Life as a theorist without a small parameter

André-Marie S. Tremblay

CIFAR
CANADIAN INSTITUTE for ADVANCED RESEARCH

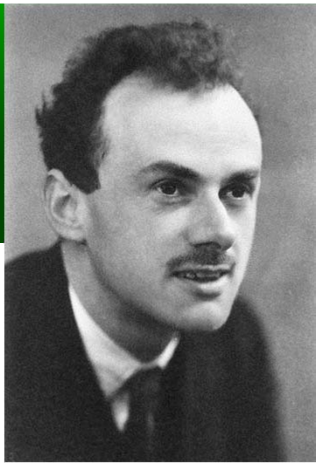
UNIVERSITÉ DE SHERBROOKE

VERITATEM IN CHARITATE

Congrès de l'association canadienne des physiciens, Sudbury
Mercredi 18 juin 2014

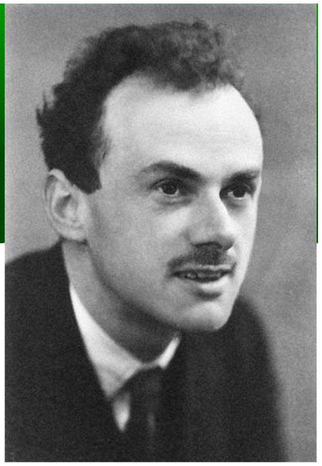
UNIVERSITÉ DE SHERBROOKE

Dirac (1902-1984)



- The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.
  - *Proceedings of the Royal Society of London. Series A, Containing Papers of a Mathematical and Physical Character, Vol. 123, No. 792* (6 April 1929)

Dirac

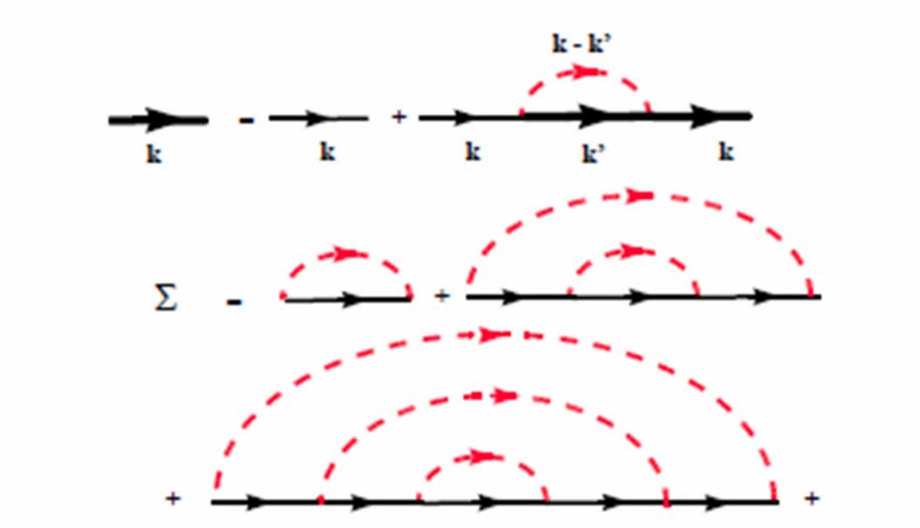


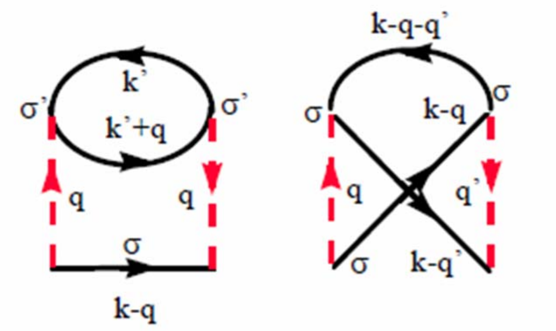
- It therefore becomes desirable that **approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation.**

The rule of the small parameter

R. Feynman:1918-1988

K.G. Wilson:1936 –2013





Computers! Monte Carlo algorithm

THE JOURNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUNE, 1953

Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*

(Received March 6, 1953)

A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

I. INTRODUCTION

THE purpose of this paper is to describe a general method, suitable for fast electronic computing machines, of calculating the properties of any substance which may be considered as composed of interacting individual molecules. Classical statistics is assumed, only two-body forces are considered, and the potential

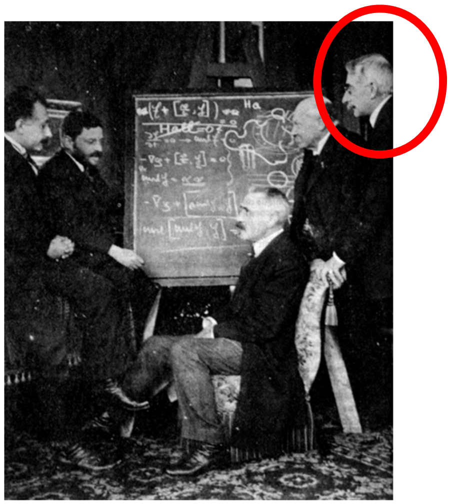
II. THE GENERAL METHOD FOR AN ARBITRARY POTENTIAL BETWEEN THE PARTICLES

In order to reduce the problem to a feasible size for numerical work, we can, of course, consider only a finite number of particles. This number N may be as high as several hundred. Our system consists of a square† containing N particles. In order to minimize the surface effects we suppose the complete substance to be periodic

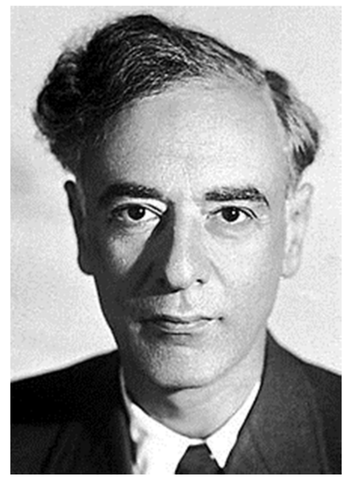
Fermions

UNIVERSITÉ DE SHERBROOKE

Broken symmetry – mean-field



Pierre Weiss: 1865 - 1940



Lev Landau: 1908-1968

The theory of everything

$$H = K + V_{e-e} + V_{e-i} + V_{i-i} + V_{s-o}$$

- 10-1000 eV vs 10 meV (3-5 orders of magnitude)
- Broken symmetry (lattice) (Bands: Bloch)
- Density Functional Theory (Hohenberg-Kohn-Sham)
  - Ground state
  - Basis for perturbation theory
- Fermi liquid theory (Landau)
- Effective Hamiltonians (e.g. spin models)
- Moore's law
- Better algorithms: beating Moore's law.

