Massively-parallel simulations of strongly-correlated materials

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strong correlations: what are they?

the many-electron *problem*

Born-Oppenheimer approximation, non-relativistic

kinetic energy

potential energy

constant

$$\hat{H}_e = -\frac{1}{2}\sum_i \nabla_i^2 + \frac{1}{2}\sum_{i \neq i'} \frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|} - \sum_{i,\alpha} \frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|} + \frac{1}{2}\sum_{\alpha \neq \alpha'} \frac{Z_\alpha Z_{\alpha'}}{|\mathbf{R}_\alpha - \mathbf{R}_{\alpha'}|}$$

electron-electron interaction

why is it a *problem*?

More Is Different

simple interactions among many particles
lead to **surprising** co-operative behavior

Nobel Prize in Physics 1977

4 August 1972, Volume 177, Number 4047

SCIENCE

More Is Different

Broken symmetry and the nature of the hierarchical structure of science.

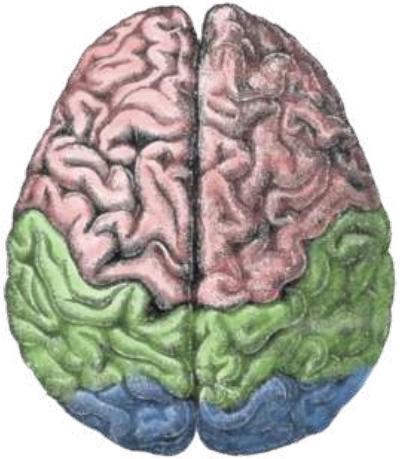
P. W. Anderson

less relevance they seem to have to the very real problems of the rest of science, much less to those of society.

The constructionist hypothesis breaks down when confronted with the twin difficulties of scale and complexity. The behavior of large and complex aggregates of elementary particles, it turns out, is not to be understood in terms of a simple extrapolation of the properties of a few particles. Instead, at each level of complexity entirely new properties appear, and the understanding of the new behaviors requires research which I think is as fundamental in its nature as any other. That is, it

co-operative phenomena

human brain



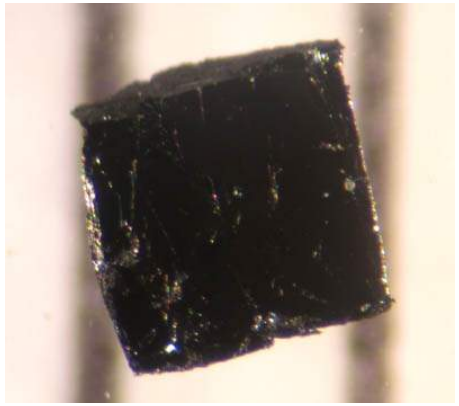
flocking

sand dunes

traffic jam

(photos from wikipedia)

in solid-state systems

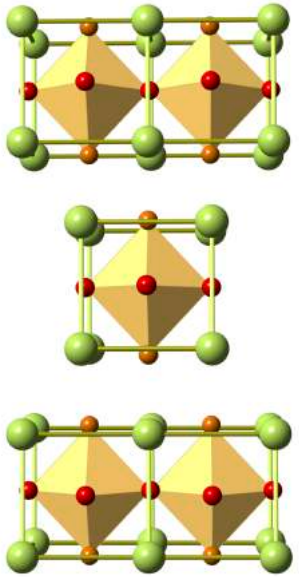


BSCCO-2223, photo from wikipedia

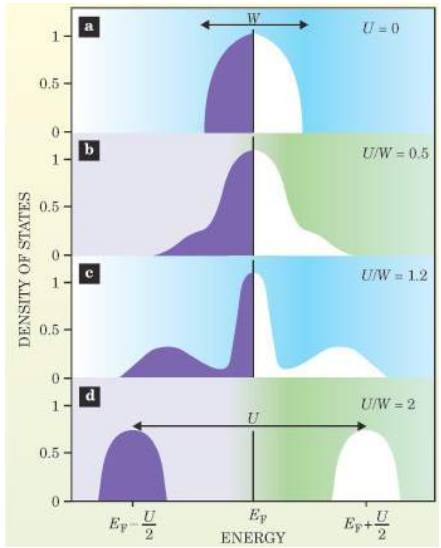
superconductivity

high-Tc superconductivity

non-conventional superconductivity

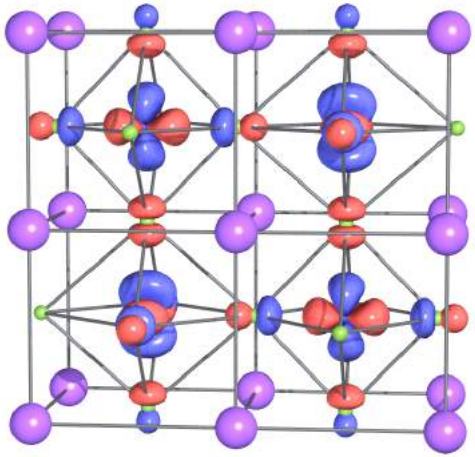


G. Zhang and E. Pavarini,
Rapid Research Letters **12**, 1800211 (2018)



Mott transition

G. Kotliar and D. Vollhardt, Physics Today **57,** 53 (2004)



orbital order

E. Pavarini, E. Koch, A.I. Lichtenstein, PRL **101**, 266405 (2008)

magnetism

photo from wikipedia

bad news: the exact solution is not an option

kinetic energy

potential energy

constant

$$\hat{H}_e = -\frac{1}{2}\sum_i \nabla_i^2 + \frac{1}{2}\sum_{i \neq i'} \frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|} - \sum_{i,\alpha} \frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|} + \frac{1}{2}\sum_{\alpha \neq \alpha'} \frac{Z_\alpha Z_{\alpha'}}{|\mathbf{R}_\alpha - \mathbf{R}_{\alpha'}|}$$

electron-electron interaction

$$\hat{H}_e \Psi_\alpha(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = E_\alpha \Psi_\alpha(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$$

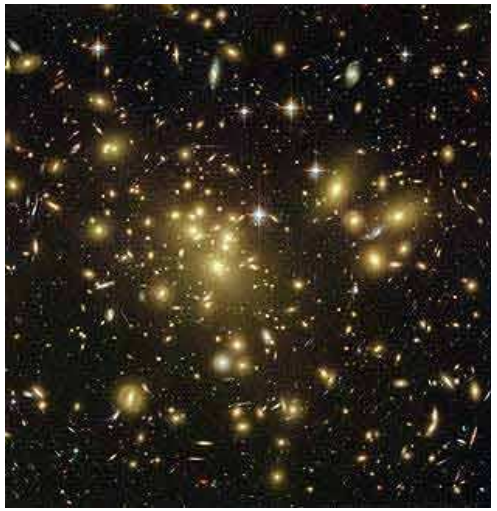
bad news: the exact solution is not an option

neutral iron, N=26

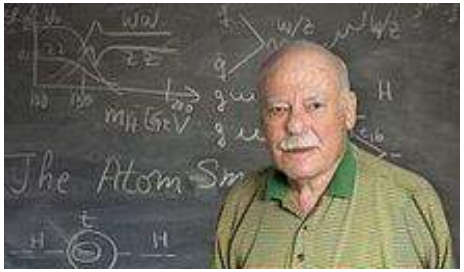
$$\Psi(\mathbf{r_1}, \mathbf{r_2}, \ldots, \mathbf{r_N})$$

The tabulation of one variable requires a page, of two variables a volume, and of three variables a library; but the full specification of a single wavefunction of neutral Fe is a function of seventy eight variables. It would be rather crude to restrict to ten the number of values at which to tabulate this function, but even so, full tabulation of it would require 10^{78} *entries, and even if this number could be reduced somewhat from considerations of symmetry, there would still not be enough atoms in the whole solar system to provide the material for printing such a table.*

D.R. Hartree (1948)



good news: it would be anyway useless



H.J. Lipkin

On the other hand, the exact solution of a many-body problem is really irrelevant since it includes a large mass of information about the system which although measurable in principle is never measured in practice.

[..] An incomplete description of the system is considered to be sufficient if these measurable quantities and their behavior are described correctly.

E. Pavarini and E. Koch, Autumn School on Correlated Electron 2013, Introduction

(photo from wikipedia)

why questions

(photo from wikipedia)

JÜLICH
FORSCHUNGSZENTRUM

what can be done then ?

$$\hat{H}_e \Psi_\alpha(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = E_\alpha \Psi_\alpha(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$$

a way out: density-functional theory

1964

PHYSICAL REVIEW VOLUME 136, NUMBER 3B 9 NOVEMEBR 1964

Inhomogeneous Electron Gas*

P. HOHENBERG†
École Normale Superieure, Paris, France
AND
W. KOHN‡
École Normale Superieure, Paris, France and Faculté des Sciences, Orsay, France
and
University of California at San Diego, La Jolla, California
(Received 18 June 1964)

This paper deals with the ground state of an inter… proved that there exists a universal functional of the … pression $E \equiv \int v(\mathbf{r})n(\mathbf{r})d\mathbf{r} + F[n(\mathbf{r})]$ has as its minimum … $v(\mathbf{r})$. The functional $F[n(\mathbf{r})]$ is then discussed for … (2) $n(\mathbf{r}) = \varphi(\mathbf{r}/r_0)$ with φ arbitrary and $r_0 \to \infty$. In bot… relation energy and linear and higher order electronic … also sheds some light on generalized Thomas-Fermi … these methods are presented.

INTRODUCTION

DURING the last decade there has been considerable progress in understanding the properties of a homogeneous interacting electron gas.[1] The point of view has been, in general, to regard the electrons as similar to a collection of noninteracting particles with the important additional concept of collective excitations.

On the other hand, there has been in existence since the 1920's a different approach, represented by the Thomas-Fermi method[2] and its refinements, in which the electronic density $n(\mathbf{r})$ plays a central role and in which the system of electrons is pictured more like a classical liquid. This approach has been useful, up to now, for simple though crude descriptions of inhomogeneous systems like atoms and impurities in metals.

Lately there have been also some important advances along this second line of approach, such as the work of Kompaneets and Pavlovskii,[3] Kirzhnits,[4] Lewis,[5] Baraff and Borowitz,[6] Baraff,[7] and DuBois and Kivelson.[8] The present paper represents a contribution in the same area.

1965

PHYSICAL REVIEW VOLUME 140, NUMBER 4A 15 NOVEMBER 1965

Self-Consistent Equations Including Exchange and Correlation Effects*

W. KOHN AND L. J. SHAM
University of California, San Diego, La Jolla, California
(Received 21 June 1965)

From a theory of Hohenberg and Kohn, approximation methods for treating an inhomogeneous system of interacting electrons are developed. These methods are exact for systems of slowly varying or high density. For the ground state, they lead to self-consistent equations analogous to the Hartree and Hartree-Fock equations, respectively. In these equations the exchange and correlation portions of the chemical potential of a uniform electron gas appear as additional effective potentials. (The exchange portion of our effective potential differs from that due to Slater by a factor of $\frac{2}{3}$.) Electronic systems at finite temperatures and in magnetic fields are also treated by similar methods. An appendix deals with a further correction for systems with short-wavelength density oscillations.

I. INTRODUCTION

IN recent years a great deal of attention has been given to the problem of a homogeneous gas of interacting electrons and its properties have been established with a considerable degree of confidence over a wide range of densities. Of course, such a homogeneous gas represents only a mathematical model, since in all real systems (atoms, molecules, solids, etc.) the electronic density is nonuniform.

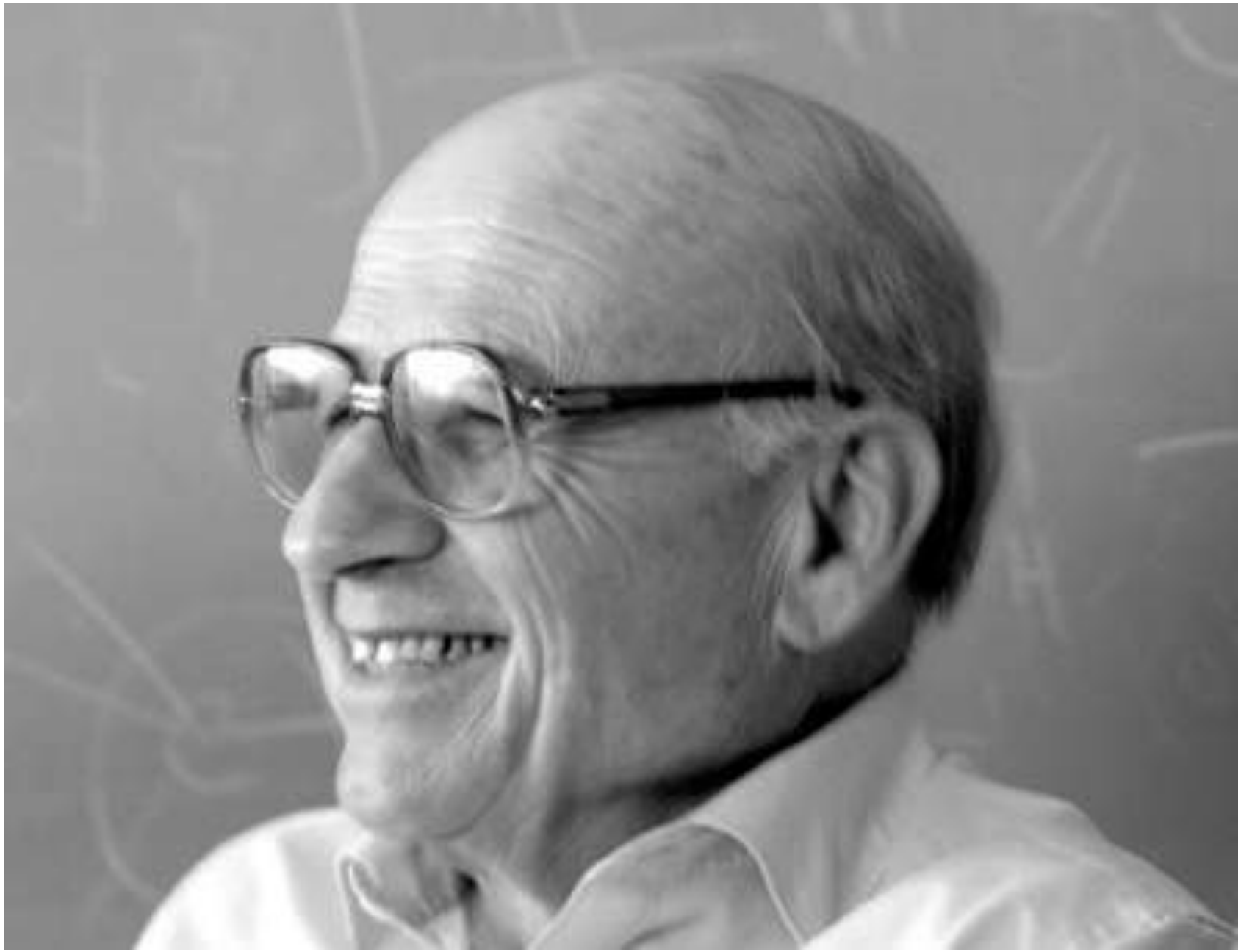
It is then a matter of interest to see how properties of the homogeneous gas can be utilized in theoretical

In Secs. III and IV, we describe the necessary modifications to deal with the finite-temperature properties and with the spin paramagnetism of an inhomogeneous electron gas.

