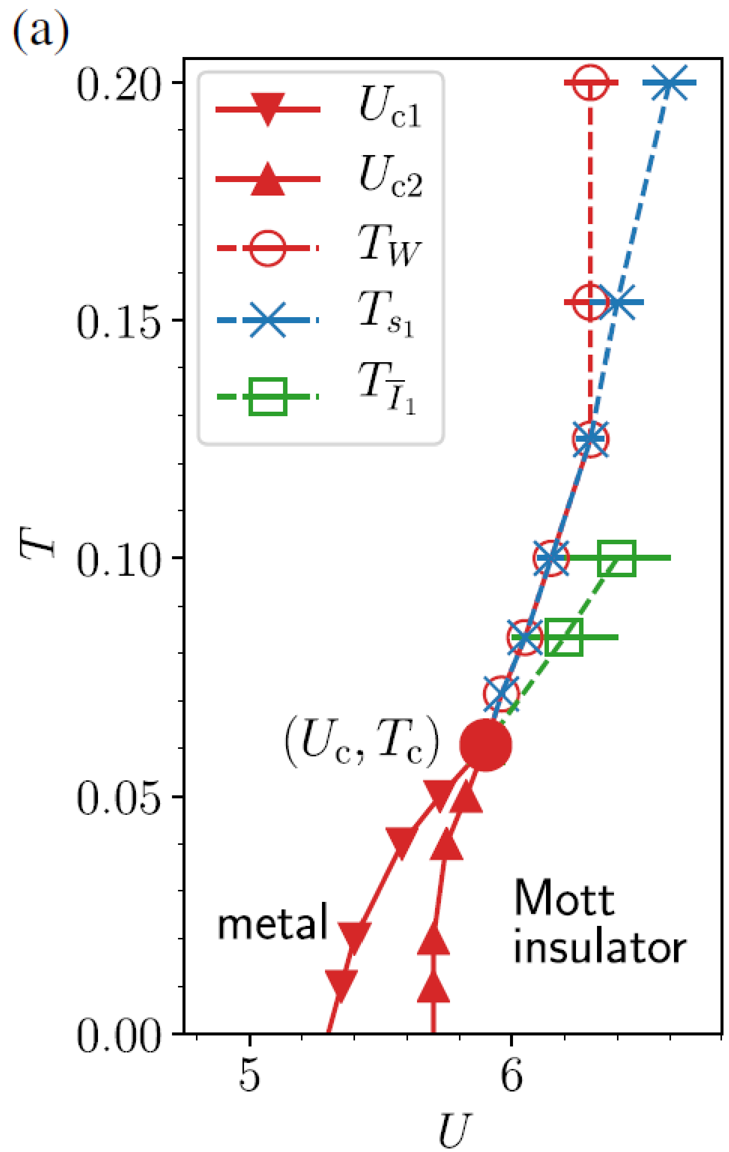
EXP:

Cocchi et al., Phys. Rev. X 7, 031025 (2017)

Transition and crossovers

- The Mott transition
- The effect of *J* that leads to larger mutual information in the insulating than in the metallic state
- Critical exponent (not usually the case)
- Crossover to the pseudogap
- Associated high-temperature crossovers,
  – Without knowledge of the order parameter of the transition

PRL 122, 067203 (2019)



Total mutual information in superconducting state

PNAS, 118 (25), e2104114118/1-6, 14 June (2021).

Total mutual information

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

Caitlin Walsh

Patrick Sémon

David Poulin

Giovanni Sordi

PNAS, 118 (25), e2104114118, (2021).

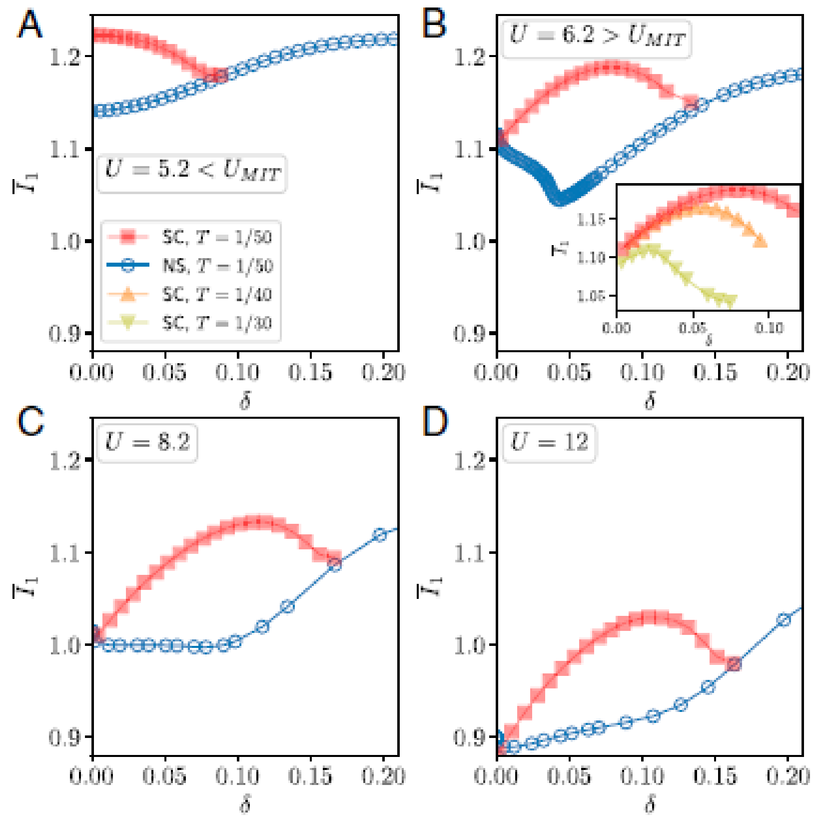


Fig. 4. Total mutual information $\bar{I}_1$ as a function of doping, for $U = 5.2 < U_{MIT}$ (*A*), $U = 6.2 > U_{MIT}$ (*B*), $U = 8.2$ (*C*), and $U = 12$ (*D*). Data in all main panels are at $T = 1/50$ for the normal and superconducting states (open circles and shaded squares, respectively). *B*, *Inset* shows $\langle\bar{I}_1(\delta)\rangle_{SC}$ at $U = 6.2$ for $T = 1/50$, $T = 1/40$, and $T = 1/30$ (squares, up triangles, and down triangles, respectively). Normal-state data for $U = 6.2$ are reproduced from ref. 18.

Take home messages

- In doped Mott insulators, solid state physics methods fail

- Condensation energy : kinetic energy ($J = 4t^2/U$)
- Information theoretic measures contain signs of the phase diagram

- Highly quantum mechanical
  - One band
  - Spin ½
  - Pairing interaction and Cooper pairs from same electrons
  - Particle-wave duality (Mott transition)
  - Mutual information (Entanglement) is modified in the different phases

Merci
Thank you

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