Superconductivity

Leon Cooper

John Bardeen*

Robert Schrieffer

High temperature superconductors

Failure of

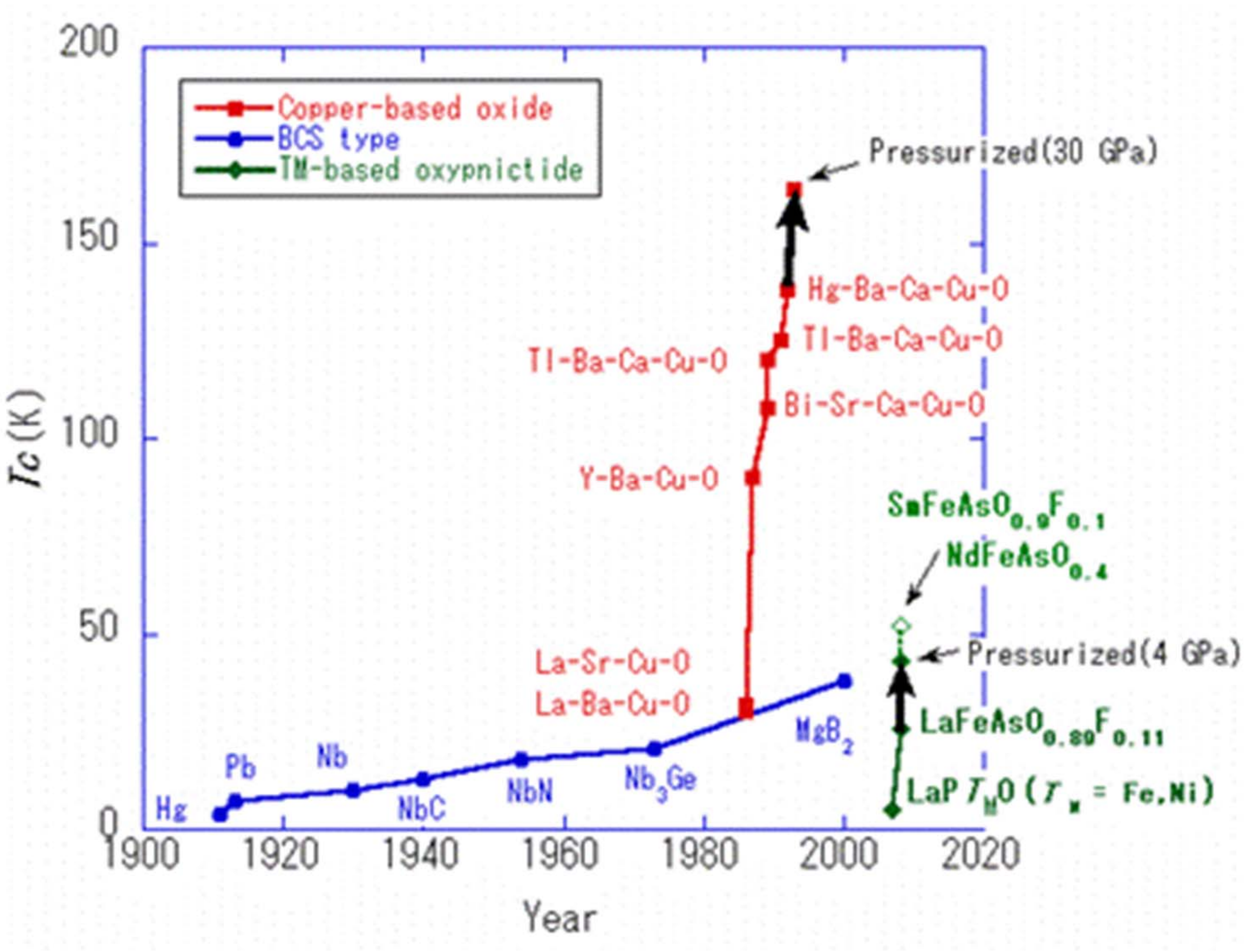
BCS theory

Band structure

and more

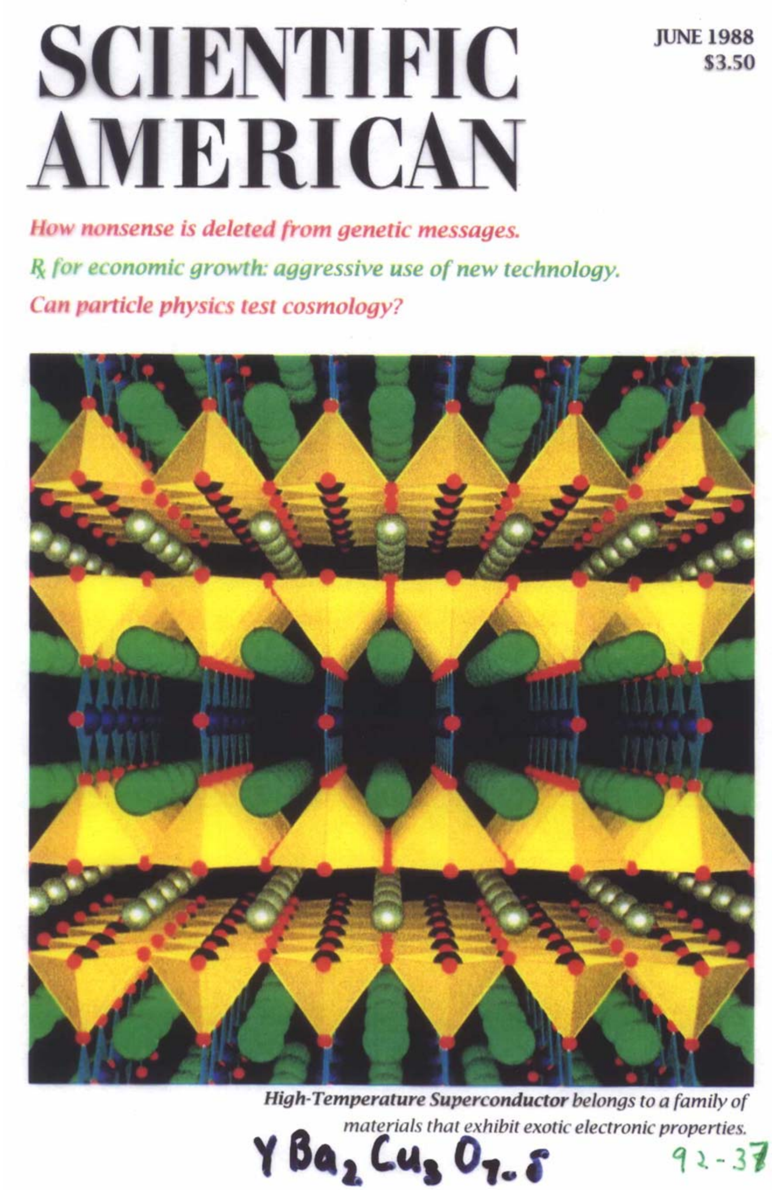
UNIVERSITÉ DE
SHERBROOKE

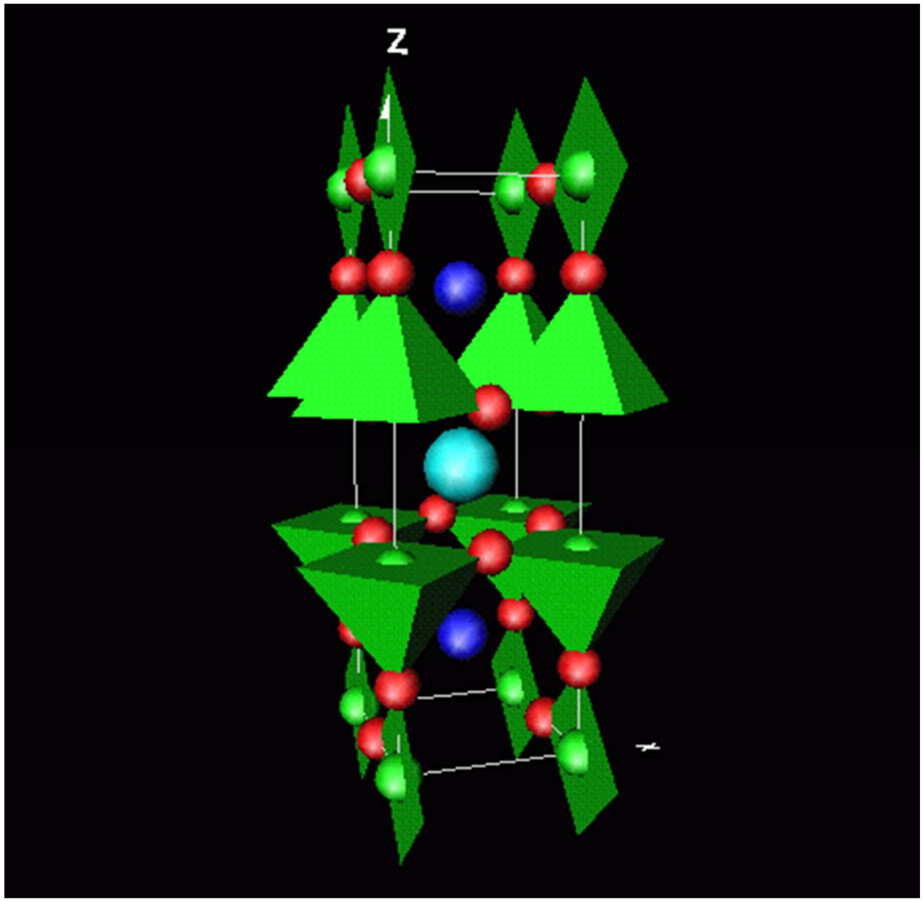
New and old superconductors



H. Takahashi: JPSJ Online—News and Comments [June 10, 2008]

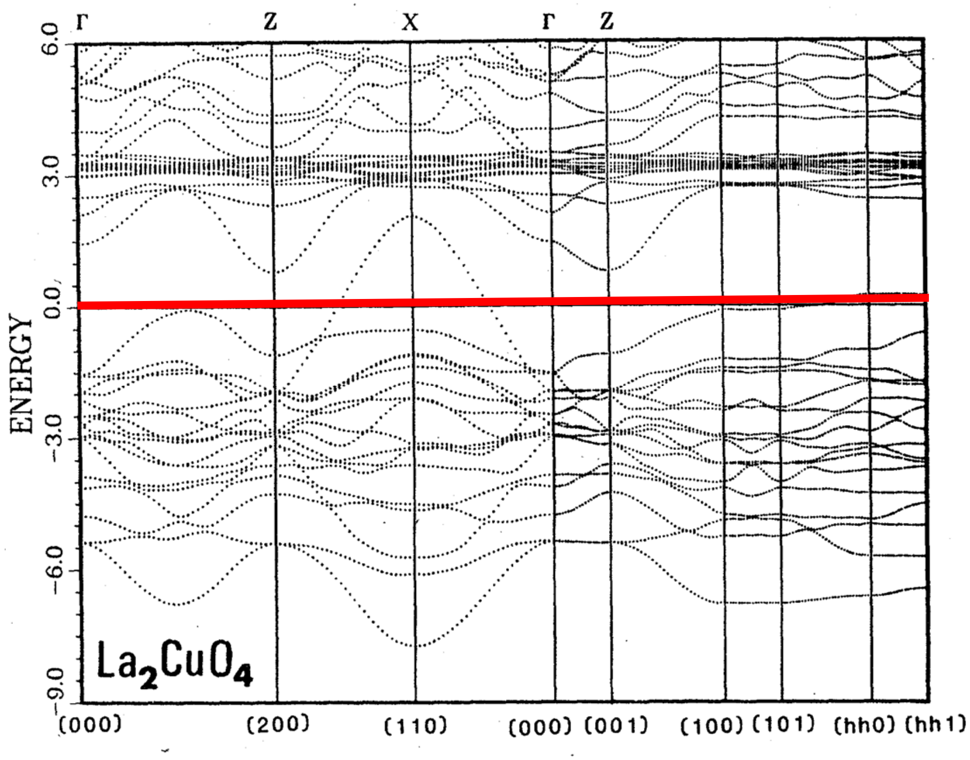
Atomic structure





UNIVERSITÉ DE SHERBROOKE

Band structure for high Tc

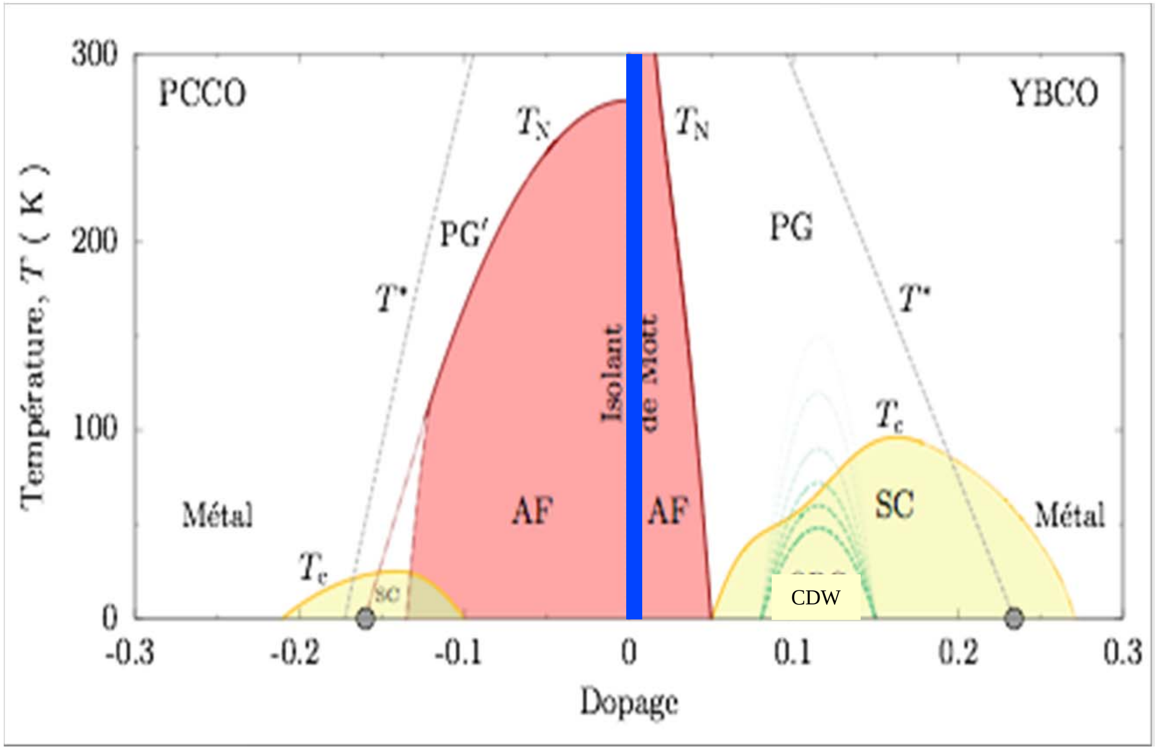


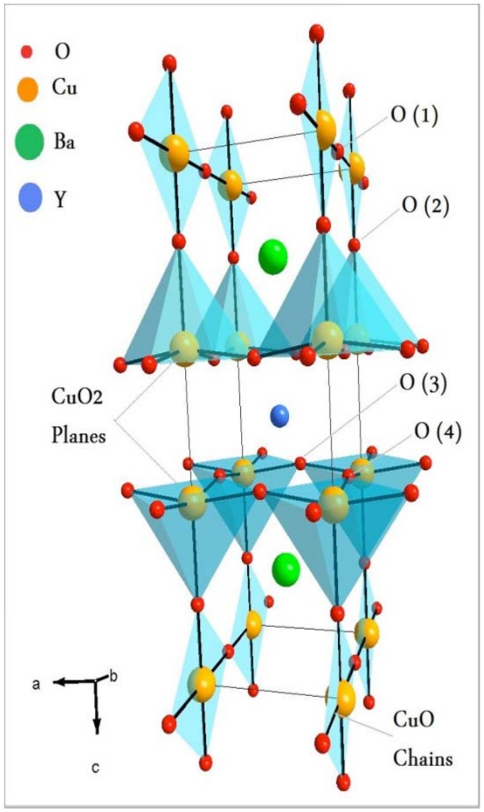
W. Pickett, Rev. Mod. Phys. 1989

UNIVERSITÉ DE SHERBROOKE

A puzzeling phase diagram

Thèse de Francis Laliberté, Université de Sherbrooke





Breakdown of band theory:
Half-filled band is metallic

Half-filled band: Not always a metal

NiO, Boer and Verway

Peierls, 1937

Mott, 1949

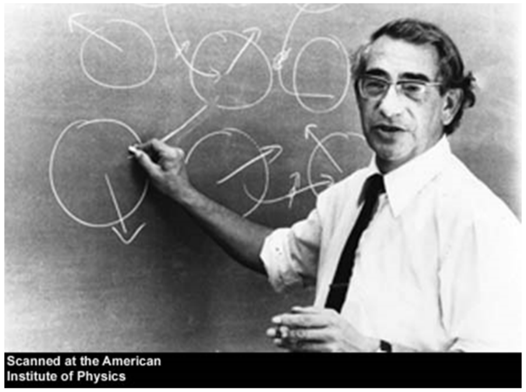
UNIVERSITÉ DE SHERBROOKE

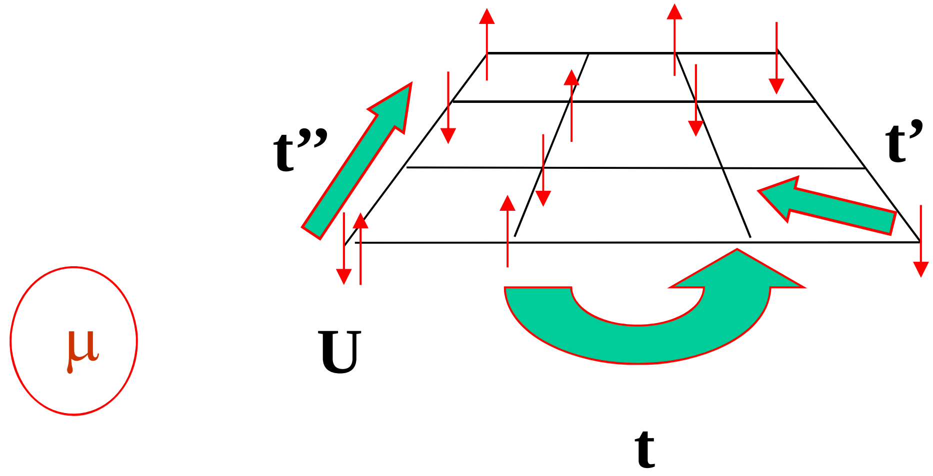
Outline

- The model
- Beyond perturbation theory
  - Weak to intermediate correlations TPSC
    - Electron-doped cuprates
  - Strong correlations DMFT
    - Hole-doped cuprates

2. The model

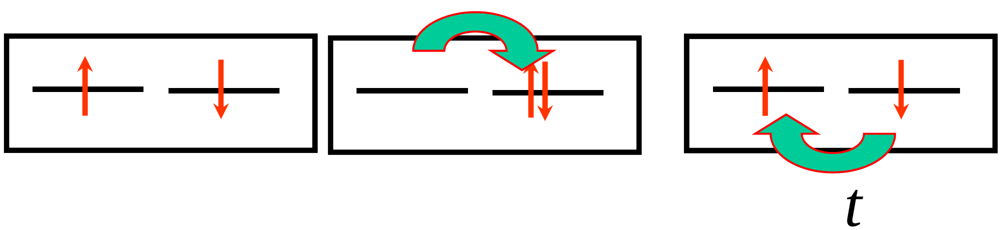
Hubbard model





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

Theoretical considerations

UNIVERSITÉ DE SHERBROOKE

Another way to look at the many-particle problem

$$F[\phi] = -T \ln Z[\phi] = -T \ln \mathrm{Tr}\left[e^{-\beta(H-\mu N)} T_\tau e^{-\int\int \psi^\dagger(\bar{1})\phi(\bar{1},\bar{2})\psi(\bar{2})} \right]$$

$$\frac{1}{T}\frac{\delta F[\phi]}{\delta\phi(1,2)} = \mathcal{G}(2,1)$$

$$\Omega[\mathcal{G}] = F[\phi] - \mathrm{Tr}[\phi\mathcal{G}] \qquad \frac{1}{T}\frac{\delta\Omega[\mathcal{G}]}{\delta\mathcal{G}(1,2)} = -\phi(2,1)$$

$$\Omega[\mathcal{G}] = \Phi[\mathcal{G}] - \mathrm{Tr}\left[\left(\mathcal{G}_0^{-1} - \mathcal{G}^{-1}\right)\mathcal{G}\right] + \mathrm{Tr}\left[\ln\left(\frac{-\mathcal{G}}{-\mathcal{G}_\infty}\right)\right]$$

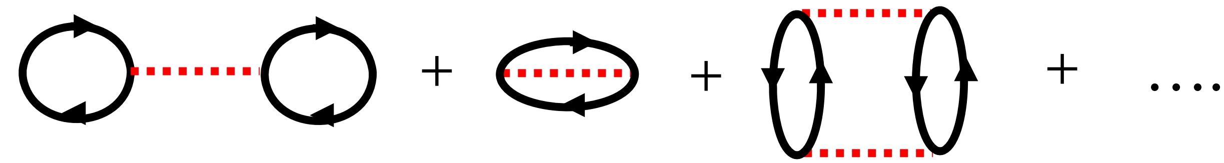
$$\frac{1}{T}\frac{\delta\Phi[\mathcal{G}]}{\delta\mathcal{G}(1,2)} = \Sigma(2,1)$$