Of course, the simple methods which are here proposed in general involve errors. These are of two general origins[4]: a too rapid variation of density and, for finite systems, boundary effects. Refinements aimed at reducing the first type of error are briefly discussed in Appendix II.

II. THE GROUND STATE

1998: Nobel Prize in Chemistry to Walter Kohn



the *standard model*: density-functional theory

$$\hat{H}_e \Psi_\alpha(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = E_\alpha \Psi_\alpha(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$$

$$n_G(\mathbf{r}), \qquad E_G[n(\mathbf{r})], \qquad \ldots$$

1998: Nobel Prize in Chemistry to Walter Kohn

In my view DFT makes two kinds of contribution to the science of multi-particle quantum systems, including problems of electronic structure of molecules and of condensed matter:

The first is in the area of fundamental *understanding*. Theoretical chemists and physicists, following the path of the Schroedinger equation, have become accustomed to think in a truncated *Hilbert space of single particle orbitals*. The spectacular advances achieved in this way attest to the fruitfulness of this perspective. However, when high accuracy is required, so many Slater determinants are required (in some calculations up to ~ 10^{9}!) that *comprehension* becomes difficult. DFT provides a complementary perspective. It focuses on quantities in the real, 3-dimensional coordinate space, principally on the electron density $n(r)$ of the groundstate. Other quantities of great interest

(from the Nobel lecture)

the Kohn-Sham eigenvalues

$$\hat{H}_e = \sum_i \hat{H}_i^0 + \sum_{i \neq i'} \frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|} \quad \longrightarrow \quad \hat{\mathcal{H}}_e = \sum_i \hat{\mathcal{H}}_i^0$$

Kohn-Sham auxiliary Hamiltonian

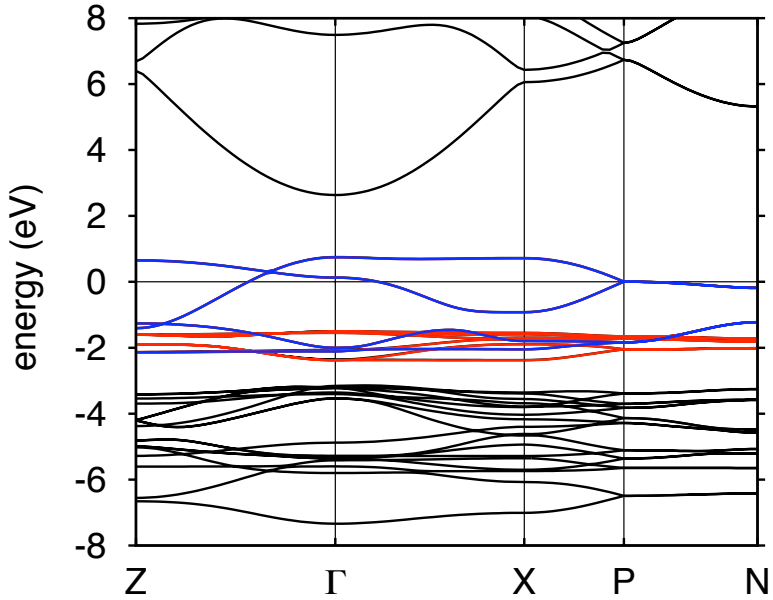
$$\hat{h}_e = \sum_i \left[-\frac{1}{2}\nabla_i^2 + v_R(\boldsymbol{r}_i) \right] = \sum_i \hat{h}_e(\boldsymbol{r}_i)$$

$$v_R(\boldsymbol{r}) = -\sum_\alpha \frac{Z_\alpha}{|\boldsymbol{r} - \boldsymbol{R}_\alpha|} + \int d\boldsymbol{r}' \frac{n(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|} + \frac{\delta E_{\mathrm{xc}}[n]}{\delta n} = v_{en}(\boldsymbol{r}) + v_H(\boldsymbol{r}) + v_{xc}(\boldsymbol{r})$$

(in practice: LDA,GGA,…)

unexpected successes of DFT

Kohn-Sham eigenvalues as *elementary excitations!*



band structures, material trends, prediction

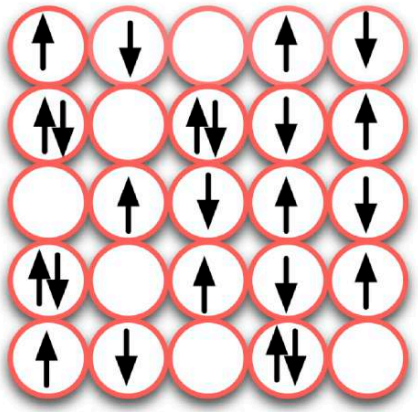
unexpected successes of DFT

Kohn-Sham eigenvalues as *elementary excitations!*

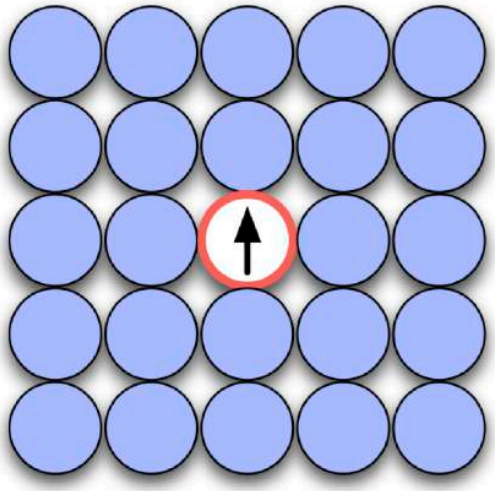
successes of the independent electron picture

Kohn-Sham auxiliary Hamiltonian

$$\hat{h}_e = \sum_i \left[-\frac{1}{2}\nabla_i^2 + v_R(\boldsymbol{r}_i) \right] = \sum_i \hat{h}_e(\boldsymbol{r}_i)$$



mean-field-like Hamiltonian

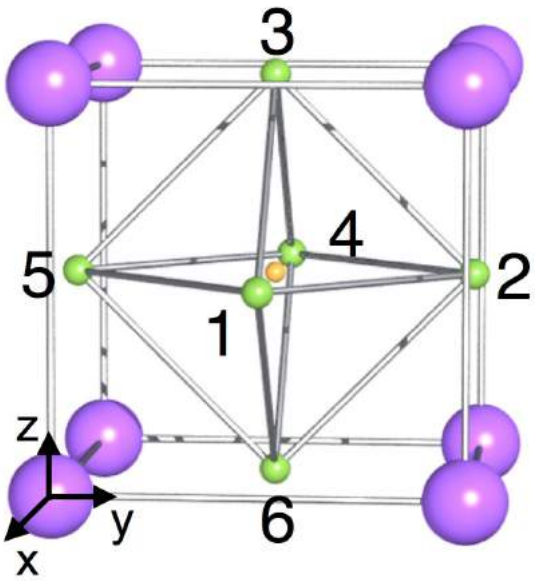


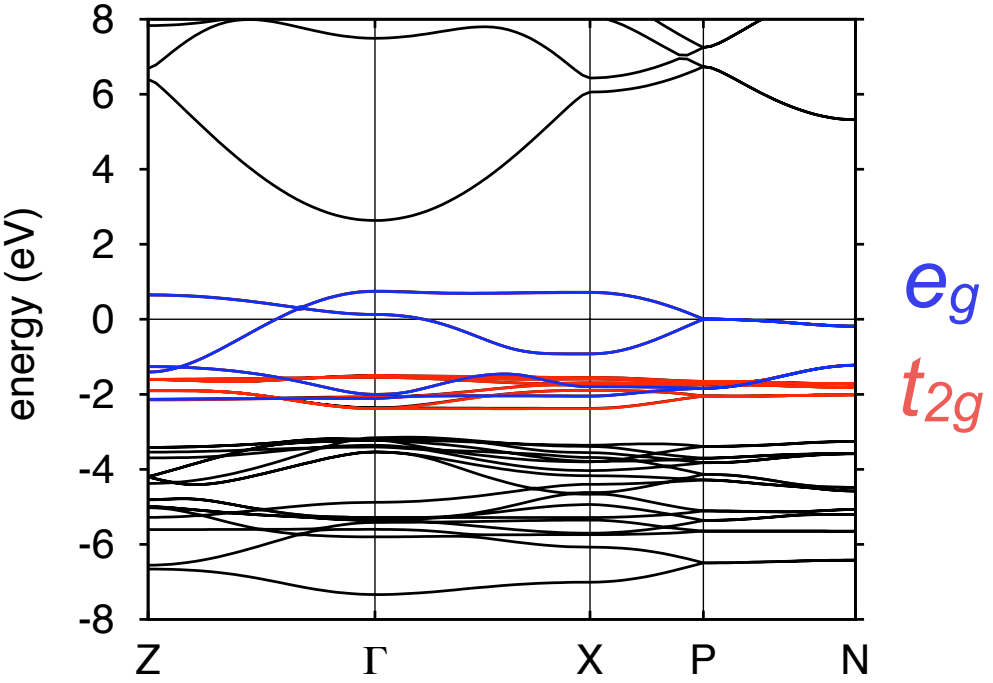
strongly-correlated systems:
those for which the KS approximation fails

deep problems: Mott systems

$KCuF_3$

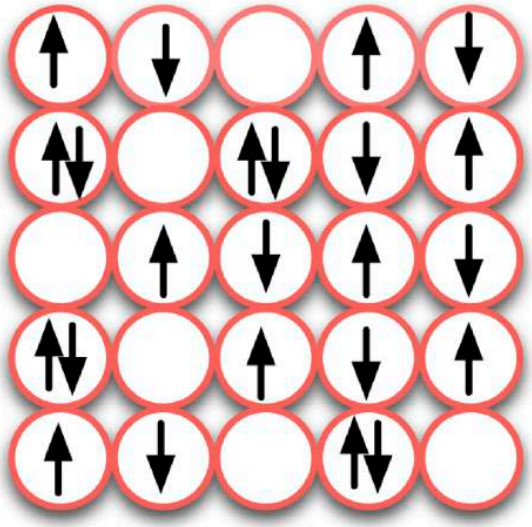
DFT (LDA): it is a metal!



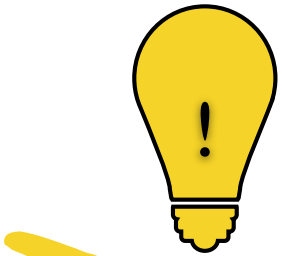


Experiments: insulator! Above 40 K a **paramagnetic** insulator

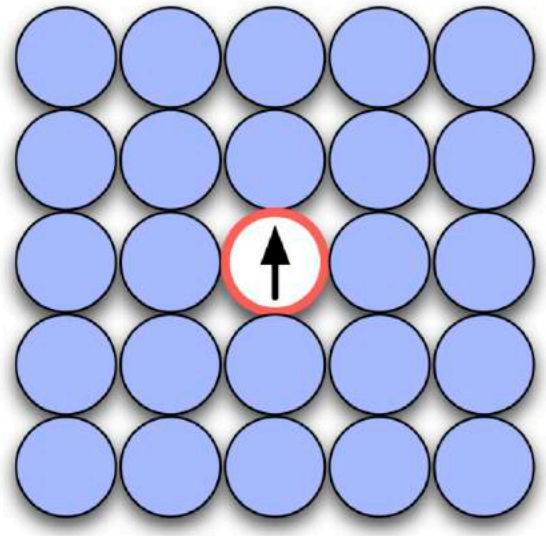
origin of failures: one-electron picture



$$\hat{H}_e = \sum_i \hat{H}_i^0 + \sum_{i \neq i'} \frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|}$$



$$\hat{H}_e = \sum_i \hat{\mathcal{H}}_i^0$$



the whole is more than the sum of its parts

Mott transition

ab-initio Kohn-Sham approximation fails…

editorial

The Hubbard model at half a century

Models are abundant in virtually all branches of physics, with some achieving iconic status. The Hubbard model, celebrating its golden jubilee this year, continues to be one of the most popular contrivances of theoretical condensed-matter physics.

Capturing the essence of a phenomenon while being simple: the ingredients of a top model in physics. Since the early days of quantum mechanics, many models, Hamiltonians and theories aiming to provide a deeper understanding of various properties of condensed matter have been put forward — with varying degrees of success and fame. One truly legendary model is the Hubbard model, independently conceived by Martin Gutzwiller[1], Junjiro Kanamori[2] and, of course, John Hubbard[3] — their original papers all appearing in 1963. The refine his model. His 'Electron correlations in narrow energy bands' would eventually comprise six installments. 'Hubbard III'[4] became especially important as it showed that for one electron per lattice site — the Hubbard model at half filling — the Mott (or Mott–Hubbard) transition is reproduced. This is a type of metal–insulator transition that could not be understood in terms of conventional band theory (which predicts that a half-filled band always results in a conducting state).