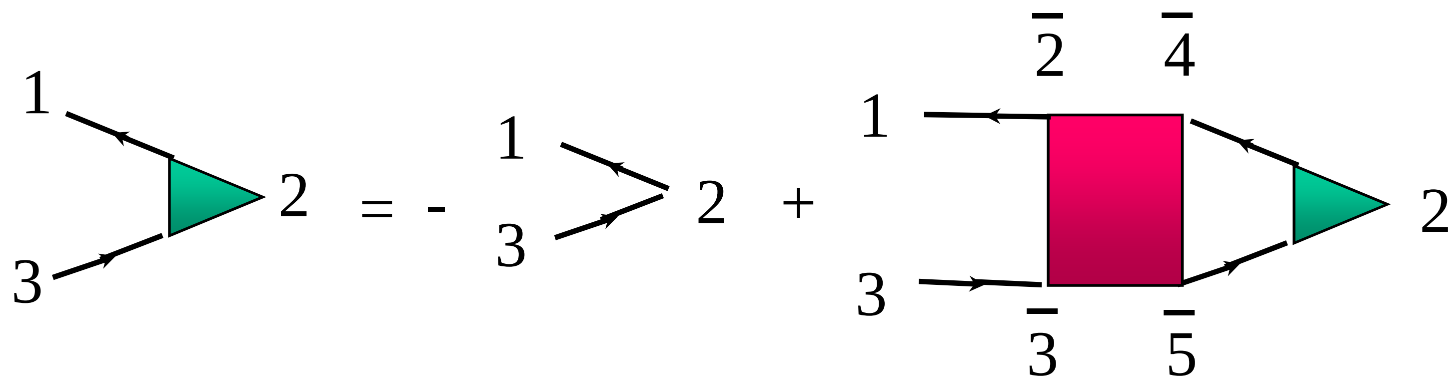
$$U_{sp} = \frac{\delta\Sigma_\uparrow}{\delta G_\downarrow} - \frac{\delta\Sigma_\uparrow}{\delta G_\uparrow}$$

J. Schwinger: 1918-1994

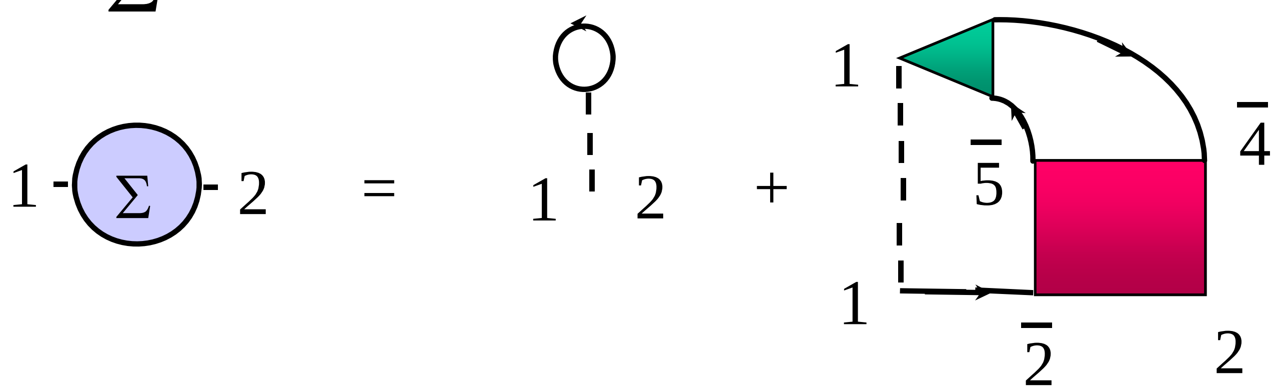
Focus on physically meaningful quantities

$\Phi[G] =$





$$\frac{\delta\Phi[G]}{\delta G} = \Sigma$$



Luttinger and Ward 1960, Baym and Kadanoff (1961)

Two-Particle Self-Consistent Theory (Vilk)

Yury Vilk

UNIVERSITÉ DE SHERBROOKE

Two-Particle Self-Consistent Theory (how it works, $U < 8t$)

- General philosophy
  - Impose constraints and sum rules to find vertex
    - Conservation laws
    - $U_{sp} = U \frac{\langle n_\uparrow n_\downarrow \rangle}{\langle n_\uparrow \rangle \langle n_\downarrow \rangle}$
    - Pauli principle $\langle {n^2}_\sigma \rangle = \langle n_\sigma \rangle$
    - Local moment and local density sum-rules

Vilk, AMT J. Phys. I France, **7**, 1309 (1997);
A.M.T. Chapt. 13, in *Theoretical Methods for Strongly Correlated Systems* Ed F. Mancini A. Avella, (Mahan, third edition)

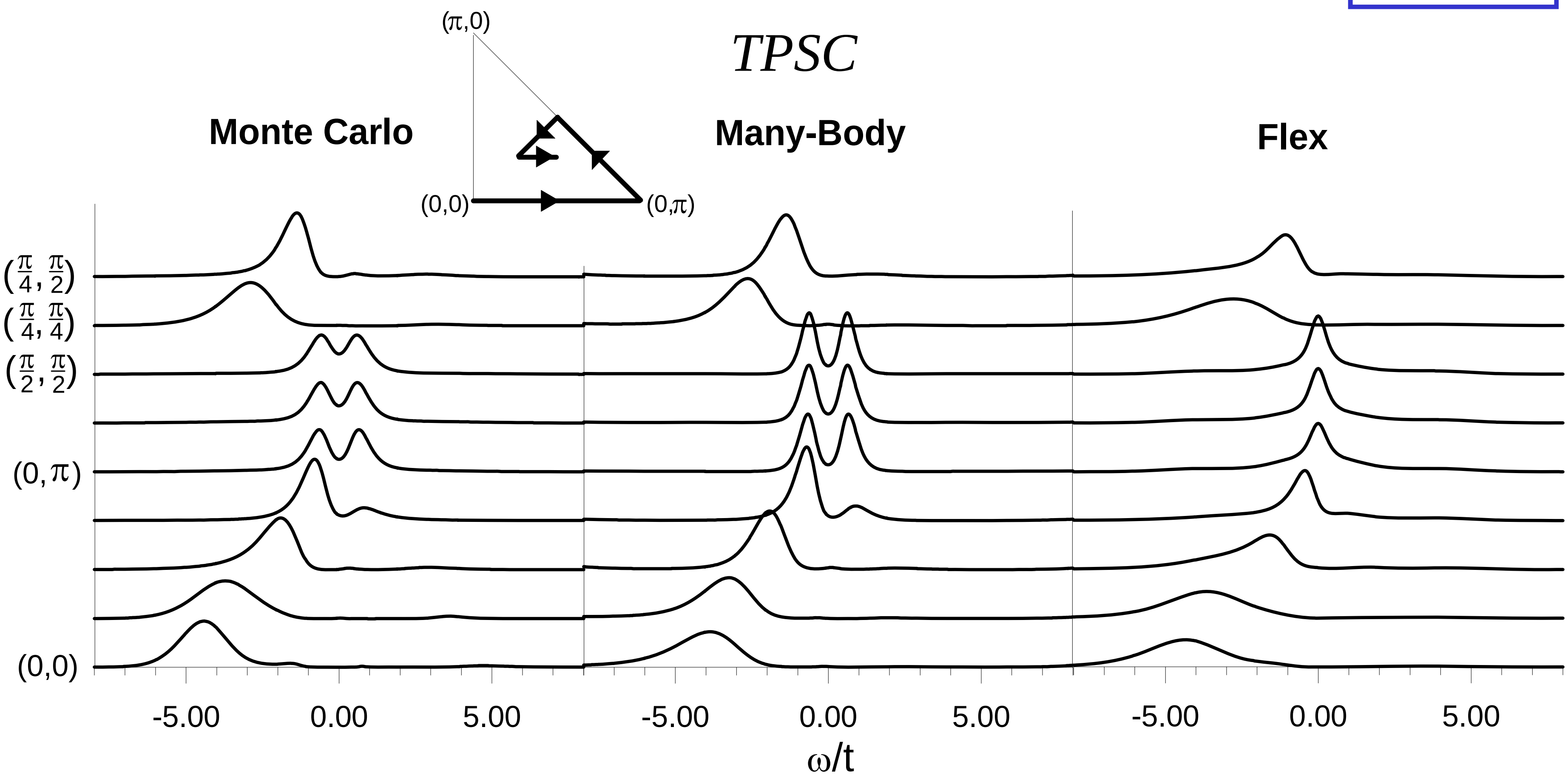
- Get for free:
  - Mermin-Wagner theorem
  - Kanamori-Brückner screening
  - Consistency between one- and two-particle $\Sigma G = U\langle n_\sigma n_{-\sigma} \rangle$

UNIVERSITÉ DE SHERBROOKE

Benchmarks for TPSC

Proofs...

U = + 4
β = 5

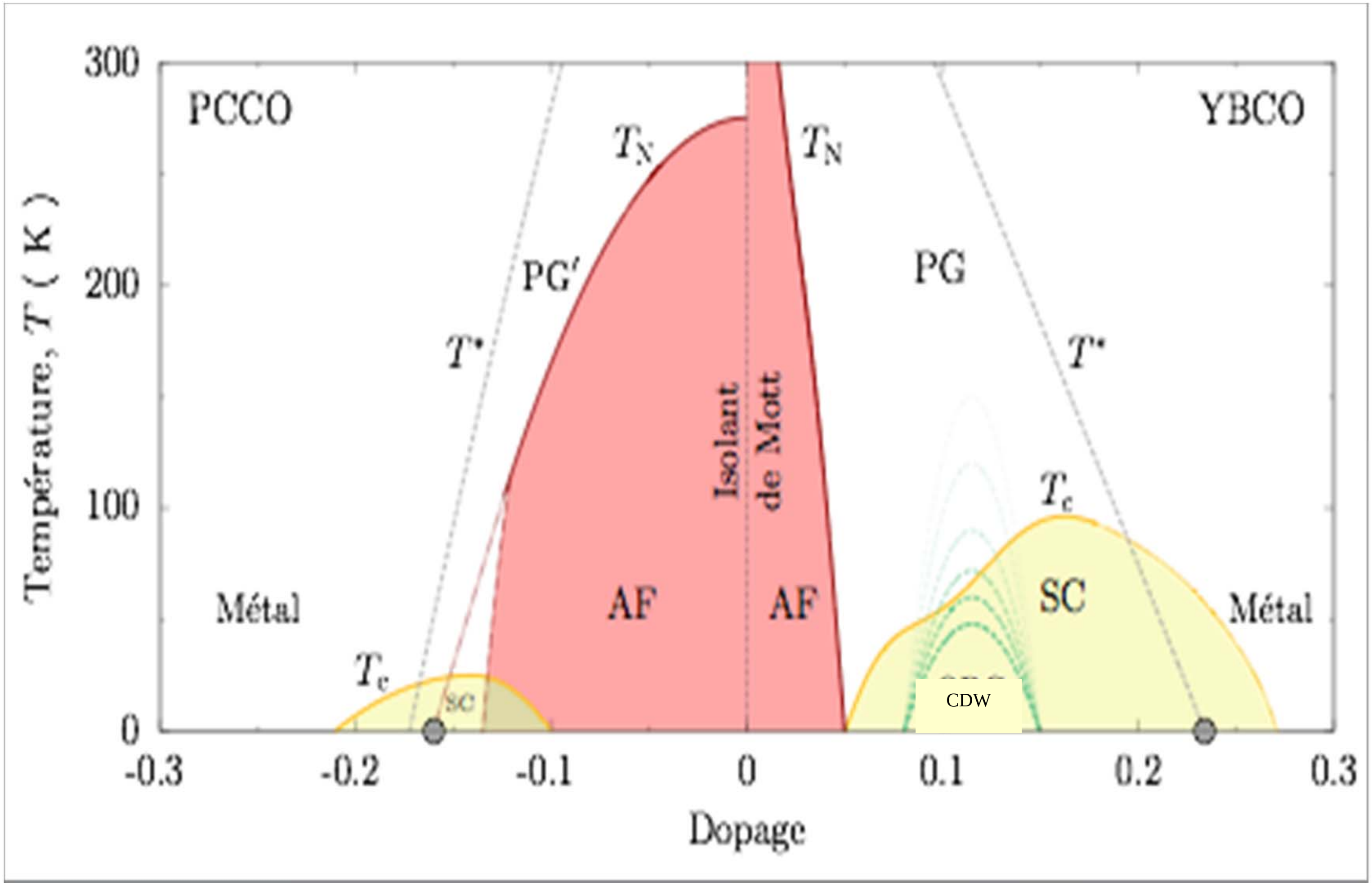


Calc. + QMC: Moukouri et al. P.R. B 61, 7887 (2000).

3. Electron-doped cuprates: normal state

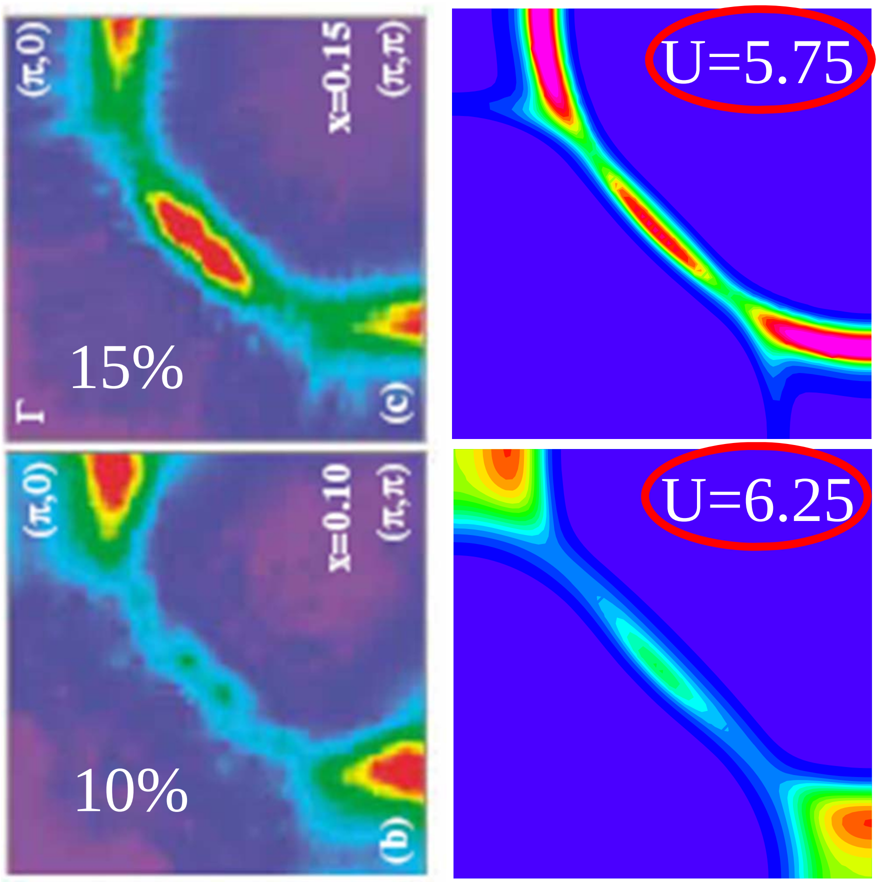
Our road map

Thèse de Francis Laliberté,
Université de Sherbrooke

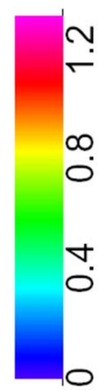


Fermi surface plots

Hubbard repulsion *U* has to…



be not too large



increase for
smaller doping

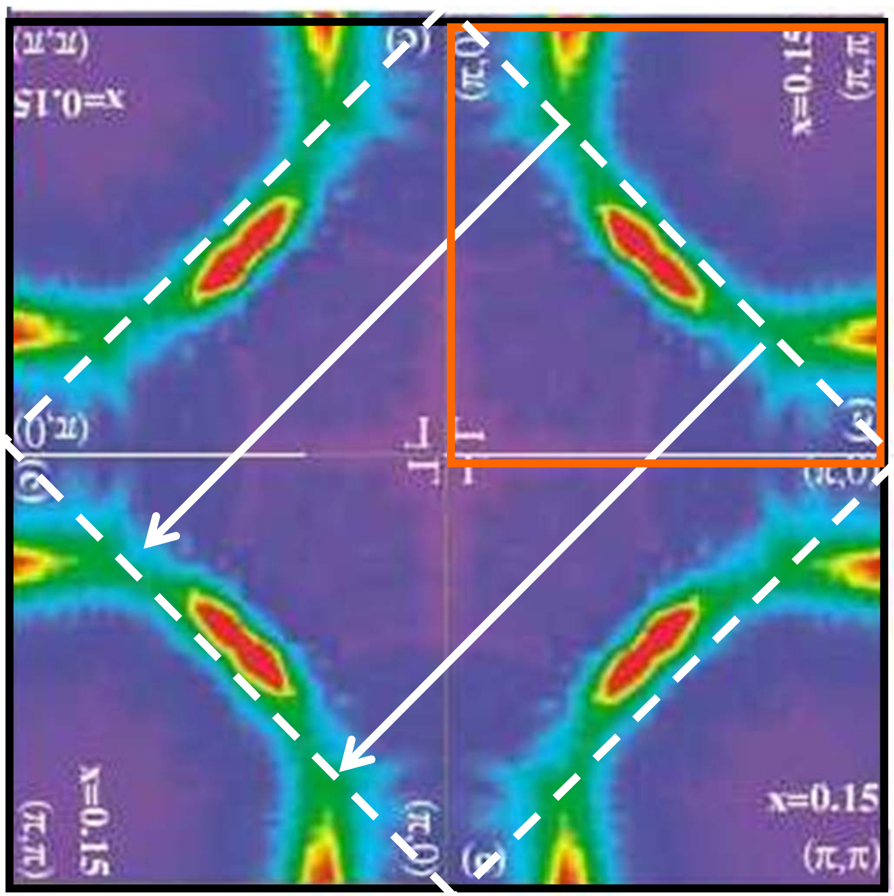
B.Kyung *et al.*,PRB **68**, 174502 (2003)

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

Hot spots from AFM quasi-static scattering

Mermin-Wagner

$d = 2$



Armitage et al. PRL 2001

Vilk, A.-M.S.T (1997)
Kyung, Hankevych,
A.-M.S.T., PRL, 2004

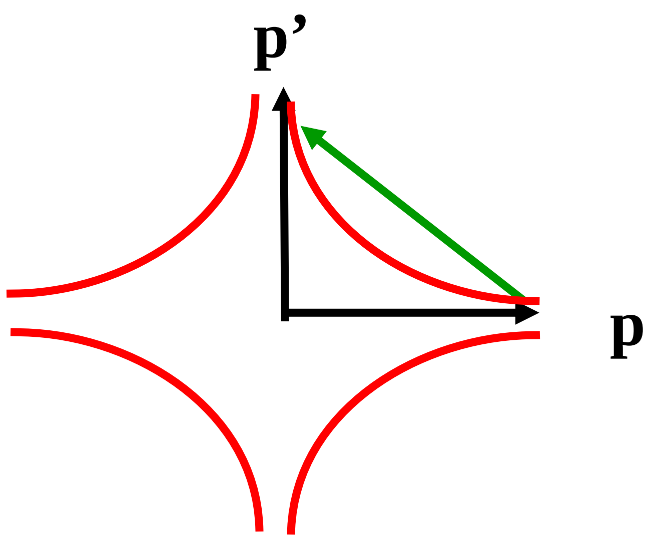
$\xi^{*} = 2.6(2)\xi_{th}$.

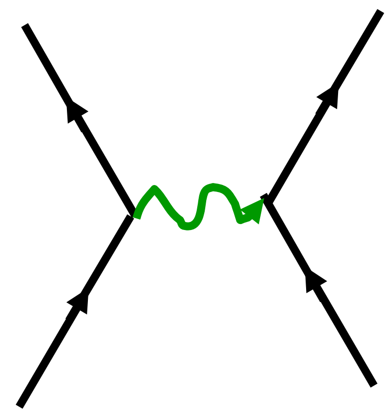
Motoyama, E. M. et al..
Nature
186–189 (2007).

4. Electron-doped cuprates: superconductivity

Cartoon « BCS » weak-coupling picture

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





Béal–Monod, Bourbonnais, Emery
P.R. B. **34**, 7716 (1986).

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).

Kohn, Luttinger, P.R.L. **15**, 524 (1965).

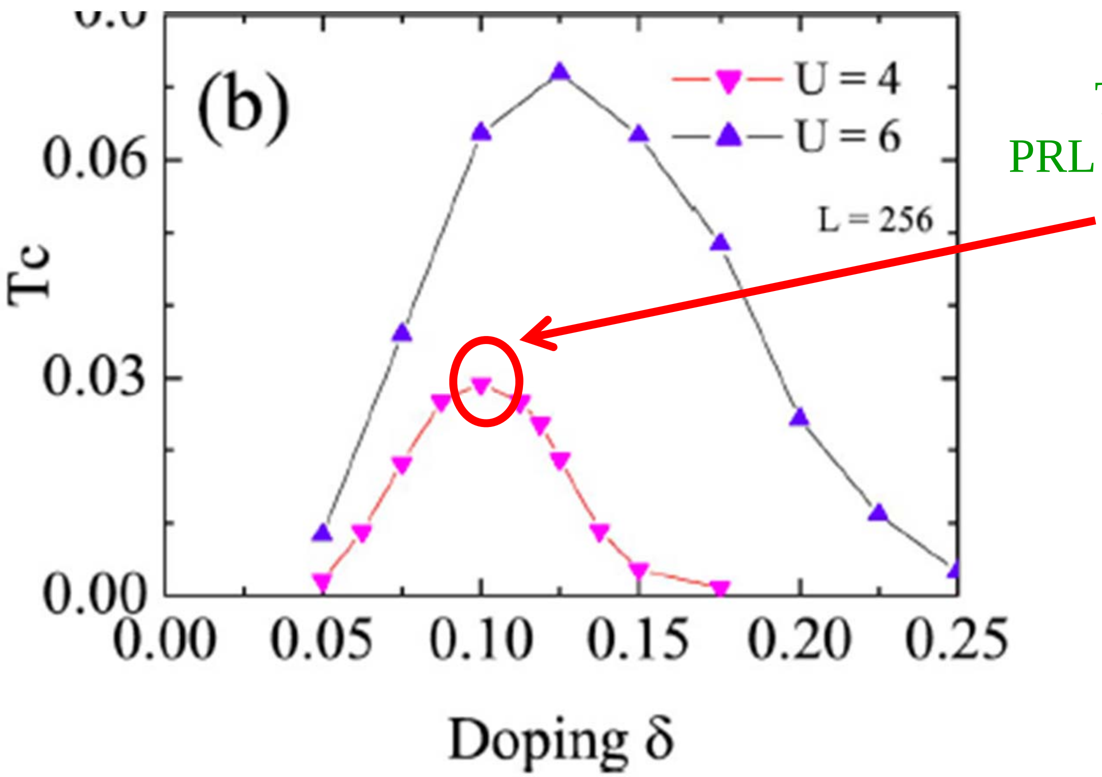
P.W. Anderson Science 317, 1705 (2007)

UNIVERSITÉ DE SHERBROOKE

Results from TPSC

Satisfies Mermin-Wagner

Tc from TPSC

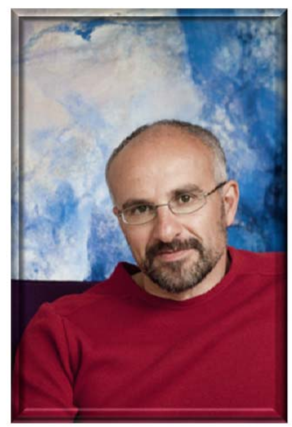


T. Maier et al.
PRL **95,** 237001 (2005)

Kyung et al. PRB **68** (2003)

5. Strong correlations: Dynamical Mean-Field Theory

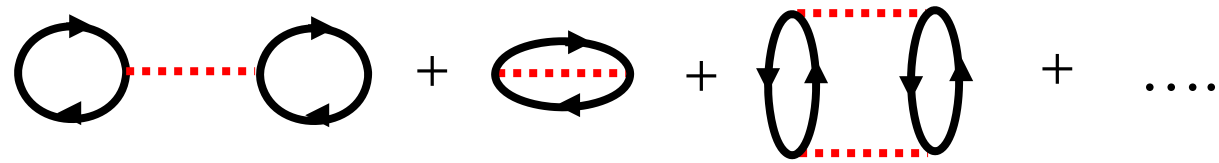
Gabriel Kotliar

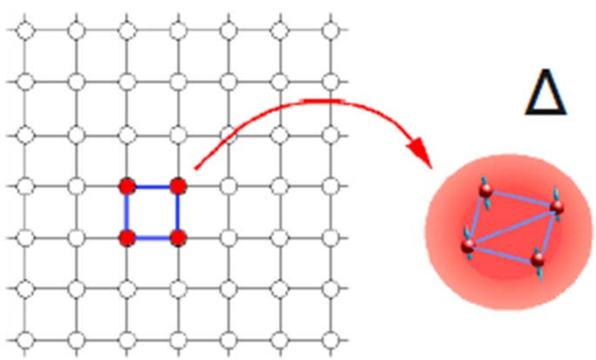


Antoine Georges

UNIVERSITÉ DE SHERBROOKE

C-DMFT

$\Phi[G] =$ 



REVIEWS

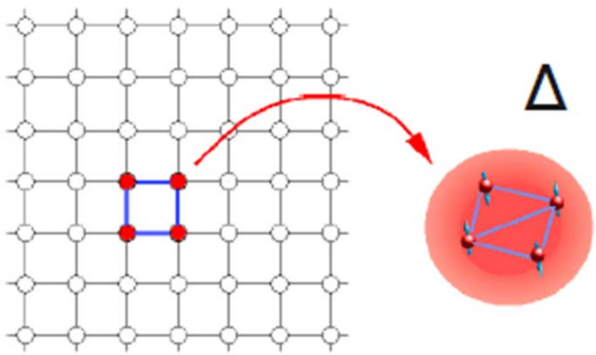
Maier, Jarrell et al., RMP. (2005)

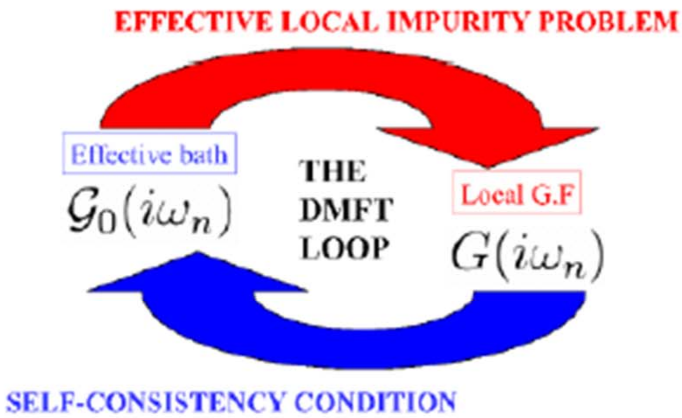
Kotliar *et al.* RMP (2006)

AMST *et al.* LTP (2006)

C-DMFT

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





Mean-field is not a trivial problem! Many impurity solvers.