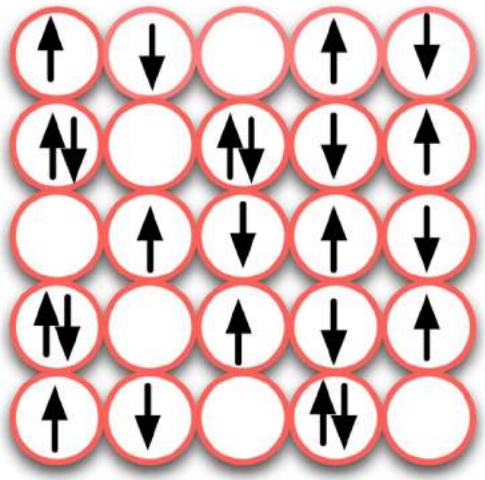
The simplicity of the Hubbard model, when written down, is deceptive. Not only when the field of cold-atom optical trapping had advanced so far that experimental realizations of the Hubbard model could be achieved. A landmark experiment demonstrated how a lattice of bosonic atoms displays a transition from a superfluid to a Mott insulator[5], a result accounted for by the Bose–Hubbard model (the Hubbard model for bosons). Many other variants of the Hubbard model, including the original model for fermions[6], have been experimentally realized by now, a development that nicely illustrates how a model can become the target of experiments

but it can be explained with simple models!

Hubbard model at half-filling

atomic hoppings atomic

$$\hat{H} = \varepsilon_d \sum_i \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c^\dagger_{i\sigma} c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} = \hat{H}_d + \hat{H}_T + \hat{H}_U$$



1. *t=0*: collection of atoms, **insulator**
2. *U=0*: half-filled band, **metal**

canonical model for Mott transition

a drastic simplification

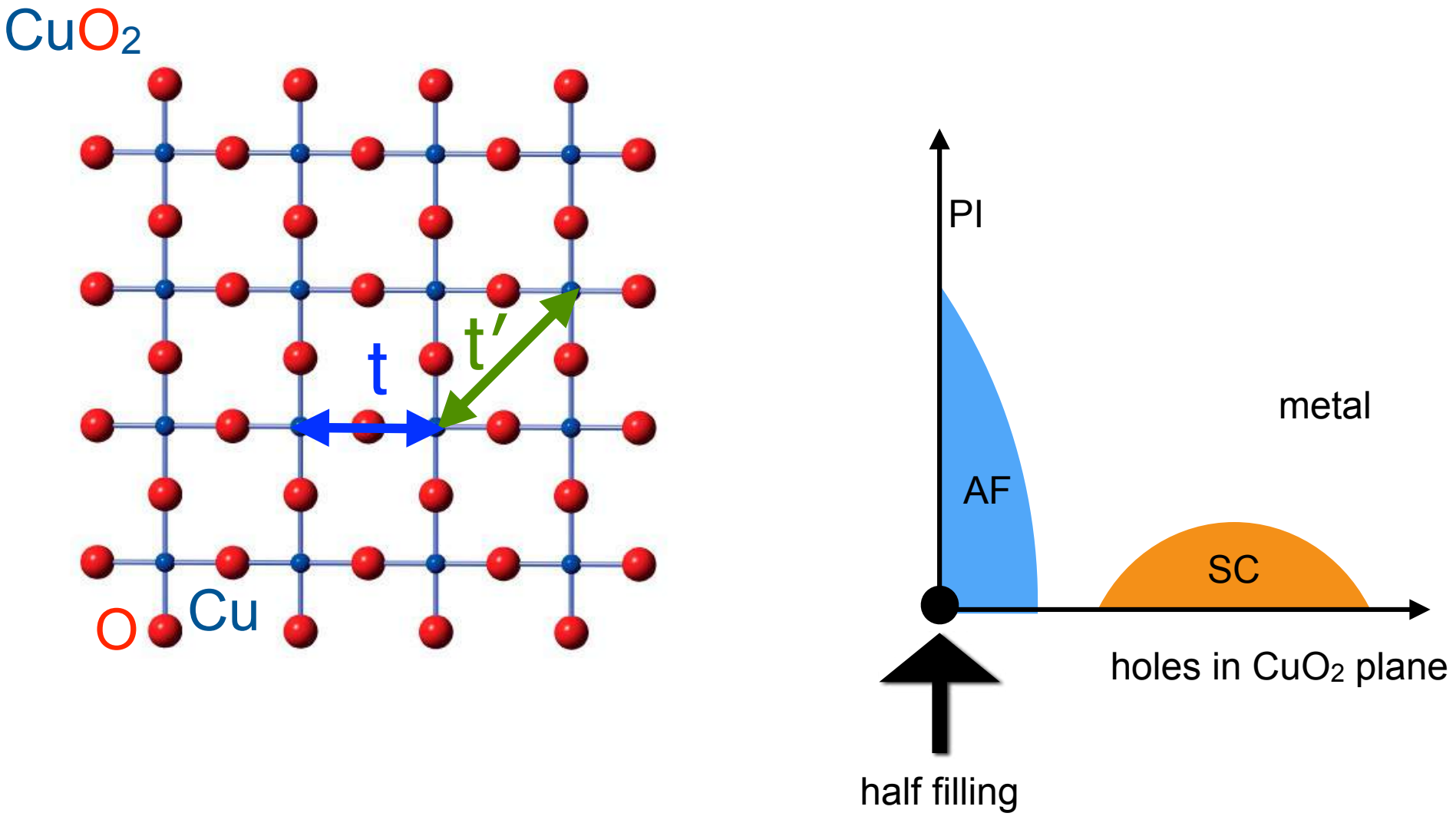
$$\hat{H}_e = \sum_i \hat{H}_i^0 + \sum_{i \neq i'} \frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|}$$

$$H = -t \sum_{\sigma} \sum_{\langle ii' \rangle} c_{i\sigma}^{\dagger} c_{i'\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow}$$

Hubbard model

high-T_c superconducting cuprates

phase diagram



1989-1992: dynamical mean-field theory

map LATTICE problem to QUANTUM IMPURITY problem

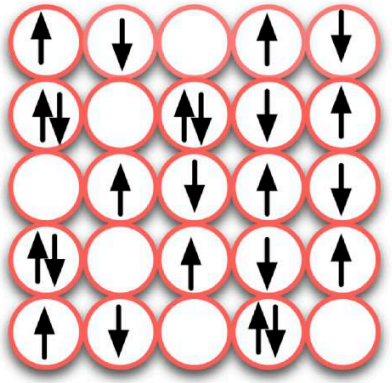
local self-energy approximation

- W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989)
- E. Müller-Hartmann, Z. Phys. B **74**, 507 (1989);
  Z. Phys. B **76**, 211 (1989); Int. J. Mod. Phys. B **3**, 2169 (1989)
- A. Georges and G. Kotliar, Phys. Rev. B **45**, 6479 (1992)
- M. Jarrell, Phys. Rev. Lett. **69**, 168 (1992)

1989-1992: dynamical mean-field theory

Hubbard model

$$\hat{H} = \varepsilon_d \sum_i \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c^\dagger_{i\sigma} c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

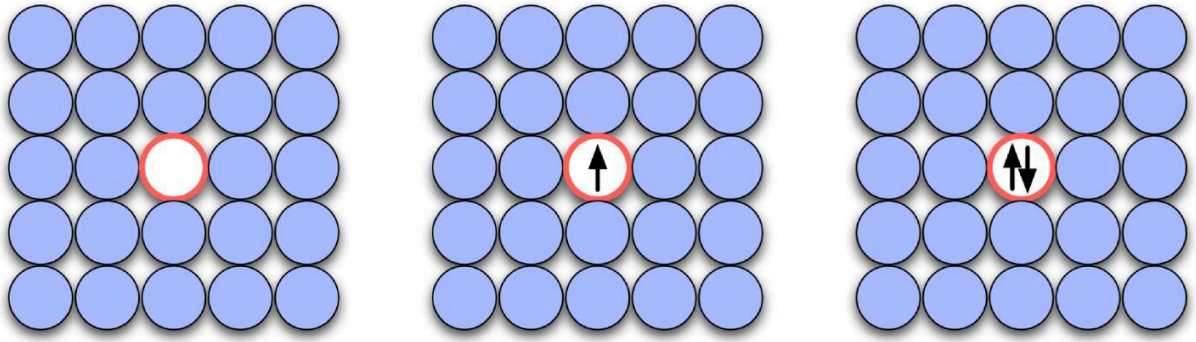


$G^{i,j}$

H^{LDA}

$U^{i,i}$

self-consistent
quantum-impurity model



$$\mathcal{G}^{-1} = G^{-1} + \Sigma$$

$$G = G^{i,i}$$

k-independent self-energy

exact in the infinite coordination number limit

Metzner and Vollhardt, PRL **62**, 324 (1989); Georges and Kotliar, PRB **45**, 6479 (1992).

dynamical mean-field theory

$$\hat{H} = \varepsilon_d \sum_i \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c^\dagger_{i\sigma} c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