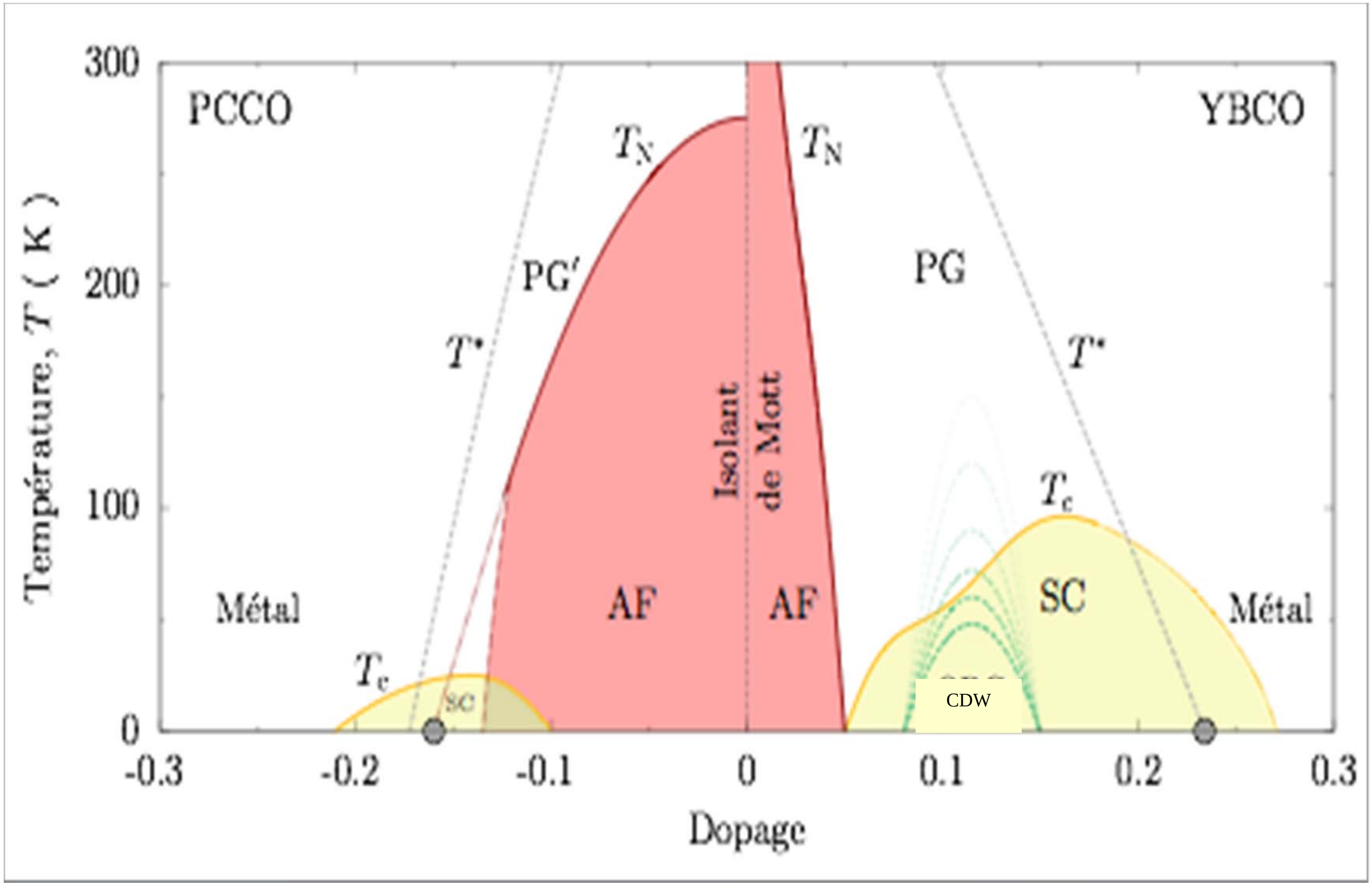
Here: continuous time QMC

P. Werner, PRL 2006
P. Werner, PRB 2007
K. Haule, PRB 2007

$$\Delta(i\omega_n) = i\omega_n + \mu - \Sigma_c(i\omega_n) - \left[\sum_{\tilde{k}} \frac{1}{i\omega_n + \mu - t_c(\tilde{k}) - \Sigma_c(i\omega_n)}\right]^{-1}$$

6. Hole-doped cuprates: normal state

Our road map

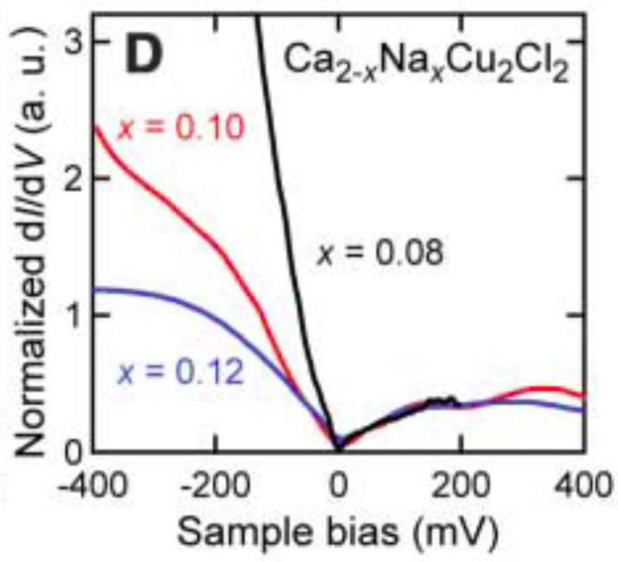


Thèse de Francis Laliberté, Université de Sherbrooke

UNIVERSITÉ DE SHERBROOKE

h-doped are strongly correlated: evidence from the normal state

Density of states (STM)



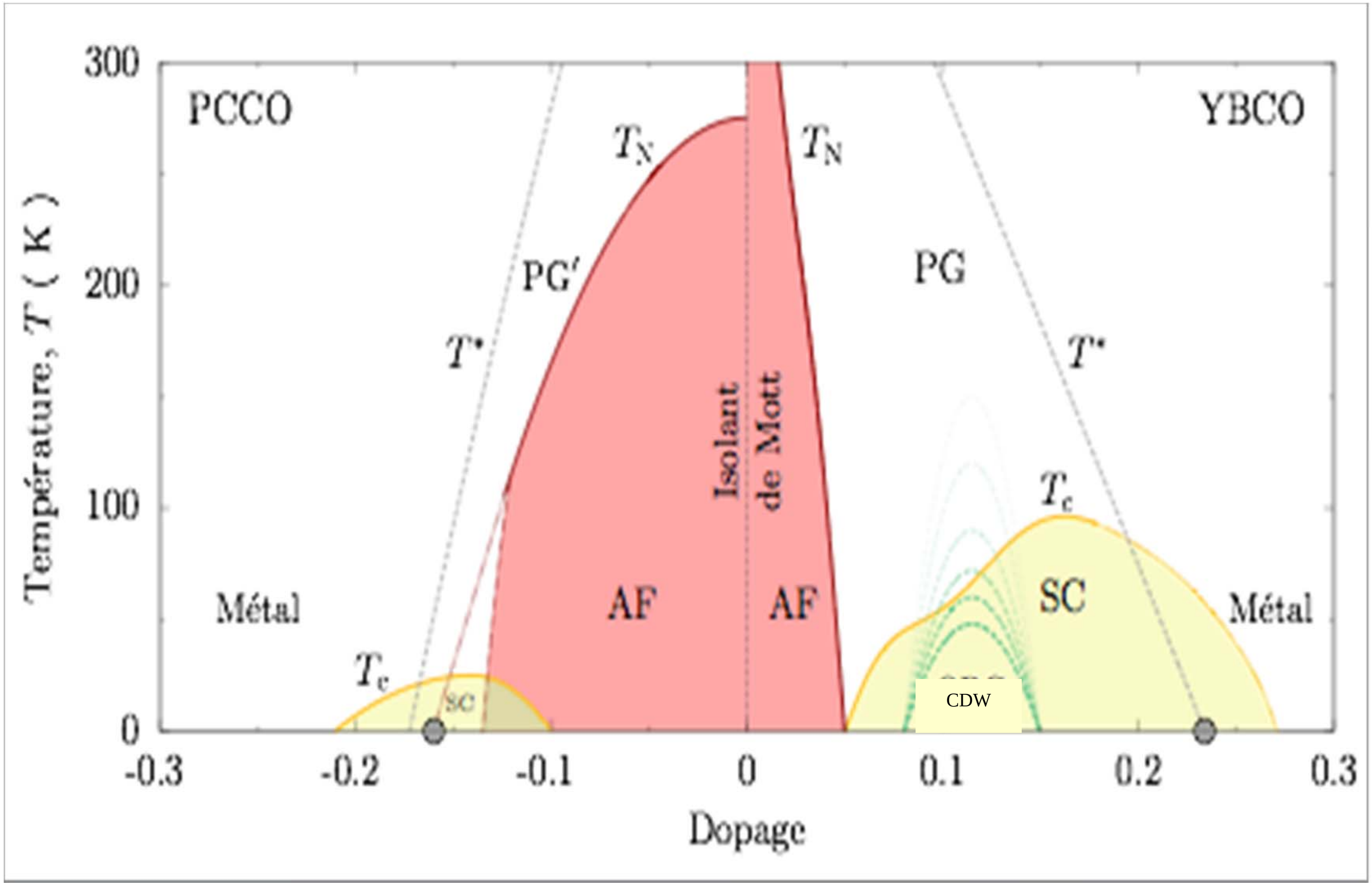
Khosaka et al. *Science* **315**, 1380 (2007);

Pseudogap (theory)

h-doped

Our road map

Thèse de Francis Laliberté, Université de Sherbrooke

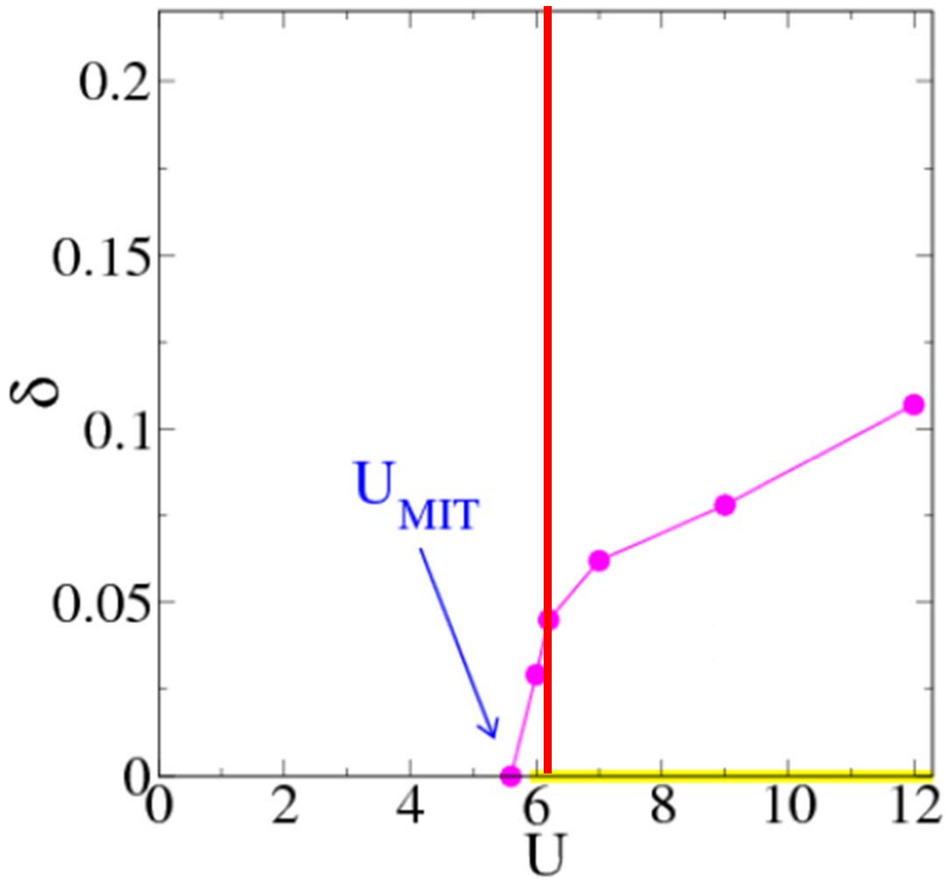


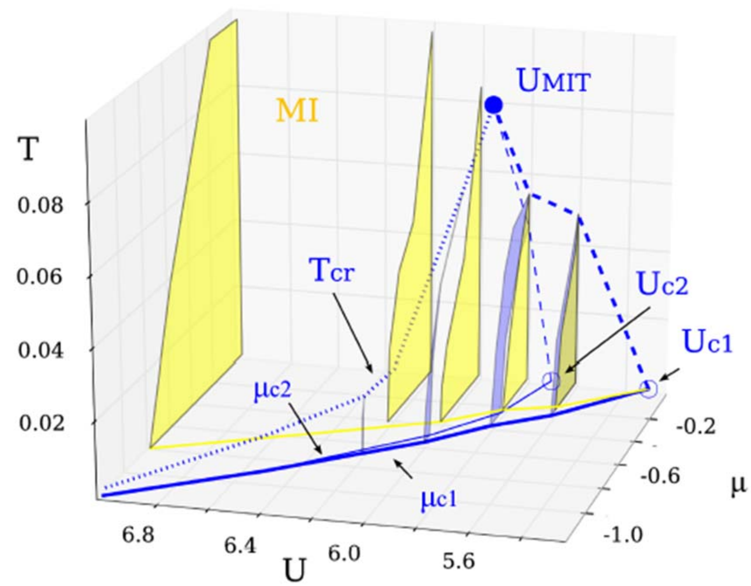
How does the pseudogap develops as a function of T ?

UNIVERSITÉ DE SHERBROOKE

Link to Mott transition up to optimal doping

Doping dependence of critical point as a function of *U*

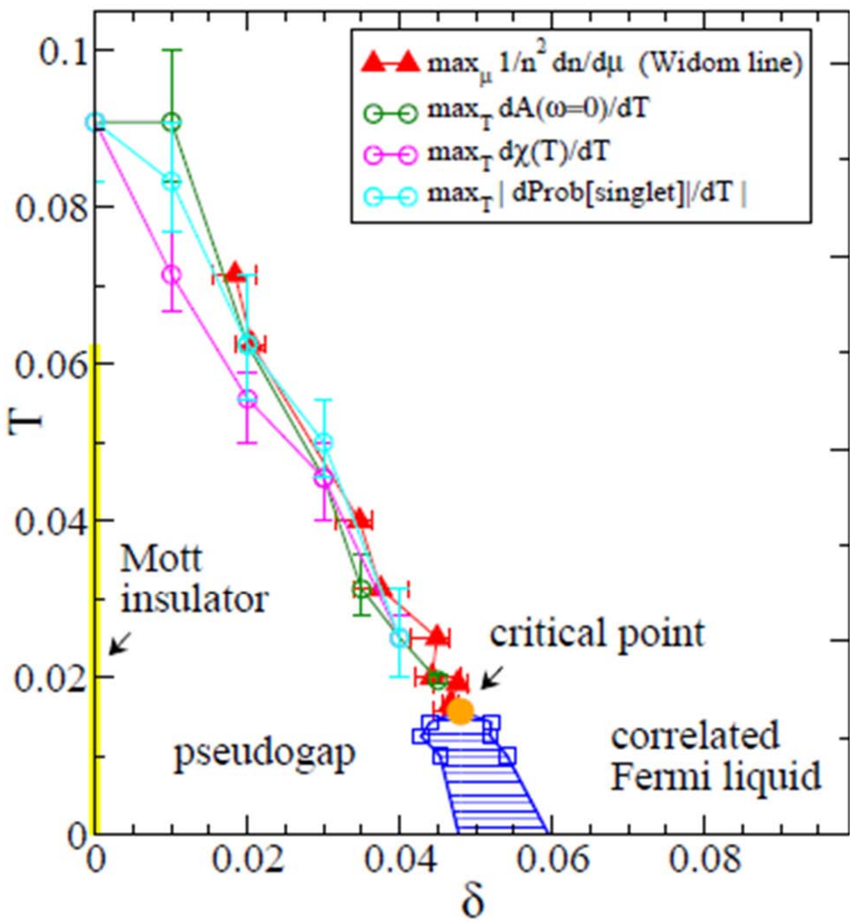


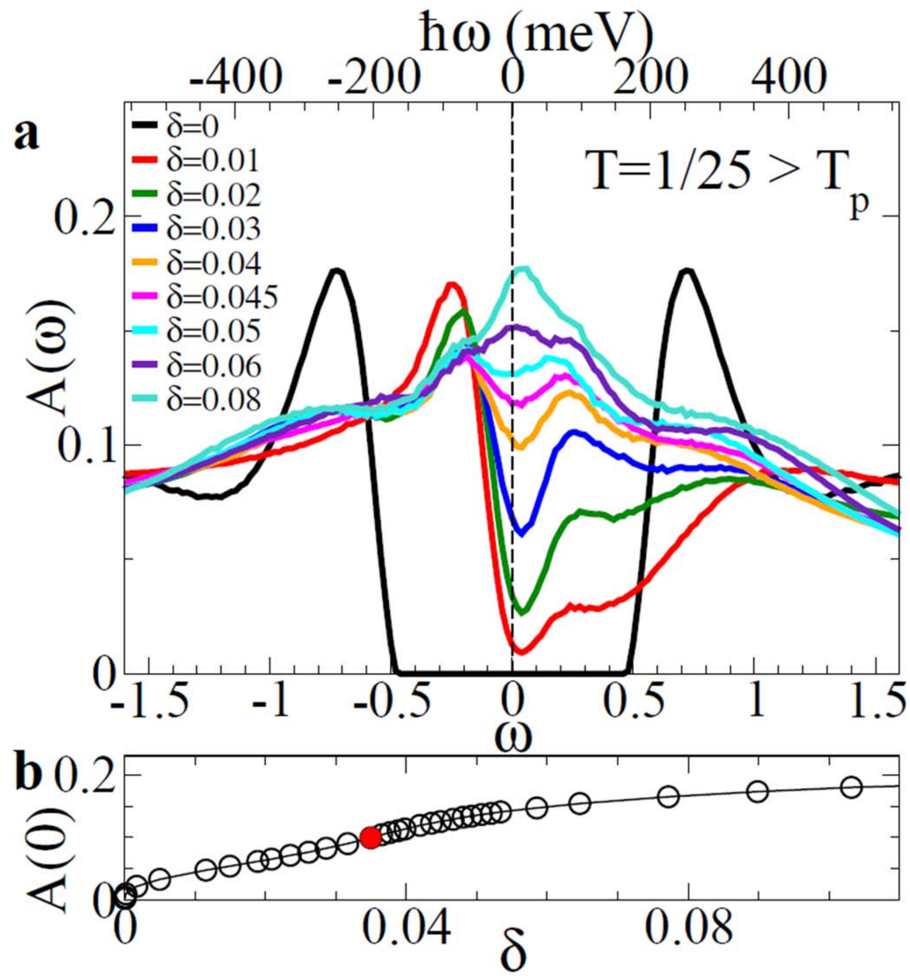


Smaller *D* and *S*

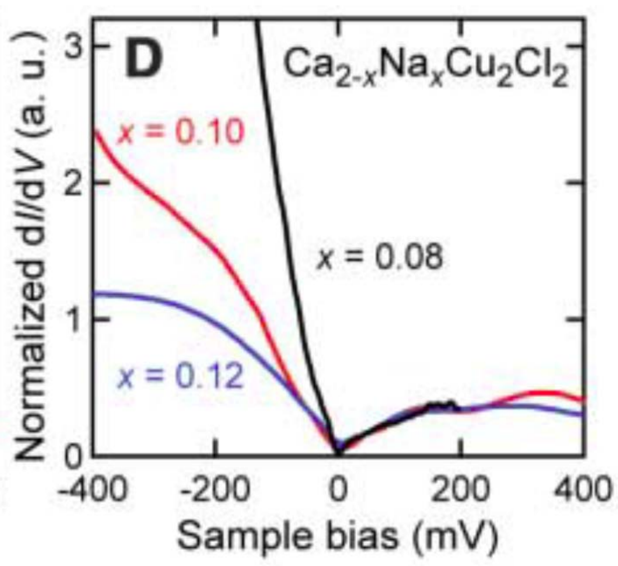
UNIVERSITÉ DE SHERBROOKE

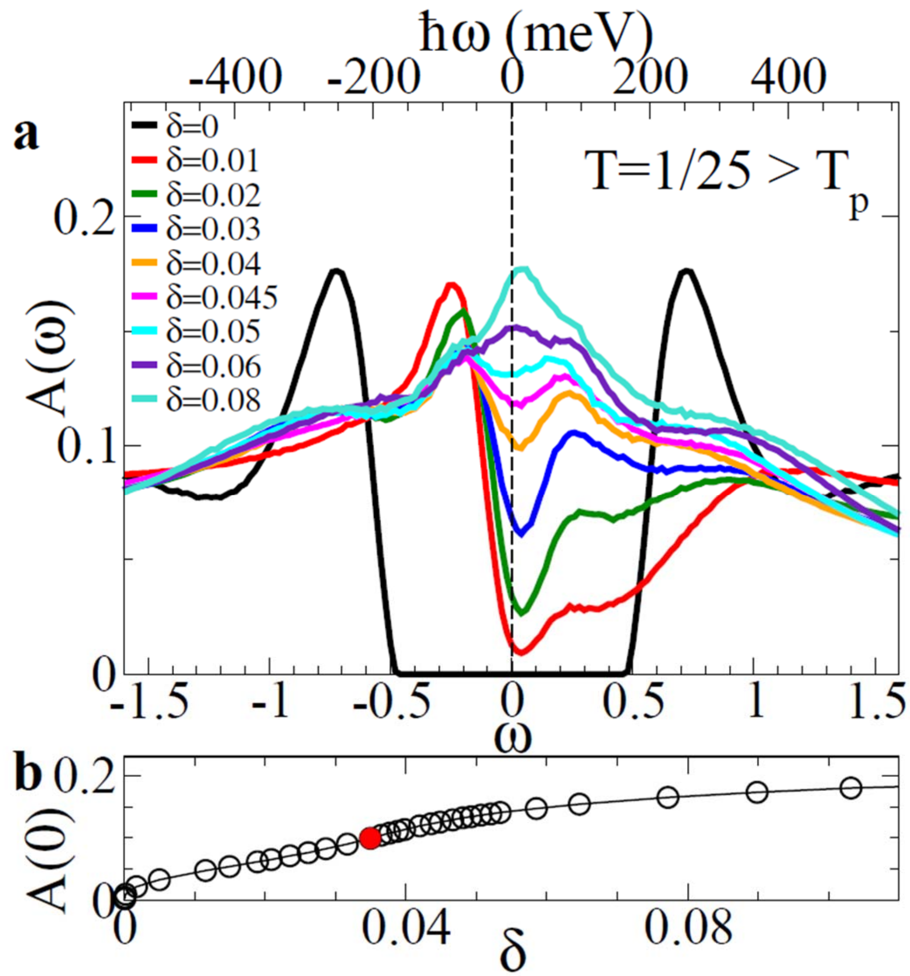
Density of states





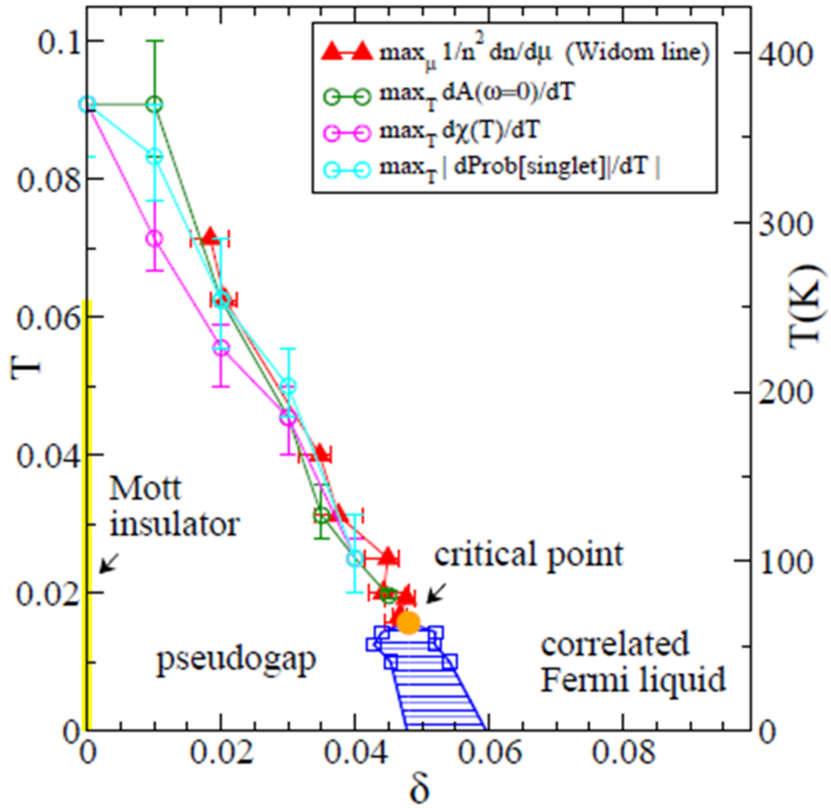
Density of states

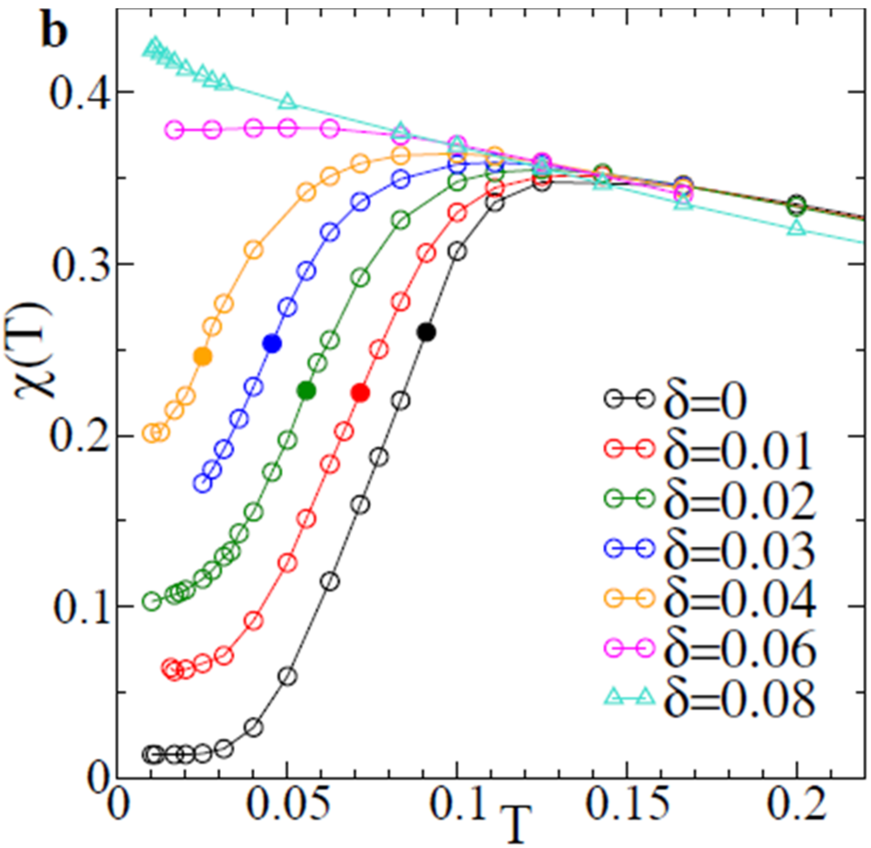




Khosaka et al. *Science* **315**, 1380 (2007);