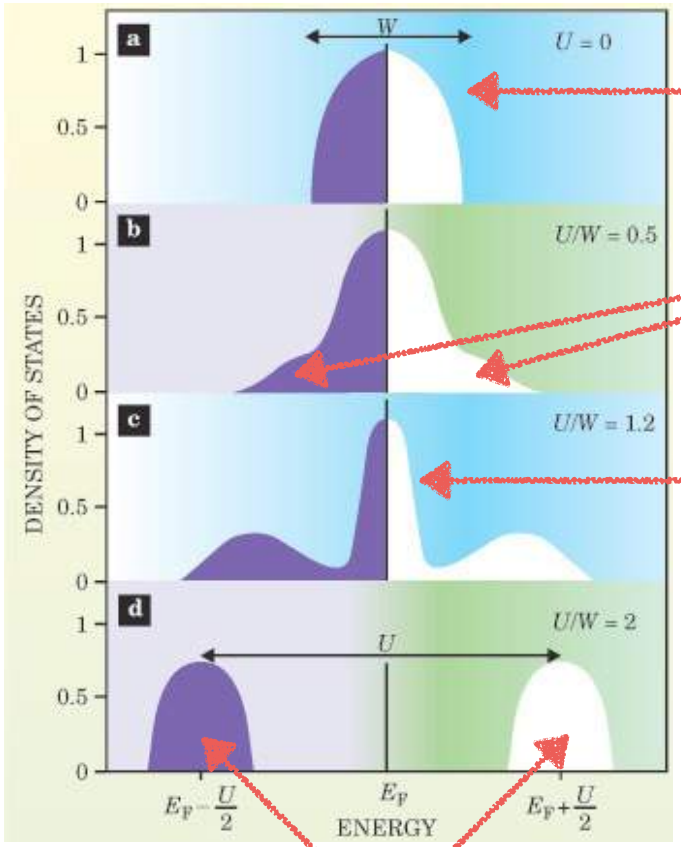
U=0

W: band width

Bethe Lattice

U~W

U>U_c



half-filled metal

spectral weight transfer

narrow quasi-particle peak

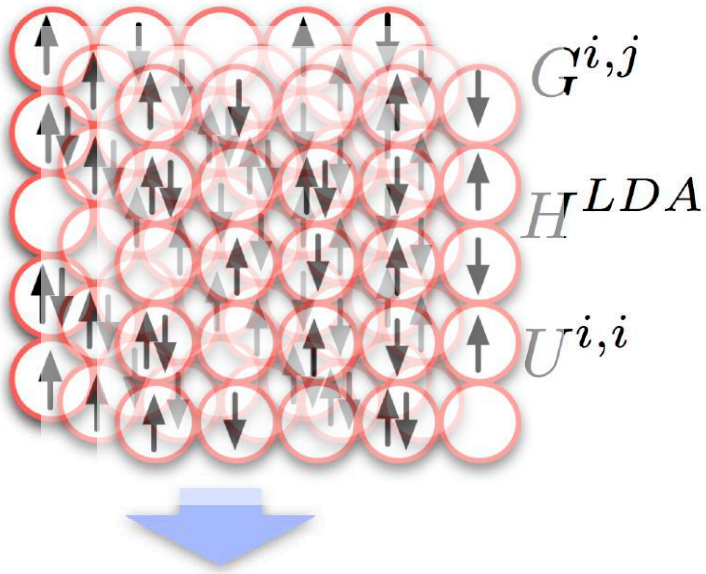
Hubbard bands

G. Kotliar and D. Vollhardt, Physics Today **57,** 53 (2004)

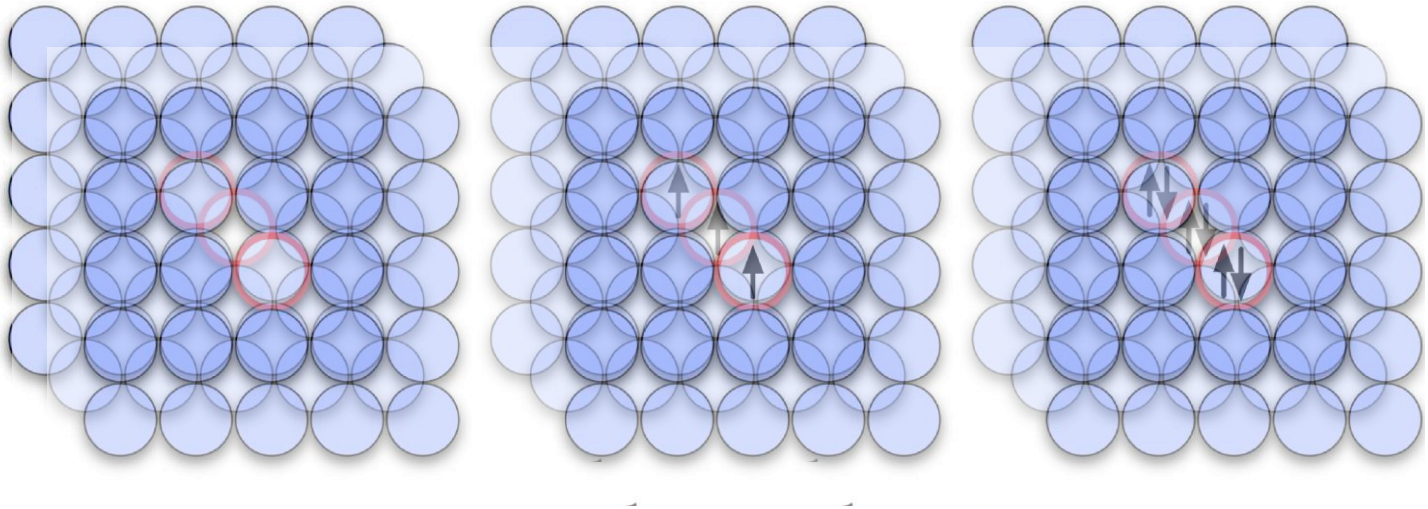
DMFT for real materials

realistic models

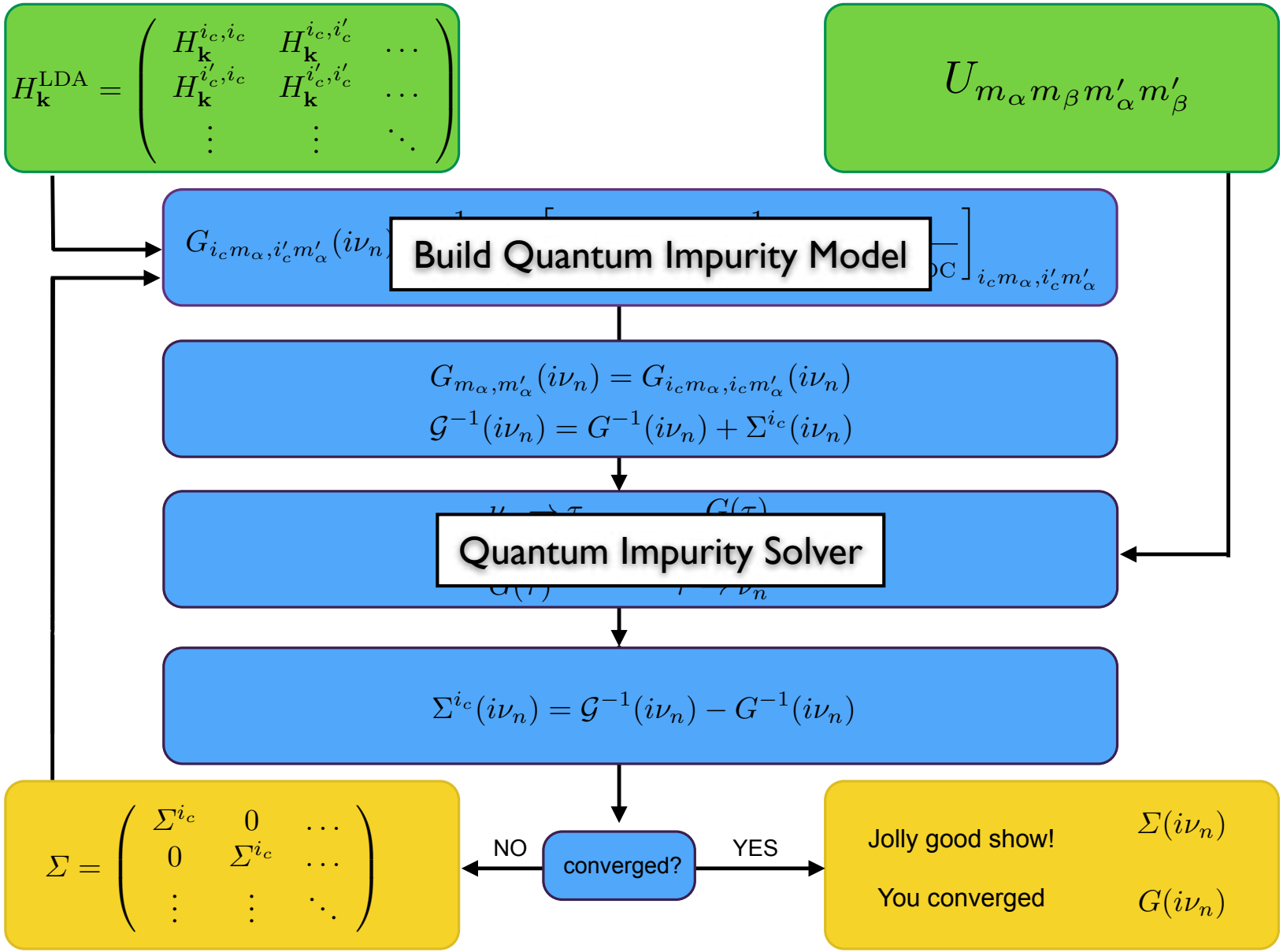
$$\hat{H}_e = \sum_{ab} t_{ab} c_a^\dagger c_b + \frac{1}{2} \sum_{cdc'd'} U_{cdd'c'} c_c^\dagger c_d^\dagger c_{c'} c_{d'}$$



realistic self-consistent quantum-impurity (QI) model



in theory, more indices



in practice, QMC-based QI solvers

computational time

limited number of orbitals/site

finite temperature

sign problem

some *interactions* are worse than others

some *bases* are worse than others

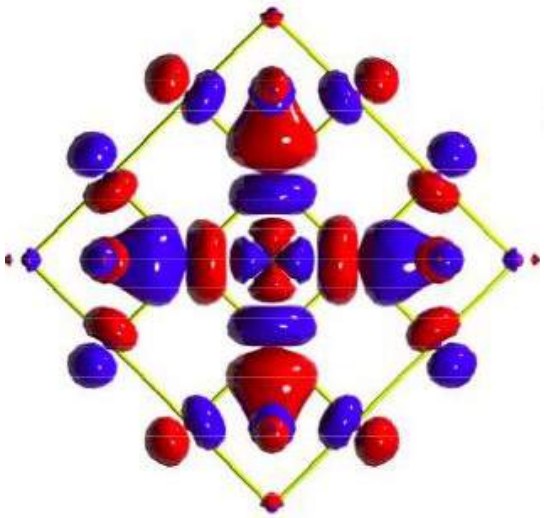
we need **minimal** material-specific models

minimal material-specific models

$$\hat{H}_e = \sum_i \hat{H}_i^0 + \sum_{i \neq i'} \frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|} \quad \Rightarrow \quad \hat{H}_e = \sum_{ab} t_{ab} c_a^\dagger c_b + \frac{1}{2} \sum_{cdc'd'} U_{cdd'c'} c_c^\dagger c_d^\dagger c_{c'} c_d$$

chose the one-electron basis in a *smart* way — minimal models

idea: DFT-based Wannier functions



- span full Hamiltonian
- good electron density
- very good description of weakly correlated states
- average and long-range Coulomb included
- information on lattice and chemistry
- allow energy- and symmetry-based downfolding

E. Pavarini *et al.*, PRL **87**, 047003 (2001); PRL **92**, 176403 (2004); New J. Phys. **7**, 188 (2005)

and (sufficiently) general QI solvers

VOLUME 92, NUMBER 17 PHYSICAL REVIEW LETTERS week ending 30 APRIL 2004

Mott Transition and Suppression of Orbital Fluctuations in Orthorhombic $3d^1$ Perovskites

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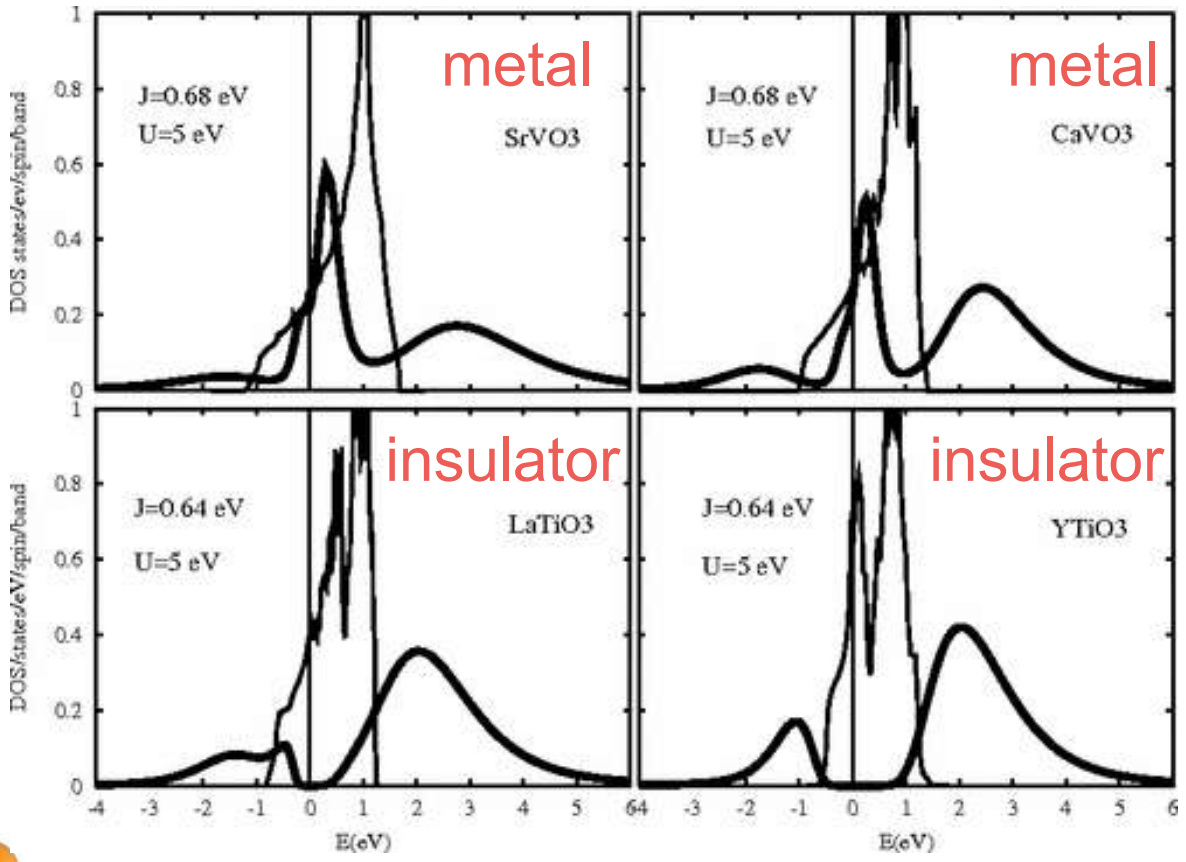
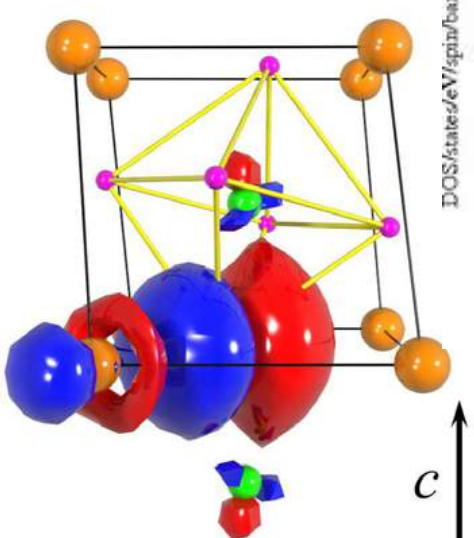
$SrVO_3$

$CaVO_3$

$LaTiO_3$

$YTiO_3$





details matter!

770 K

new QMC-based QI solvers

REVIEWS OF MODERN PHYSICS, VOLUME 83, APRIL–JUNE 2011

Continuous-time Monte Carlo methods for quantum impurity models

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Quantum impurity models describe an atom or molecule embedded in a host material with which it can exchange electrons. They are basic to nanoscience as representations of quantum dots and molecular conductors and play an increasingly important role in the theory of ''correlated electron'' materials as auxiliary problems whose solution gives the ''dynamical mean-field'' approximation to the self-energy and local correlation functions. These applications require a method of solution which provides access to both high and low energy scales and is effective for wide classes of physically realistic models. The continuous-time quantum Monte Carlo algorithms reviewed in this article meet this challenge. Derivations and descriptions of the algorithms are presented in enough detail to allow other workers to write their own implementations, discuss the strengths and weaknesses of the methods, summarize the problems to which the new methods have been successfully applied, and outline prospects for future applications.

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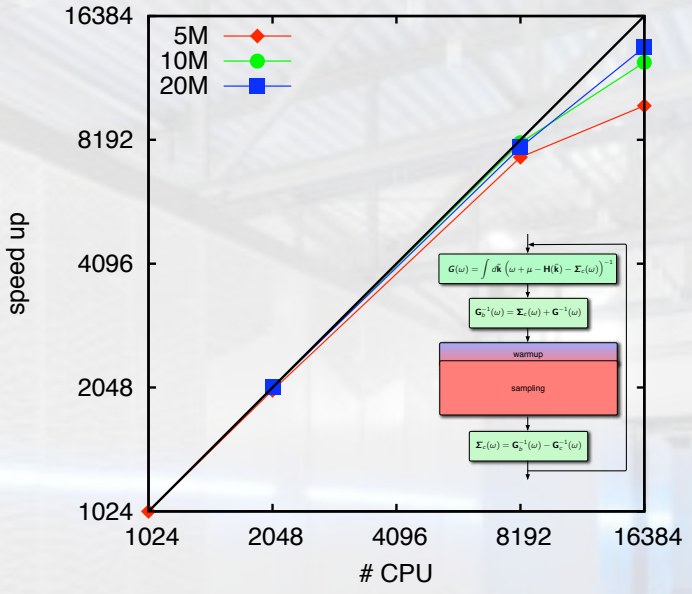
flexible and efficient solvers

$$H = -\sum_{ii'}\sum_{mm'}\sum_{\sigma} t^{ii'}_{mm'} c^{\dagger}_{im\sigma} c_{i'm'\sigma} + U\sum_{im} n_{im\uparrow} n_{im\downarrow} + \frac{1}{2}\sum_{im\neq m'\sigma\sigma'} (U - 2J - J\delta_{\sigma\sigma'}) n_{im\sigma} n_{im'\sigma'} - J\sum_{m\neq m'} (c^{\dagger}_{m\uparrow} c^{\dagger}_{m'\downarrow} c_{m'\uparrow} c_{m\downarrow} + c^{\dagger}_{m\uparrow} c^{\dagger}_{m\downarrow} c_{m'\uparrow} c_{m'\downarrow})$$

self-energy matrix in spin-orbital space

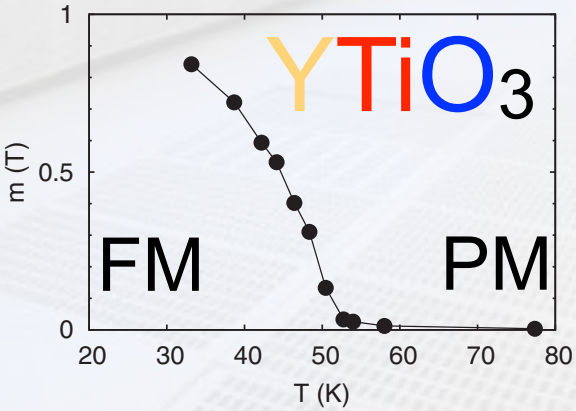


DMFT and cDMFT

generalized quantum impurity solvers:

general HF QMC
general CT-INT QMC
general CT-HYB QMC

- CT-HYB: A. Flesch, E. Gorelov, E. Koch and E. Pavarini
  Phys. Rev. B **87**, 195141 (2013)
- CT-INT: E. Gorelov et al, PRL 104, 226410 (2010)
- CT-INT+SO: G. Zhang, E. Gorelov, E. Sarvestani, and E. Pavarini,
  Phys. Rev. Lett. 116, 106402 (2016)