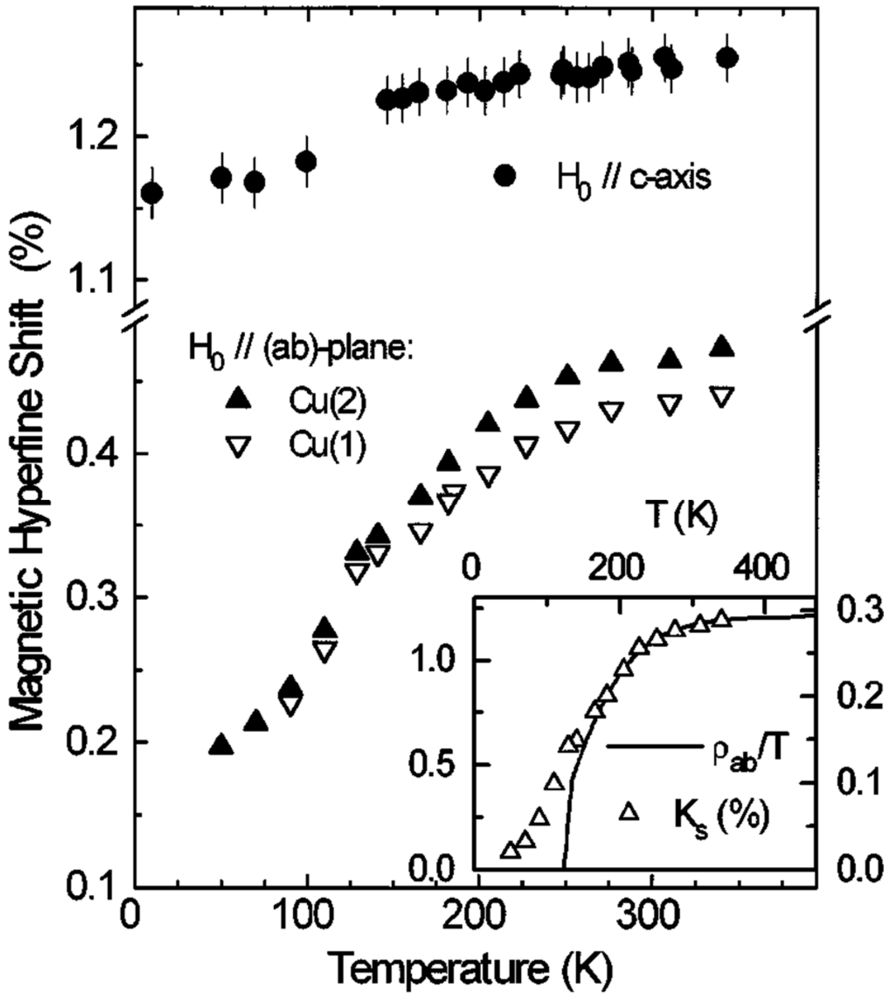
Spin susceptibility

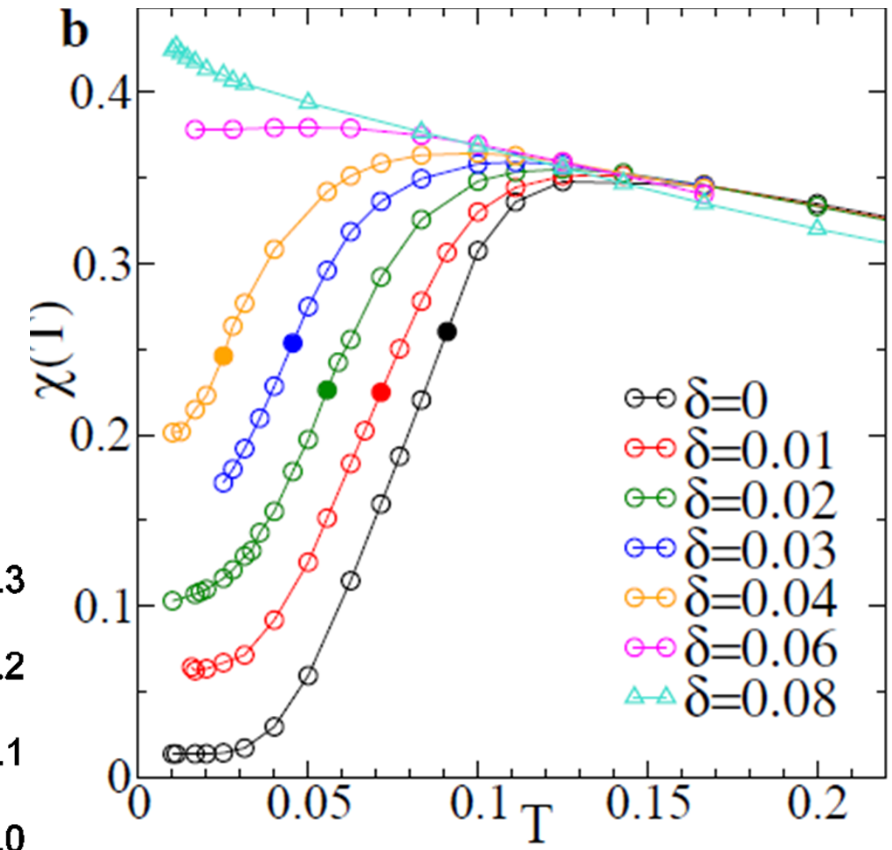




UNIVERSITÉ DE SHERBROOKE

Spin susceptibility



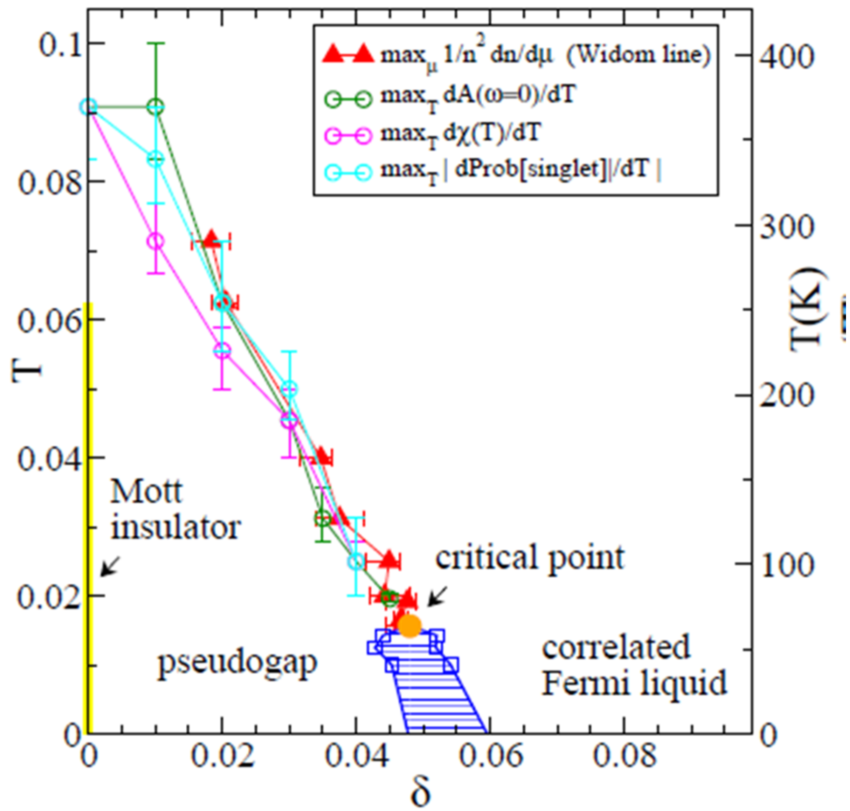


Underdoped Hg1223

Julien et al. PRL **76,** 4238 (1996)

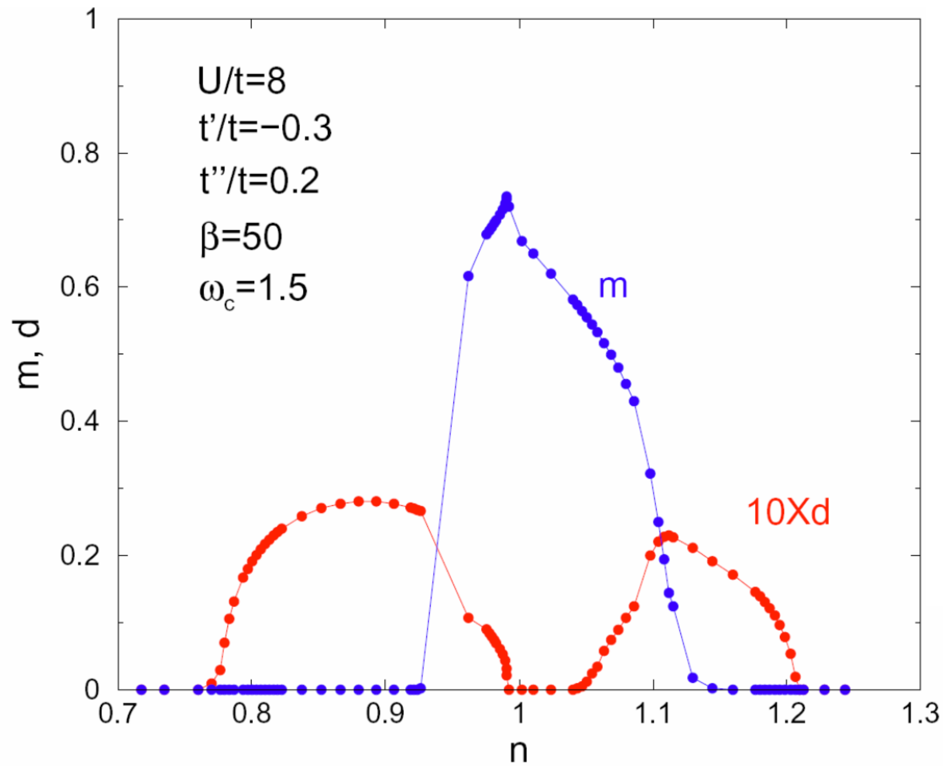
UNIVERSITÉ DE SHERBROOKE

Pseudogap *T** along the Widom line

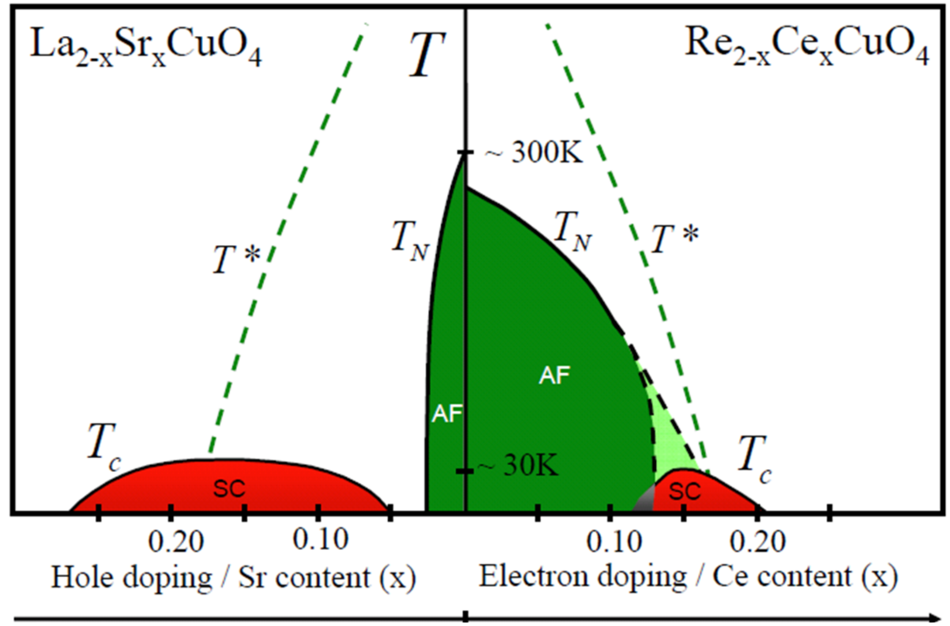


7. Hole-doped cuprates: superconductivity

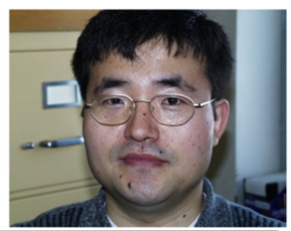
CDMFT global phase diagram

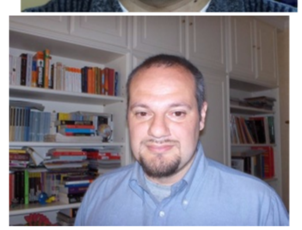


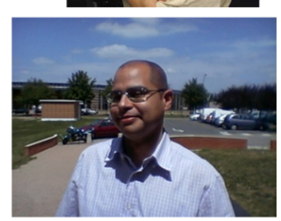
Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST Phys. Rev. B (2008)
AND Capone, Kotliar PRL (2006)



Armitage, Fournier, Greene, RMP (2009)