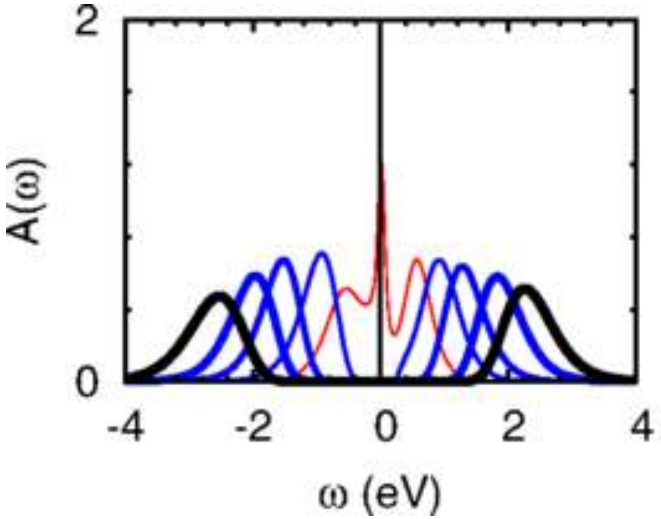


sign problem: smart adapted basis choice

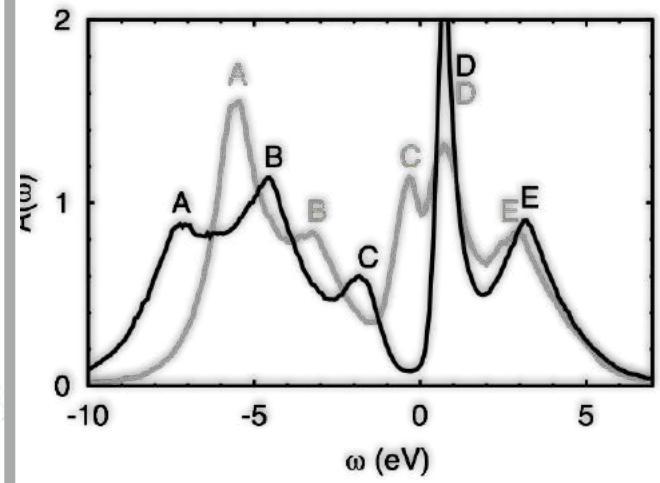
… and powerful computers

what can we do so far?

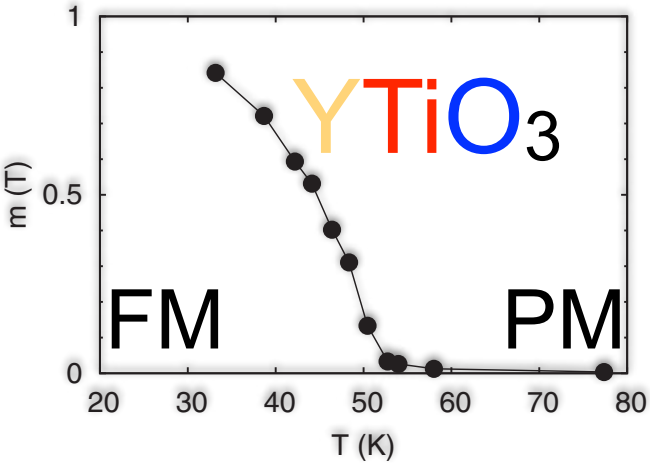
spectral functions



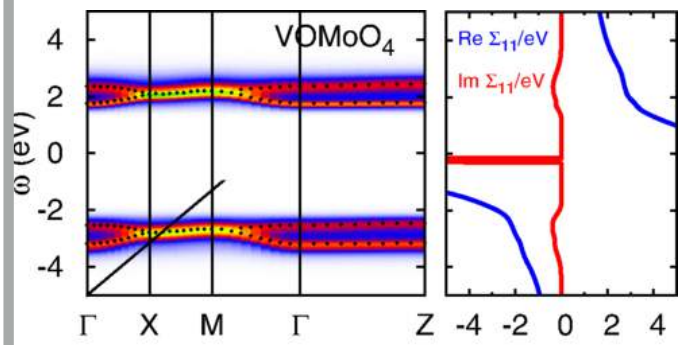
many orbitals



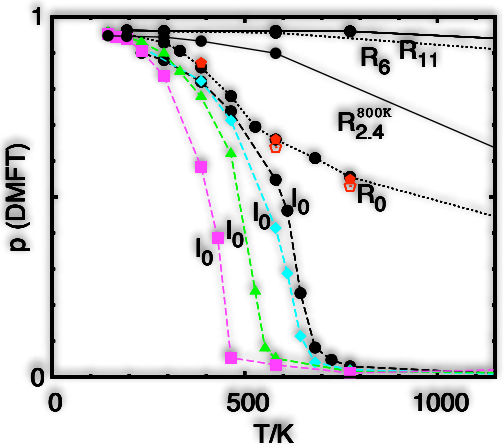
low T



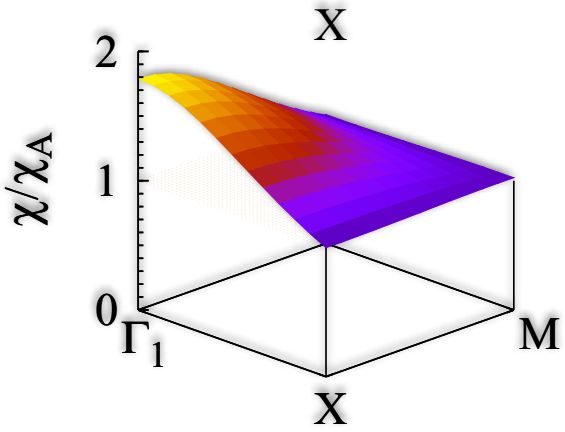
correlated bands



phase transitions

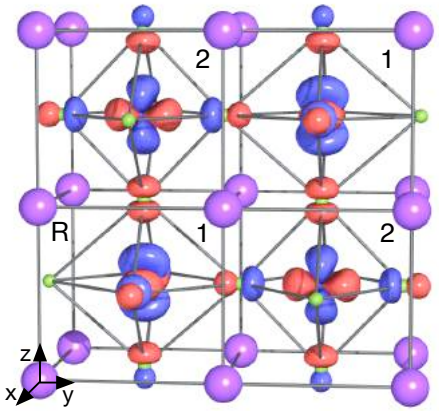


susceptibilities

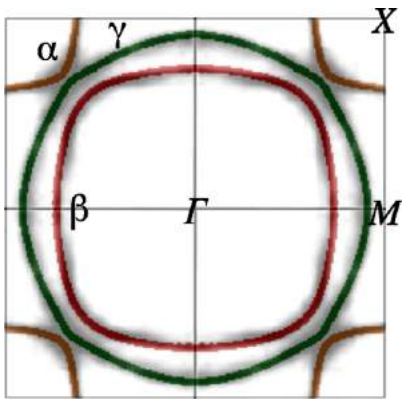


what can we do so far?

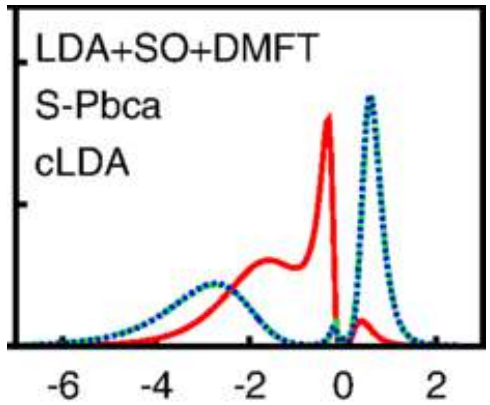
orbital order



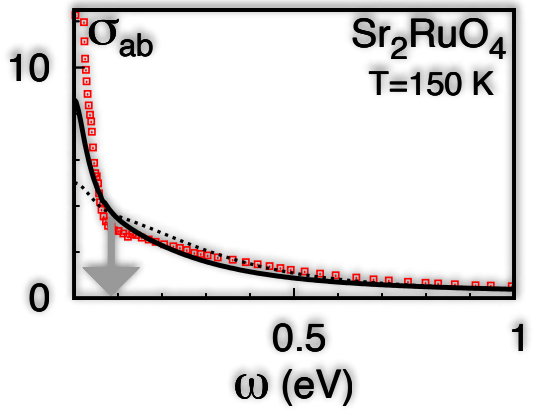
Fermi surface



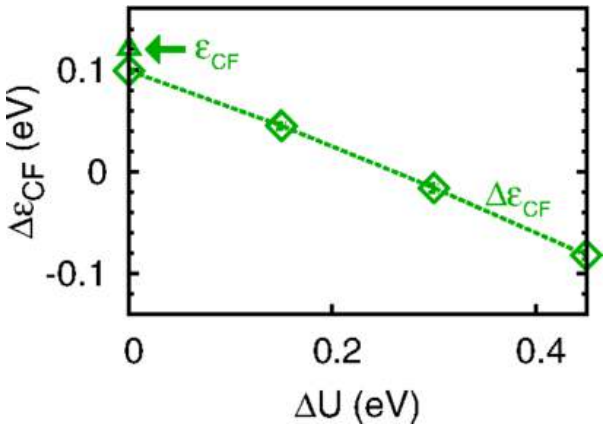
spin-orbit



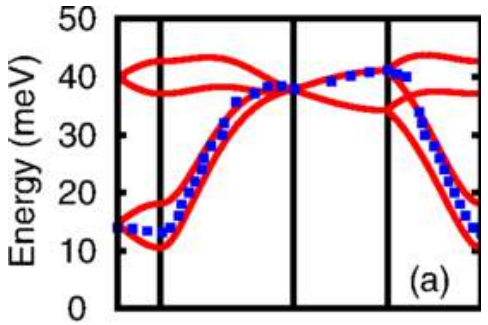
conductivity



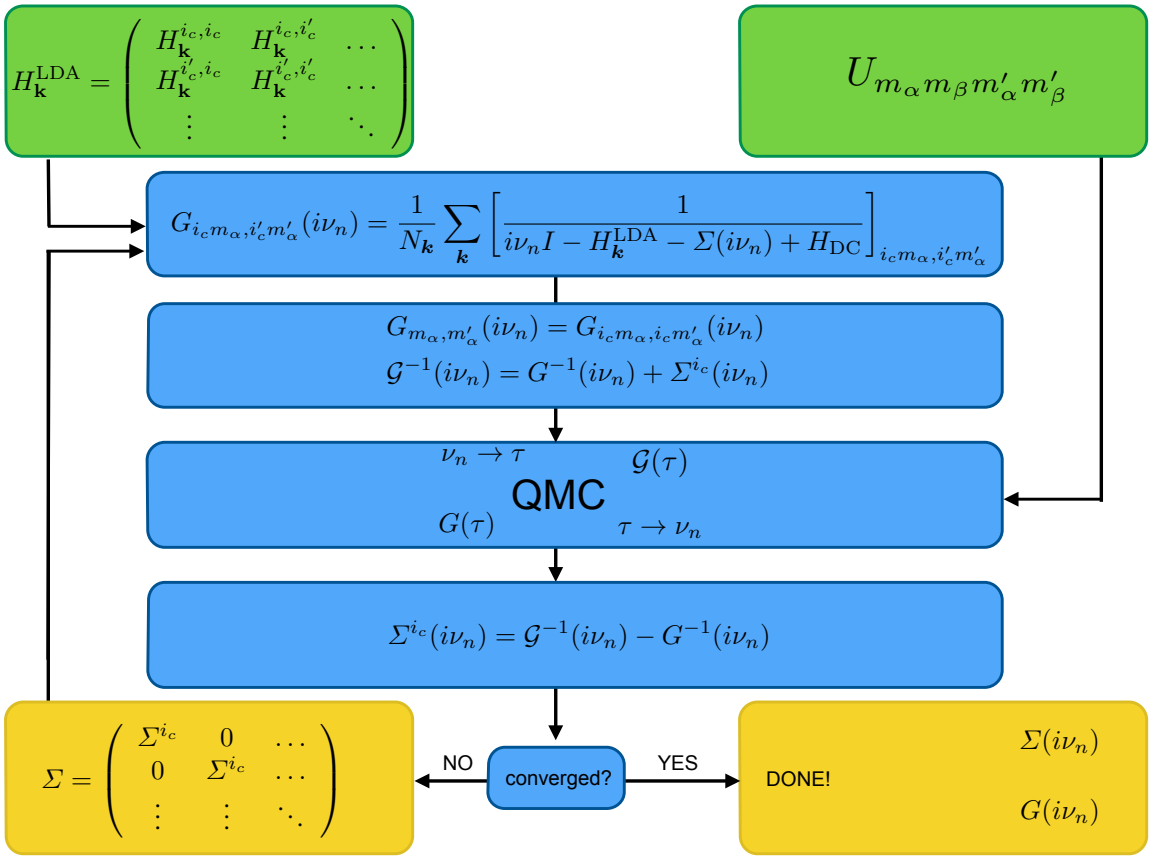
realistic Coulomb



spin waves

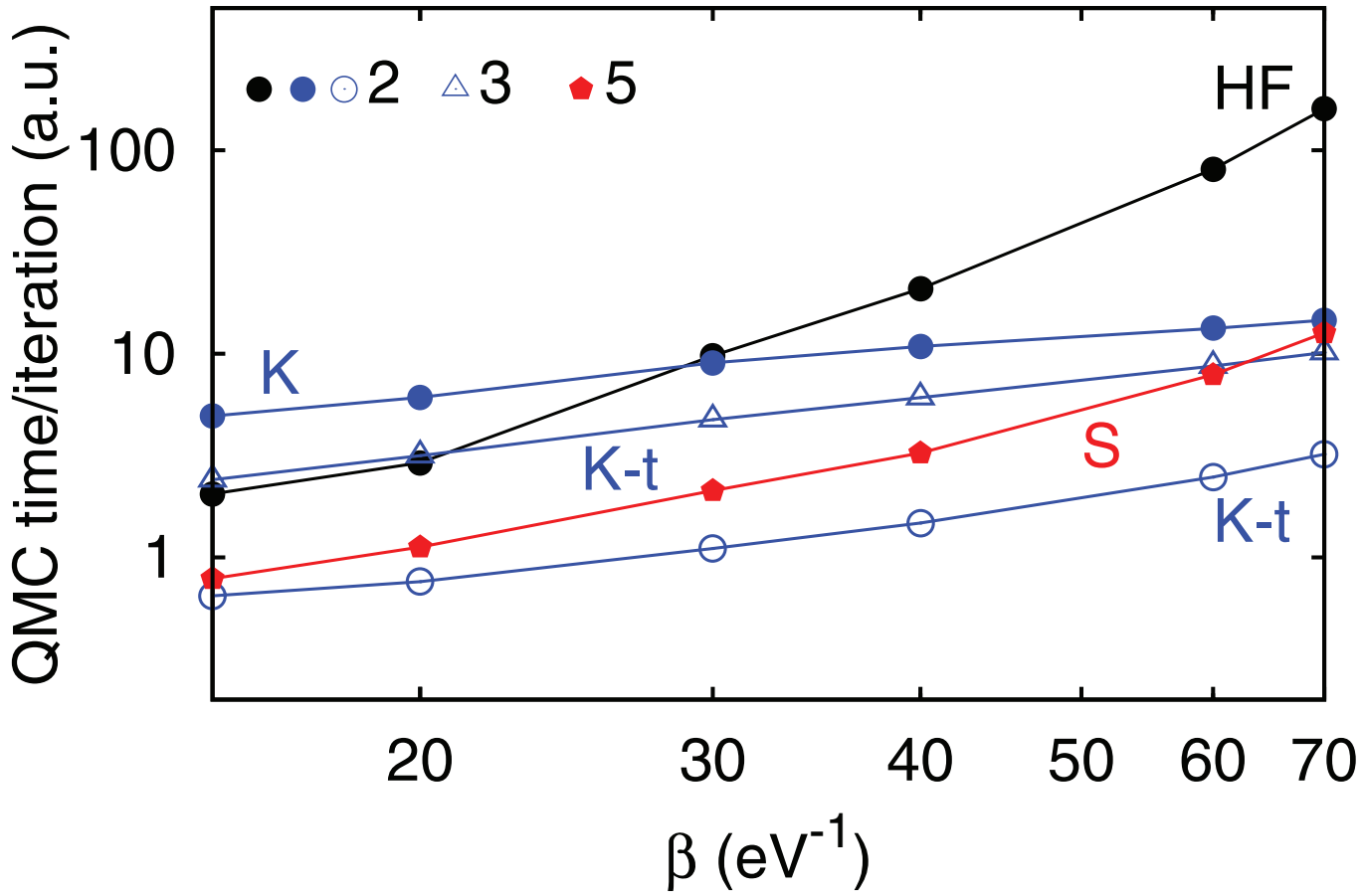


our dft+dmft package



QMC: CPU-time consuming part

CPU-time: QMC block



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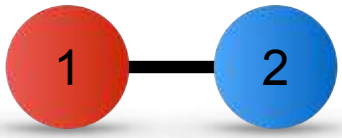
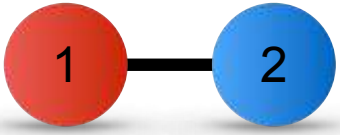
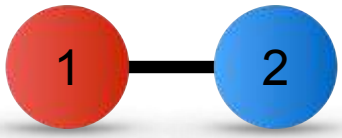


hybridization-expansion CT-QMC



$$\hat{H}^{\mathrm{QIM}} = \underbrace{\varepsilon_s \sum_{\sigma} \hat{n}_{s\sigma}}_{\hat{H}_{\mathrm{bath}}} \underbrace{-t \sum_{\sigma} \left(c^{\dagger}_{d\sigma} c_{s\sigma} + c^{\dagger}_{s\sigma} c_{d\sigma} \right)}_{\hat{H}_{\mathrm{hyb}}} + \underbrace{\varepsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d}}_{\hat{H}_{\mathrm{loc}}}$$

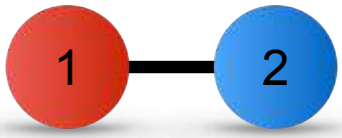


hybridization-expansion CT-QMC

$$Z = \mathrm{Tr}\left(e^{-\beta(\hat{H}_0-\mu\hat{N})}\hat{V}(\beta)\right)$$

$$\hat{V}(\beta) = \sum_m \underbrace{\int_0^\beta d\tau_1 \cdots \int_{\tau_{m-1}}^\beta d\tau_m}_{\int d\boldsymbol{\tau}^m} \underbrace{(-1)^m \prod_{l=m}^1 \hat{H}_{\mathrm{hyb}}(\tau_l)}_{\hat{O}^m(\boldsymbol{\tau})}$$

only even orders survive (m=2k)



hybridization-expansion CT-QMC

bath-impurity decoupling

$$\frac{Z}{Z_{\text{bath}}} = \sum_k \int^k d\boldsymbol{\tau} \int^k d\bar{\boldsymbol{\tau}} \sum_{\boldsymbol{\sigma},\bar{\boldsymbol{\sigma}}} d^k_{\bar{\boldsymbol{\sigma}},\boldsymbol{\sigma}}(\boldsymbol{\tau},\bar{\boldsymbol{\tau}})\, t^k_{\boldsymbol{\sigma},\bar{\boldsymbol{\sigma}}}(\boldsymbol{\tau},\bar{\boldsymbol{\tau}})$$

(d_c and t_c mark the two factors)

$$w_c = d\boldsymbol{\tau}_c\, d_c\, t_c$$

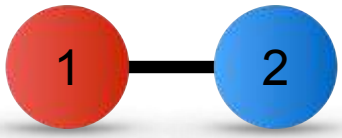
d_c

$$d^k_{\bar{\boldsymbol{\sigma}},\boldsymbol{\sigma}}(\boldsymbol{\tau},\bar{\boldsymbol{\tau}}) = \det\left(F^k_{\bar{\boldsymbol{\sigma}},\boldsymbol{\sigma}}(\boldsymbol{\tau},\bar{\boldsymbol{\tau}})\right)$$

bath hybridization function

t_c

the difficult part: local trace $t^k_{\boldsymbol{\sigma},\bar{\boldsymbol{\sigma}}}(\boldsymbol{\tau},\bar{\boldsymbol{\tau}})$

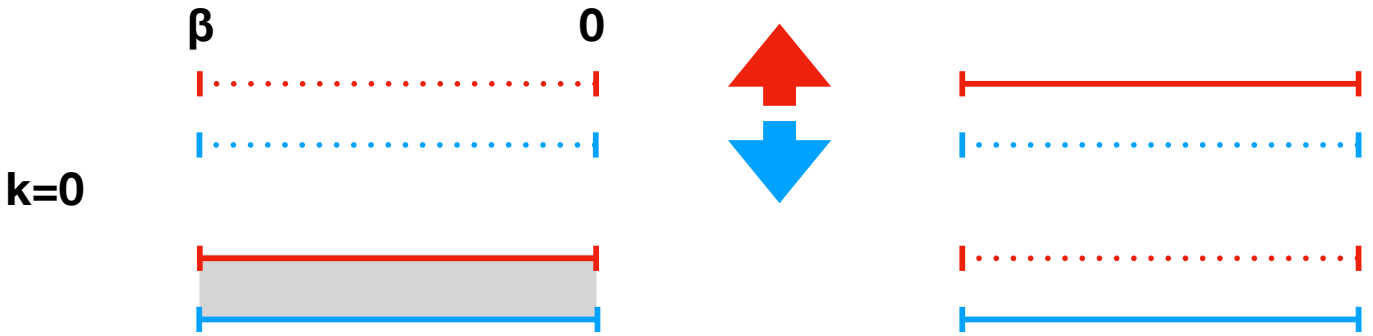


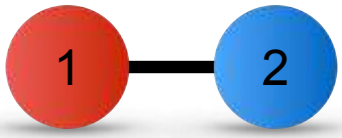
hybridization-expansion CT-QMC

local trace: segment solver

$$t^k_{\boldsymbol{\sigma},\bar{\boldsymbol{\sigma}}}(\boldsymbol{\tau},\bar{\boldsymbol{\tau}}) = \mathrm{Tr}_{\mathrm{loc}}\left(e^{-\beta(\hat{H}_{\mathrm{loc}}-\mu\hat{N}_d)}\mathcal{T}\Pi^1_{i=k}c_{d\sigma_i}(\tau_i)c^\dagger_{d\bar{\sigma}_i}(\bar{\tau}_i)\right),$$

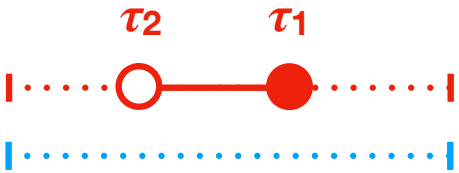
order (k) gives number of creators/annhilators

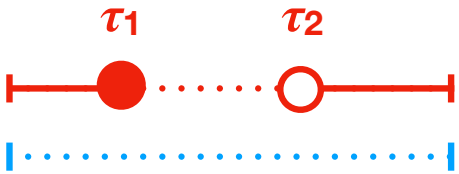


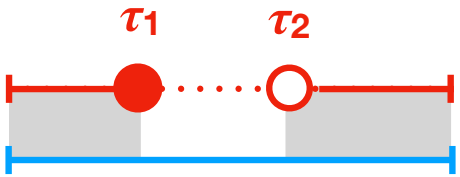


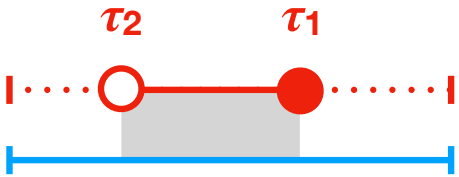
analytic expression k=1

k=1

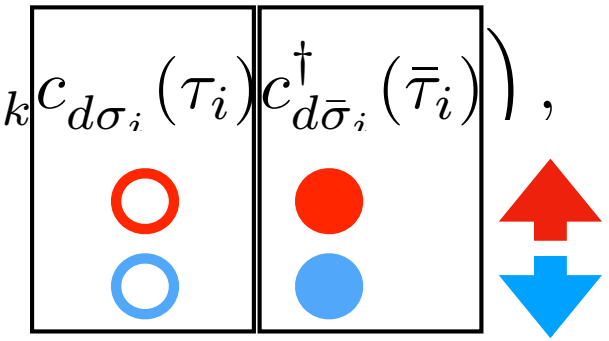




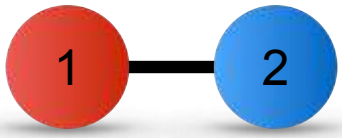




$$t^k_{\boldsymbol{\sigma},\bar{\boldsymbol{\sigma}}}(\boldsymbol{\tau},\bar{\boldsymbol{\tau}}) = \mathrm{Tr}_{\mathrm{loc}}\left(e^{-\beta(\hat{H}_{\mathrm{loc}}-\mu\hat{N}_d)}\mathcal{T}\Pi^1_{i=k} c_{d\sigma_i}(\tau_i)c^\dagger_{d\bar{\sigma}_i}(\bar{\tau}_i)\right),$$



$$t^k_{\sigma,\bar{\sigma}}(\boldsymbol{\tau},\bar{\boldsymbol{\tau}}) = \left(\prod_\sigma s^{k_\sigma}_\sigma\right) e^{-\sum_{\sigma\sigma'}((\varepsilon_d-\mu)\delta_{\sigma\sigma'}+\frac{U}{2}(1-\delta_{\sigma,\sigma'}))l_{\sigma,\sigma'}}$$



hybridization-expansion CT-QMC

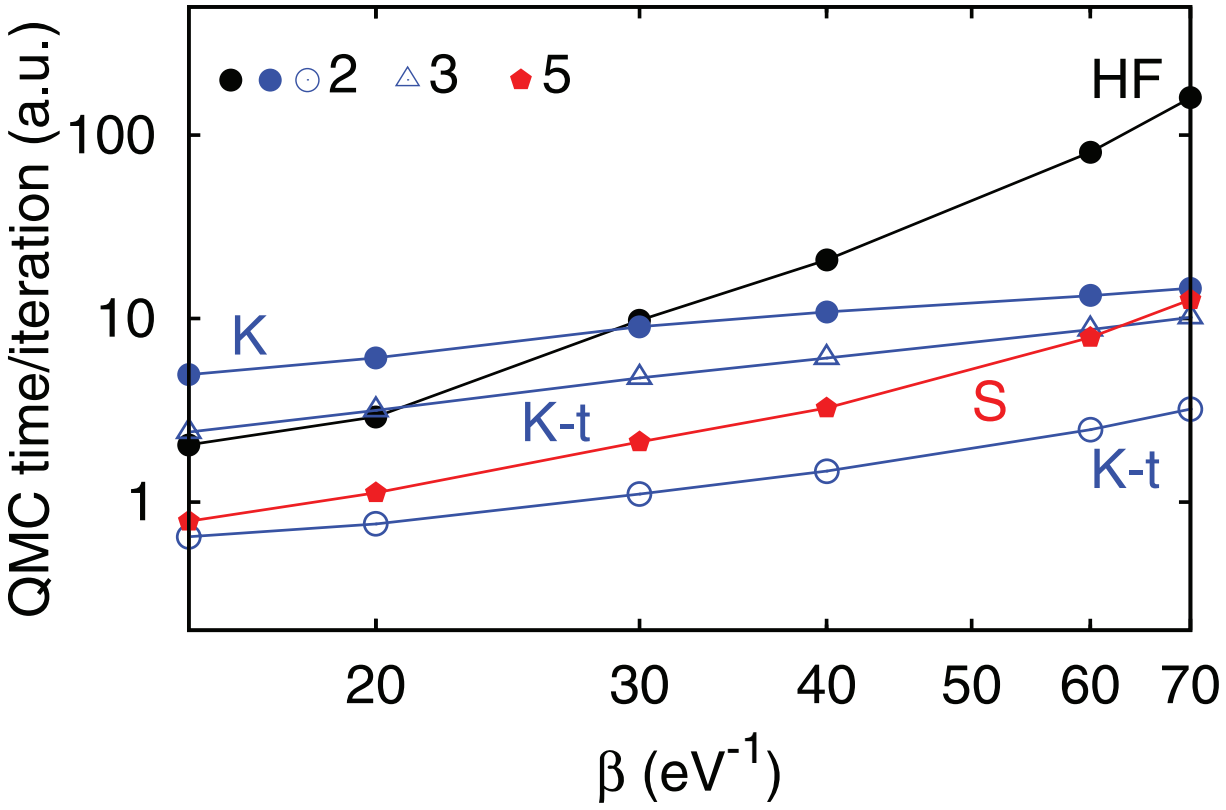
$$Z = \sum_c w_c = \sum_c |w_c| \ \mathrm{sign}\ w_c$$