UNIVERSITE DE SHERBROOKE

Giovanni Sordi

Patrick Sémon

Kristjan Haule

Finite *T* phase diagram Superconductivity

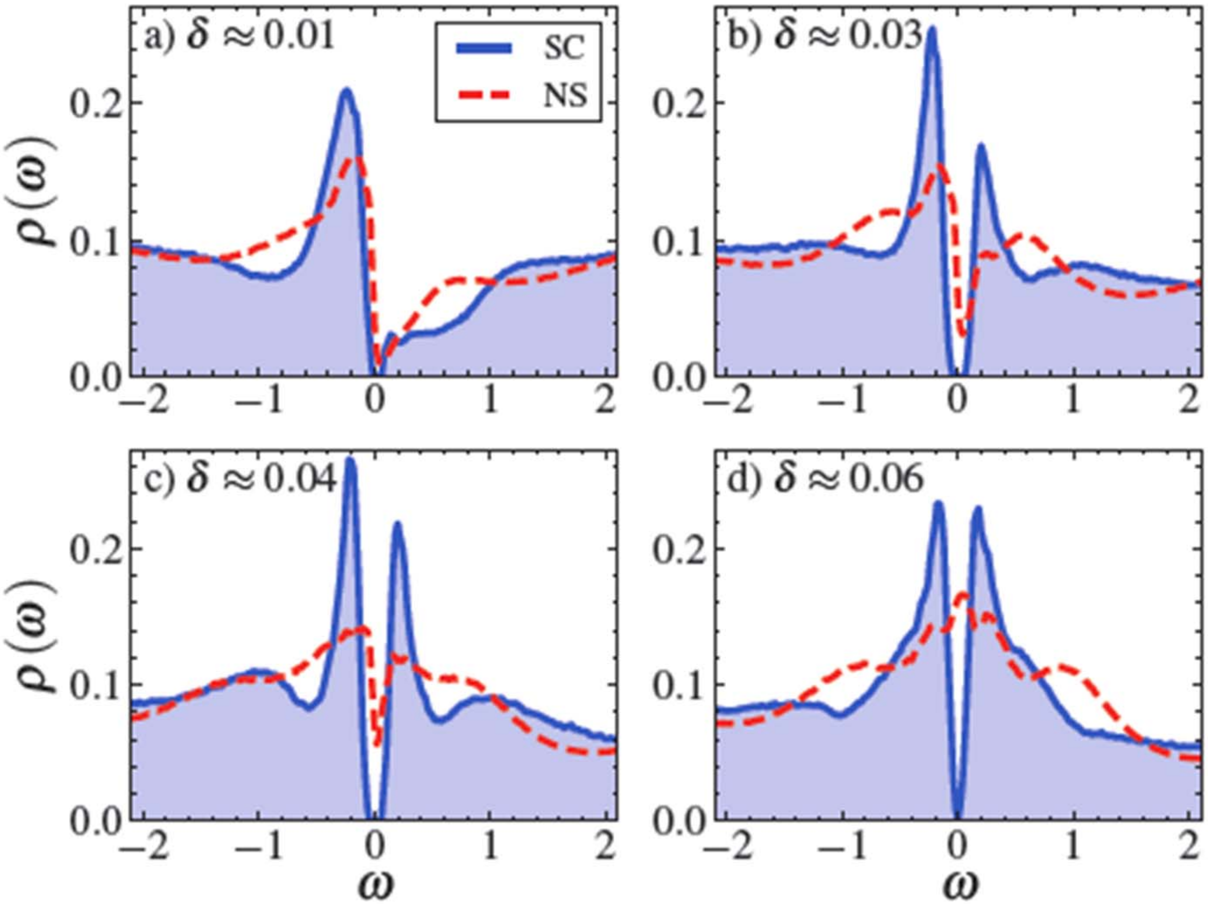
Sordi et al. PRL **108**, 216401 (2012)

UNIVERSITÉ DE SHERBROOKE

Strongly correlated superconductors

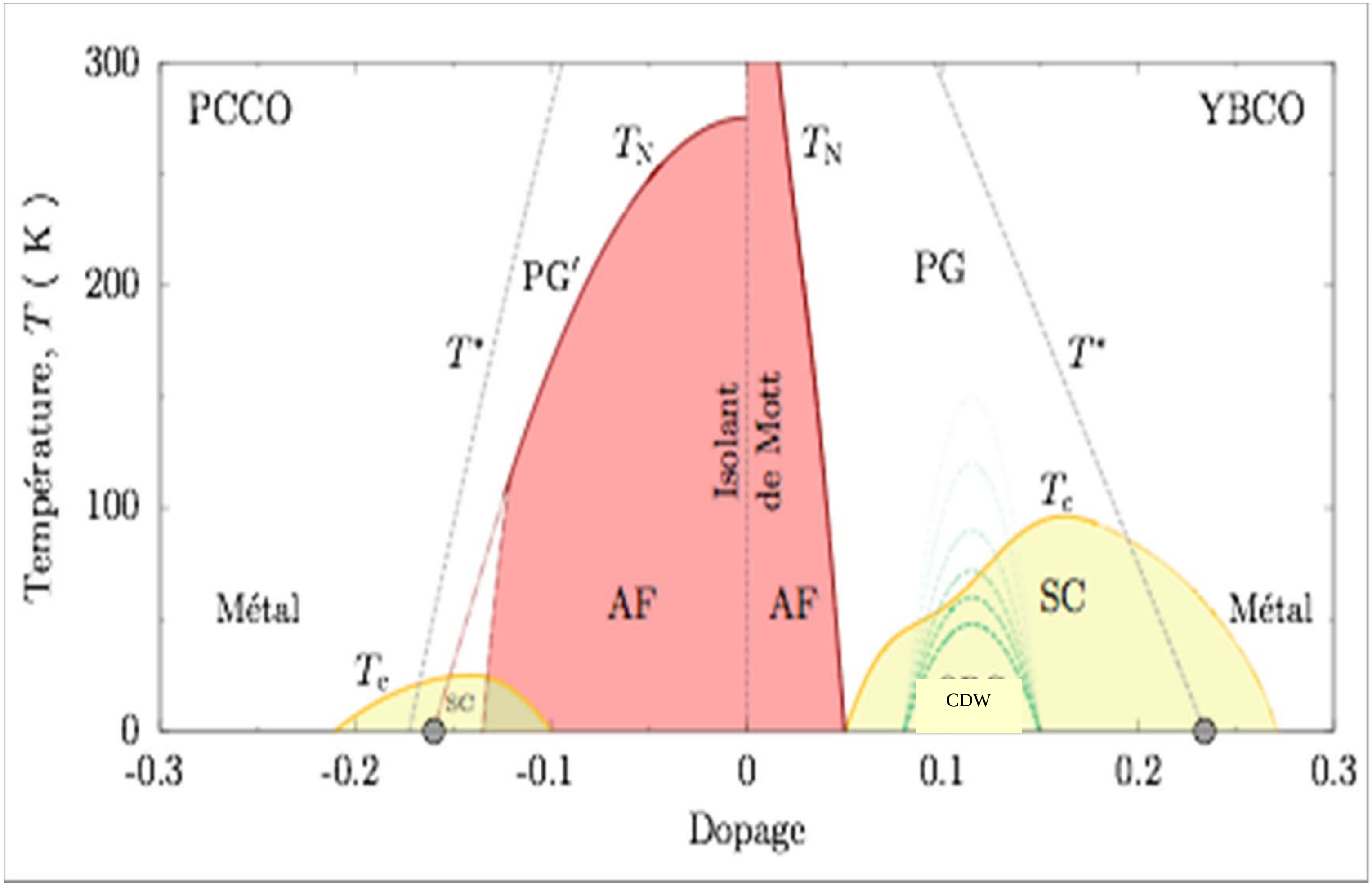
- T_c does not scale like order parameter
- Superfluid stiffness scales like doping
- Superconductivity can be largest close to the metal-insulator transition
- Resilience to near-neighbor repulsion

First-order transition leaves its mark



Open problems

Thèse de Francis Laliberté,
Université de Sherbrooke



UNIVERSITÉ DE SHERBROOKE

Conclusion

The dream

room-temperature superconductors

50–50

They would transform the grid—if they can exist at all

By Michael Moyer

You can build a coal-fired power plant just about anywhere. Renewables, on the other hand, are finicky. The strongest winds blow across the high plains. The sun shines brightest on the desert. Transporting that energy into cities hundreds of kilometers away will be one of the great challenges of the switch to renewable energy.

The most advanced superconducting cable can move those megawatts thousands of kilometers with losses of only a few percent. Yet there is a catch: the cable must be kept in a bath of liquid nitrogen at 77 kelvins (or –196 degrees Celsius). This kind of deployment, in turn, requires pumps and refrigeration units every kilometer or so, greatly increasing the cost and complexity of superconducting cable projects.

Superconductors that work at ordinary temperatures and pressures would enable a truly global energy supply. The Saharan sun could power western Europe via superconducting cables strung across the floor of the Mediterranean Sea. Yet the trick to making a room-temperature superconductor is just as much of a mystery today as it was in 1986, when researchers constructed the first superconducting materials that worked at the relatively high temperatures of liquid nitrogen (previous substances needed to be chilled down to 23 kelvins or less).

Two years ago the discovery of an entirely new class of superconductor—one based on iron—raised hopes that theorists might be able to divine the mechanism at work in high-temperature superconductors [see "An Iron Key to High-Temperature Superconductivity?" by Graham P. Collins; SCIENTIFIC AMERICAN, August 2009]. With such insights in hand, perhaps a path toward room-temperature superconductors would come into view. But progress has remained slow. The winds of change don't always blow on cue.

http://www.physique.usherbrooke.ca/taillefer/Vulgarisation.html

DFT + Methods from strongly correlated

Anisimov et al. J. Phys. **9**, 7354 (1997)
G. Kotliar et al. RMP, **78**, 865 (2006)
P. Sémon et al. arXiv:1403.7214

Materials Genome Initiative

Merci

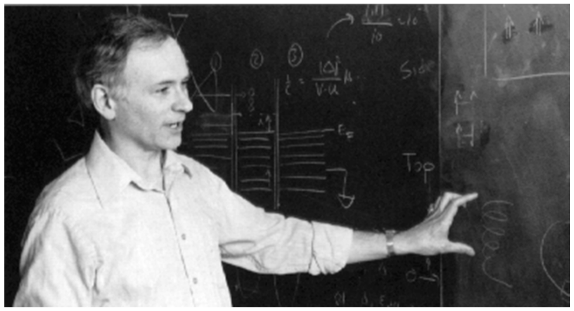
Thank you

Remerciements

Mentors

Université de Montréal

Letourneux, Depommier



Bruce Patton: MIT

Paul Martin: Harvard

Main recent collaborators


Giovanni Sordi


Kristjan Haule


David Sénéchal


Bumsoo Kyung


Alexandre Day


Marcello Civelli


Syed Hassan


Vincent Bouliane


Patrick Sémon


Dominic Bergeron


Sarma Kancharla


Massimo Capone


Gabriel Kotliar

UNIVERSITÉ DE SHERBROOKE

Anciens: professeurs

G. Slater, PhD, 1984, Ottawa, Doyen, MSRC

R. Dandoloff, PDF, 1984, Cergy-Pontoise

R.Day, PDF, 1985, Marquettte University, Michigan

B. Fourcade, PhD, 1988, ENS Lyon

A. Diaz-Guilera, PDF, 1990, Barcelone, Espagne

J.E. Llebot, PDF, 1986, Barcelone, Espagne

P. Bénard, PDF, 1993, UQTR

A.-M. Daré, PhD, 1994, Marseille

R. Côté PDF, 1994, UdeS

L. Chen PDF, 1995, Ottawa

A. Blais PhD, 2002, UdeS

A. Nevidomskyy, PDF, 2007 Rice University

S.R. Hassan, PDF, 2008 IMSc, Chennai, India

G. Sordi PDF, 2010, Royal Holloway

http://www.physique.usherbrooke.ca/pages/tremblay

Université de Sherbrooke

Anciens: industrie

P. Breton, MSc, 1987,
Investissements XLCAP

C. Brillon, MSc, 2007
Spécialiste contrôle non-destructif
Olympus NDT Canada

A. Veilleux MSc, 1994,
Directeur, CCS, Mammouth

B. Kyung PDF, 2009,
RBC, analyste financier

V. Hankevych, PDF, 2008,
Vice President, Structured
Product Development -
Quantitative Analysis,
RBC Capital Markets.

D. Chassé, PhD, 2009,
Gestion de risque,
Caisse de dépôt et placement.

S. Roy, PhD, 2008
Spécialiste de recherche
opérationnelle, Kronos,
Montréal.

S. Allen, PhD, 2006,
Analyste, CCS, Mammouth

Anciens, suite

Réal Tremblay, PhD, 1992
Manager, Natural Language Understanding R&D, Nuance

Yury Vilk, PDF, 1995
Senior SAS Programmer and Analyst
Department of Population Medicine
Boston, MA

Hugues Nélisse, MSc 1991
Prévention des risques mécaniques et physiques
IRSST

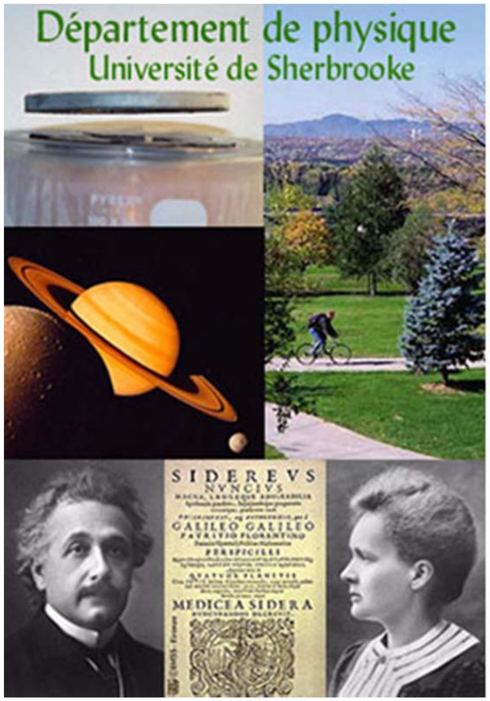
Serge Robillard, MSc 1986
Reconnaissance de la parole, Yahoo

Daniel Boies, PhD 1994
Principal Scientist
Microsoft
Natural Language Understanding, Information Extraction, Speech Recognition, Dialog Systems

François Lemay, PhD 2000
Physicien, Environnement Canada

Maxim Marienko PDF 2005
Quantitative Risk Management
at CME Group

André-Marie Tremblay



CANADA RESEARCH CHAIRS
CHAIRES DE RECHERCHE DU CANADA

RQMP

Le regroupement québécois sur les matériaux de pointe

CIFAR
CANADIAN INSTITUTE
for ADVANCED RESEARCH

UNIVERSITÉ DE
SHERBROOKE

Sponsors:

CRSNG NSERC

Fonds FCAR

RQCHP

Fondation canadienne pour l'innovation

UNIVERSITÉ DE
SHERBROOKE

Mammouth

Éducation, Loisir et Sport
Québec

Canada Foundation for Innovation
Fondation canadienne pour l'innovation

compute • calcul CANADA
High Performance Computing
CREATING KNOWLEDGE
DRIVING INNOVATION
BUILDING THE DIGITAL ECONOMY
Le calcul de haute performance
CRÉER LE SAVOIR
ALIMENTER L'INNOVATION
BÂTIR L'ÉCONOMIE NUMÉRIQUE

Calcul Québec

UNIVERSITÉ DE SHERBROOKE

Guylaine Séguin

UNIVERSITÉ DE SHERBROOKE

Merci

Thank you