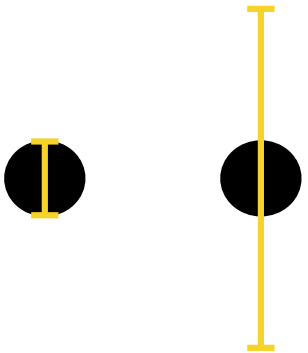
configuration *c*: expansion order & flavors

$$\langle \hat{O} \rangle = \frac{\sum_c \langle \hat{O} \rangle_c |w_c| \mathrm{sign}\ w_c}{\sum_c |w_c| \mathrm{sign}\ w_c} = \frac{\sum_c \langle \hat{O} \rangle_c |w_c| \mathrm{sign}\ w_c / \sum_c |w_c|}{\sum_c |w_c| \mathrm{sign}\ w_c / \sum_c |w_c|} \approx \frac{\frac{1}{N_c} \sum_c^{N_c} \langle \hat{O} \rangle_c \mathrm{sign}\ w_c}{\frac{1}{N_c} \sum_c \mathrm{sign}\ w_c}$$

why not half the number of sweeps?

$$\langle \hat{O} \rangle = \frac{\sum_c \langle \hat{O} \rangle_c |w_c| \text{sign } w_c}{\sum_c |w_c| \text{sign } w_c} = \frac{\sum_c \langle \hat{O} \rangle_c |w_c| \text{sign } w_c / \sum_c |w_c|}{\sum_c |w_c| \text{sign } w_c / \sum_c |w_c|} \approx \frac{\frac{1}{N_c} \sum_c^{N_c} \langle \hat{O} \rangle_c \text{sign } w_c}{\frac{1}{N_c} \sum_c \text{sign } w_c}$$





$$\sigma_{\langle O \rangle} \sim \frac{1}{\sqrt{N_{sweeps}}} \sim \frac{1}{\sqrt{t_{CPU}}}$$

sign problem

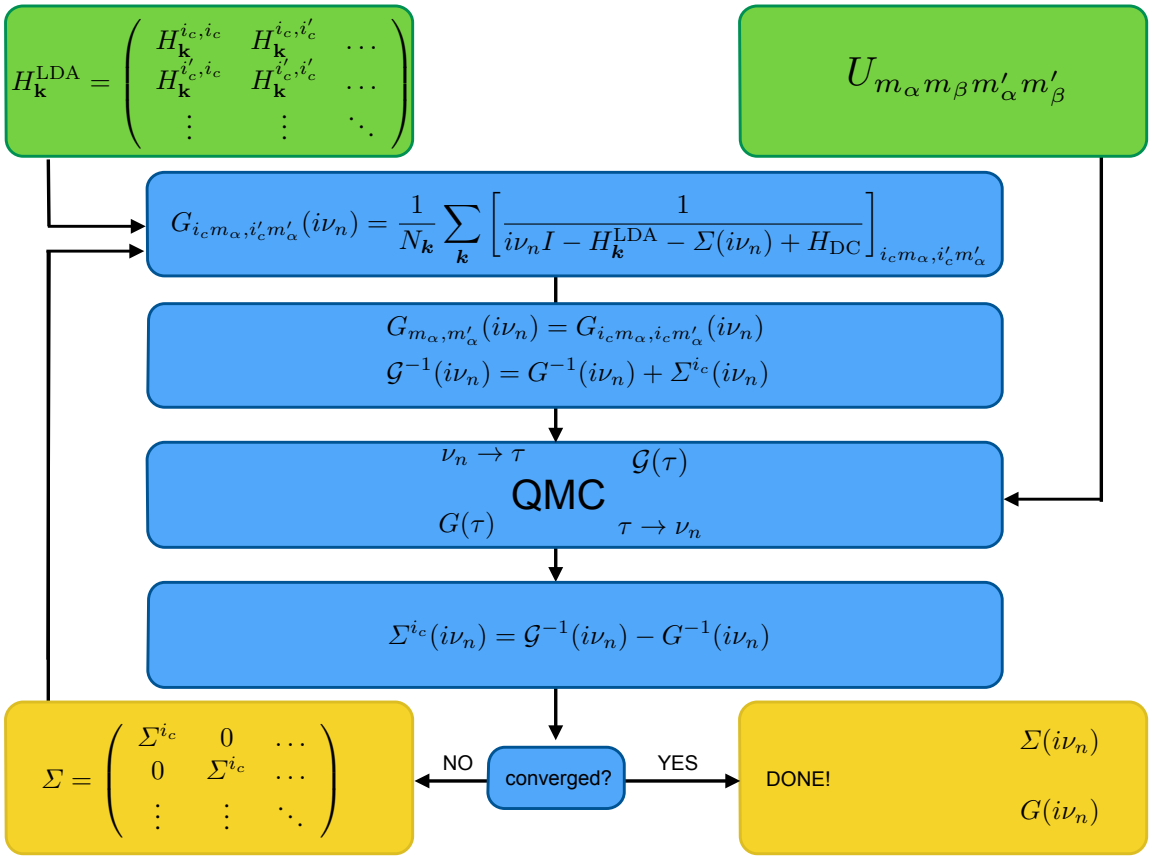
$$\langle \hat{O} \rangle = \frac{\sum_c \langle \hat{O} \rangle_c |w_c| \text{sign } w_c}{\sum_c |w_c| \text{sign } w_c} = \frac{\sum_c \langle \hat{O} \rangle_c |w_c| \text{sign } w_c / \sum_c |w_c|}{\sum_c |w_c| \text{sign } w_c / \sum_c |w_c|} \approx \frac{\frac{1}{N_c} \sum_c^{N_c} \langle \hat{O} \rangle_c \text{sign } w_c}{\frac{1}{N_c} \sum_c \text{sign } w_c}$$

$$\langle \text{sign} \rangle = \frac{\sum_c |w_c| \text{sign } w_c}{\sum_c |w_c|} \sim \exp(-\Delta \beta N)$$

$$\sigma_{\langle \text{sign} \rangle} \sim \frac{1}{\sqrt{t_{CPU}}} \qquad \frac{\sigma_{\langle \text{sign} \rangle}}{\langle \text{sign} \rangle} \ll 1$$

$$t_{CPU} \gg \exp(2\Delta \beta N)$$

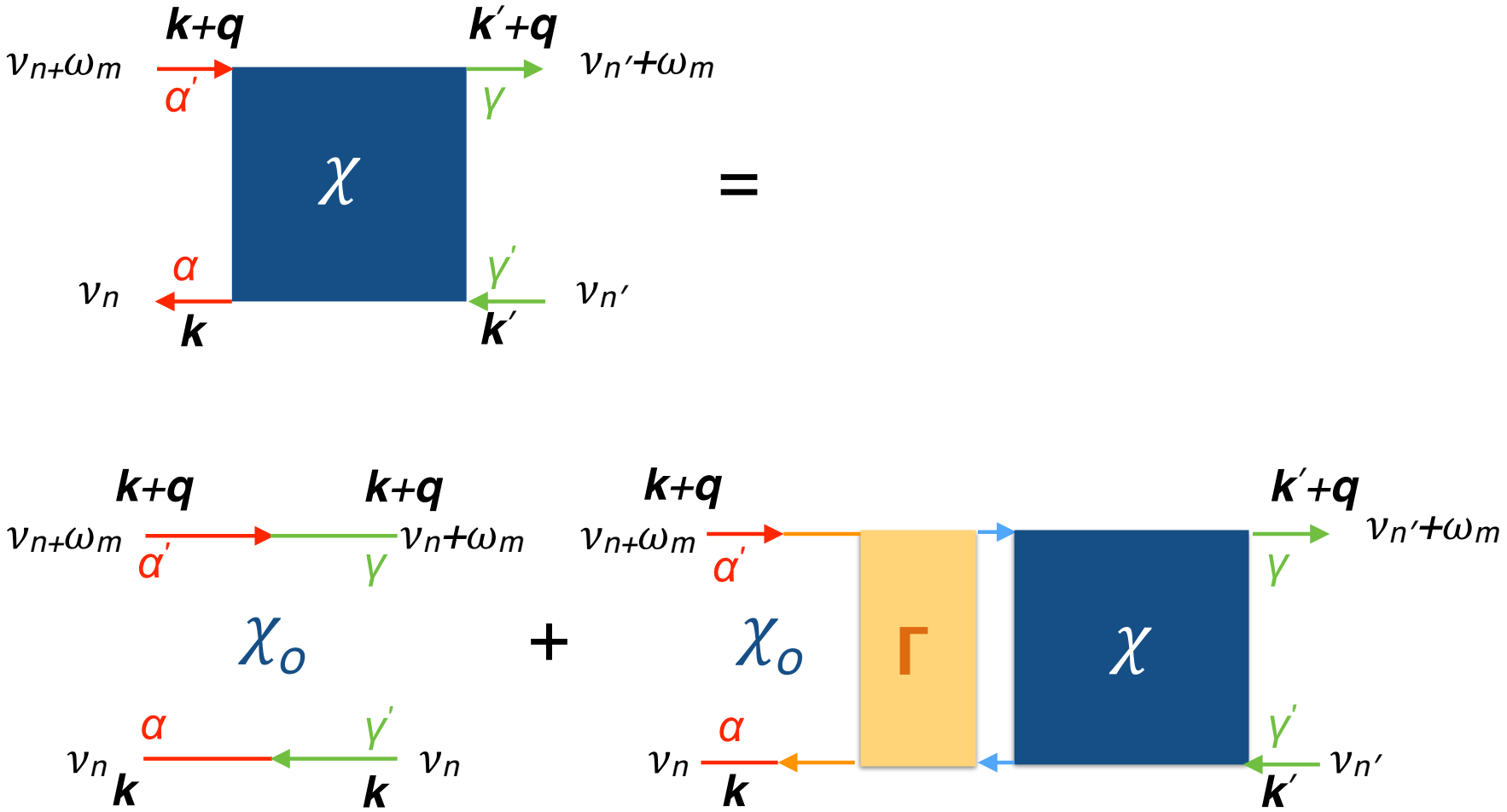
our dft+dmft package



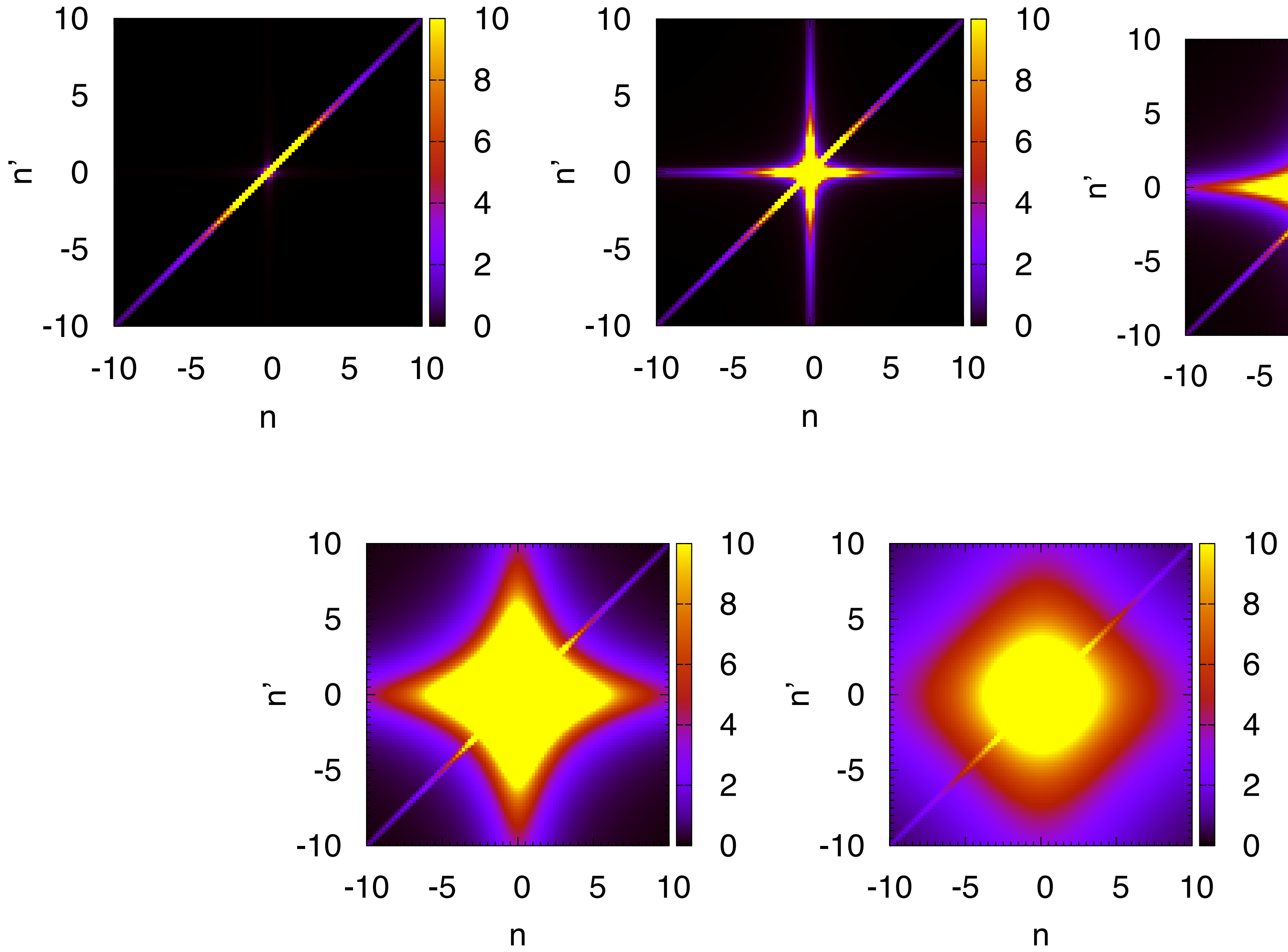
QMC: CPU-time consuming part

even harder: response functions

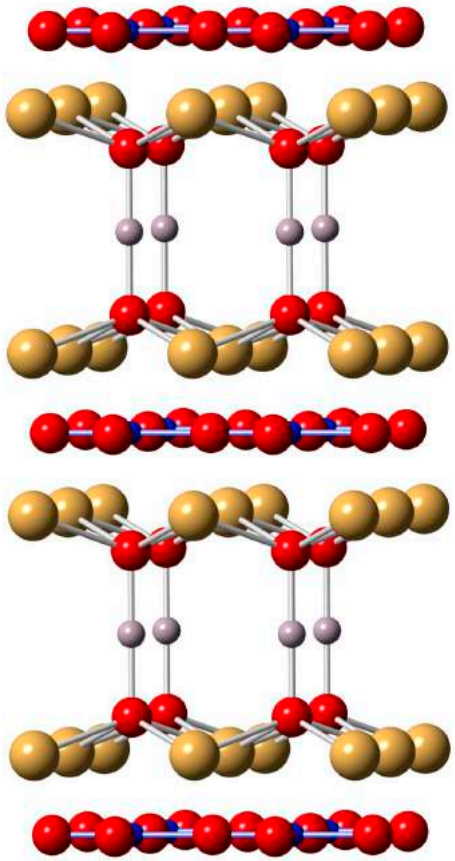
Bethe-Salpeter equations

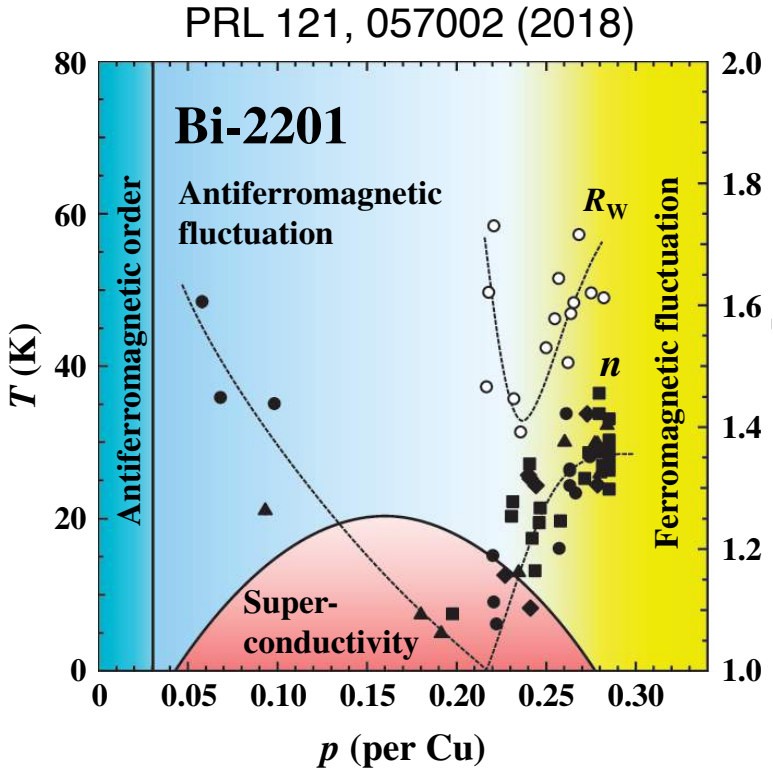


atomic limit, increasing U



high-T_c superconducting cuprates (e_g^9)

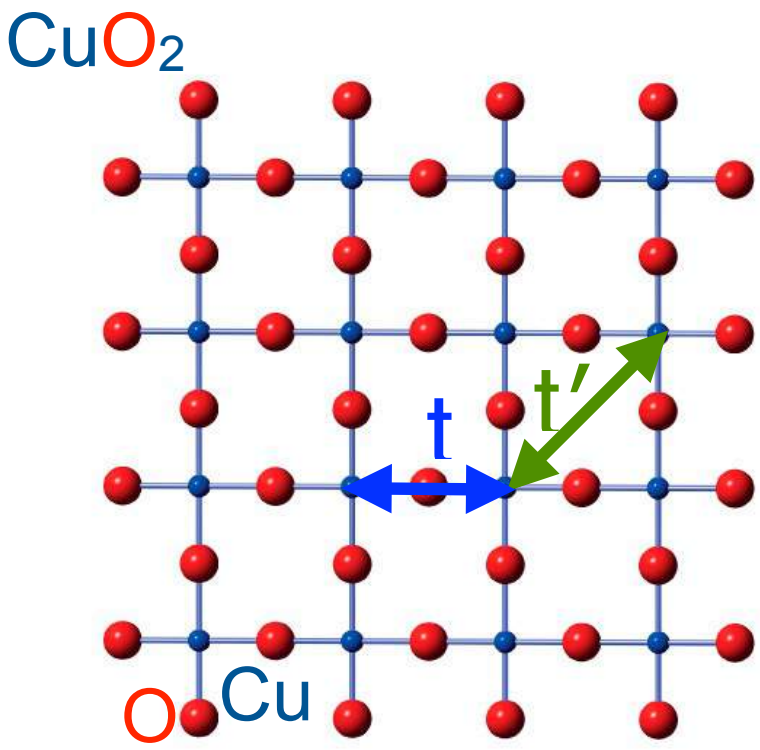


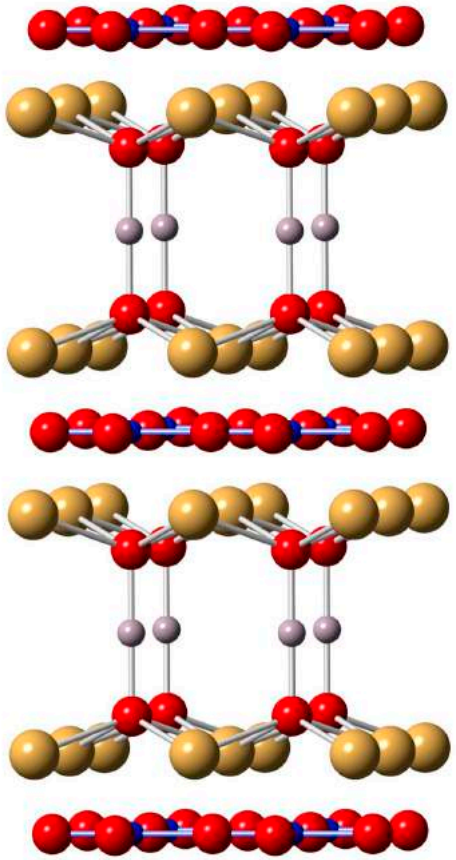


goal: spin-spin correlations

JÜLICH
FORSCHUNGSZENTRUM

high-T_c superconducting cuprates (e_g^9)





$$H = -\sum_{\sigma}\sum_{\langle ii' \rangle} t_{i,i'} c^{\dagger}_{i\sigma} c_{i'\sigma} + \sum_{i} U n_{i\uparrow} n_{i\downarrow}$$

high-T_c superconducting cuprates

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Band-Structure Trend in Hole-Doped Cuprates and Correlation with $T_{c\,\max}$

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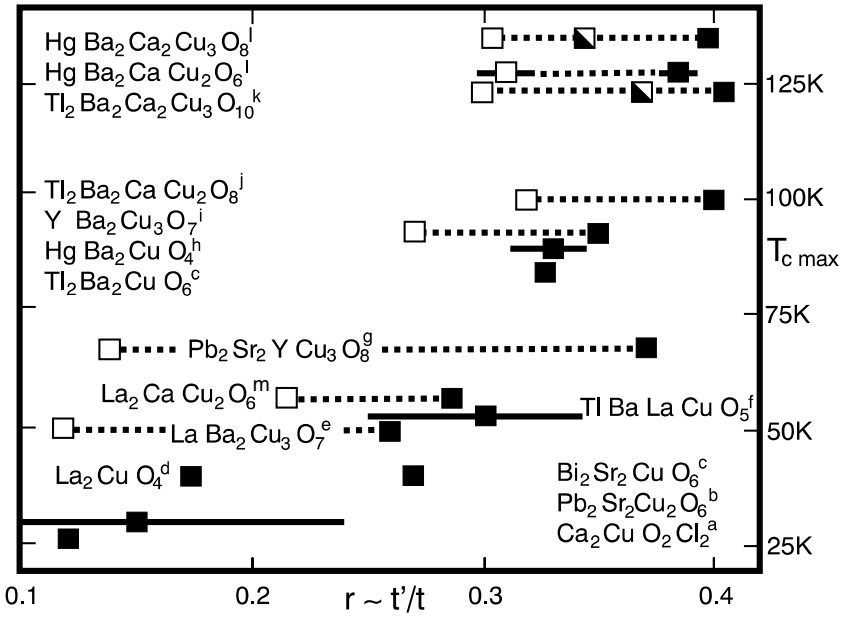
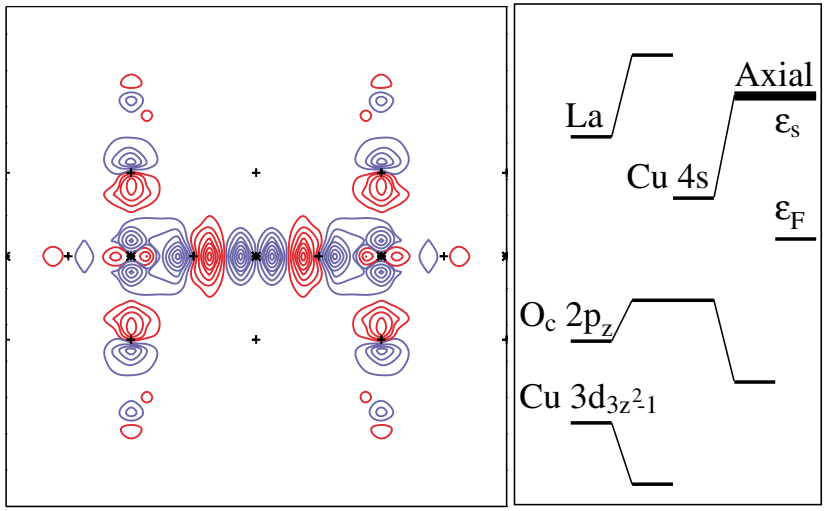
(Received 4 December 2000; published 10 July 2001)

By calculation and analysis of the bare conduction bands in a large number of hole-doped high-temperature superconductors, we have identified the range of the intralayer hopping as the essential, material-dependent parameter. It is controlled by the energy of the axial orbital, a hybrid between Cu 4*s*, apical-oxygen $2p_z$, and farther orbitals. Materials with higher $T_{c\,\max}$ have larger hopping ranges and axial orbitals more localized in the CuO_2 layers.



the axial orbital



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the single fluid picture

PHYSICAL REVIEW B VOLUME 43, NUMBER 1 1 JANUARY 1991

Cu and O NMR studies of the magnetic properties of $YBa_2Cu_3O_{6.63}$ ($T_c = 62$ K)

M. Takigawa,* A. P. Reyes,† P. C. Hammel, J. D. Thompson, R. H. Heffner, Z. Fisk, and K. C. Ott

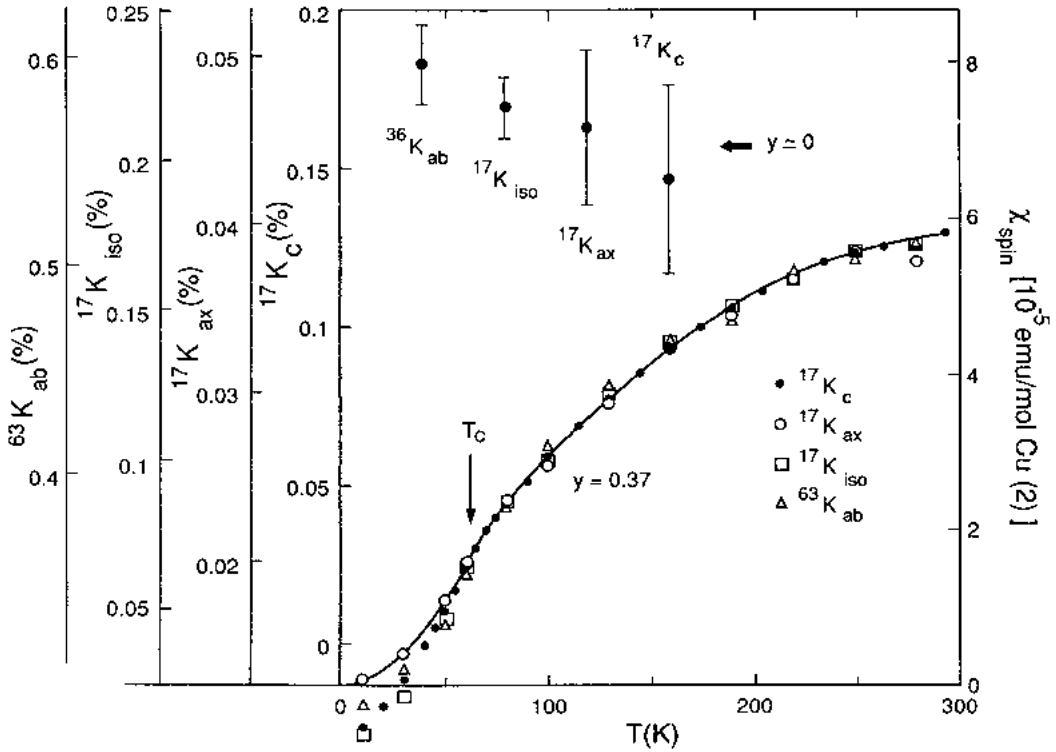

FIG. 8. Various components of the Cu and O Knight shift are plotted against temperature with different vertical scales and origins. The T-independent values of spin Knight shifts in the $y \simeq 0$ material (from Refs. 6 and 25) are also plotted with the same vertical scales.

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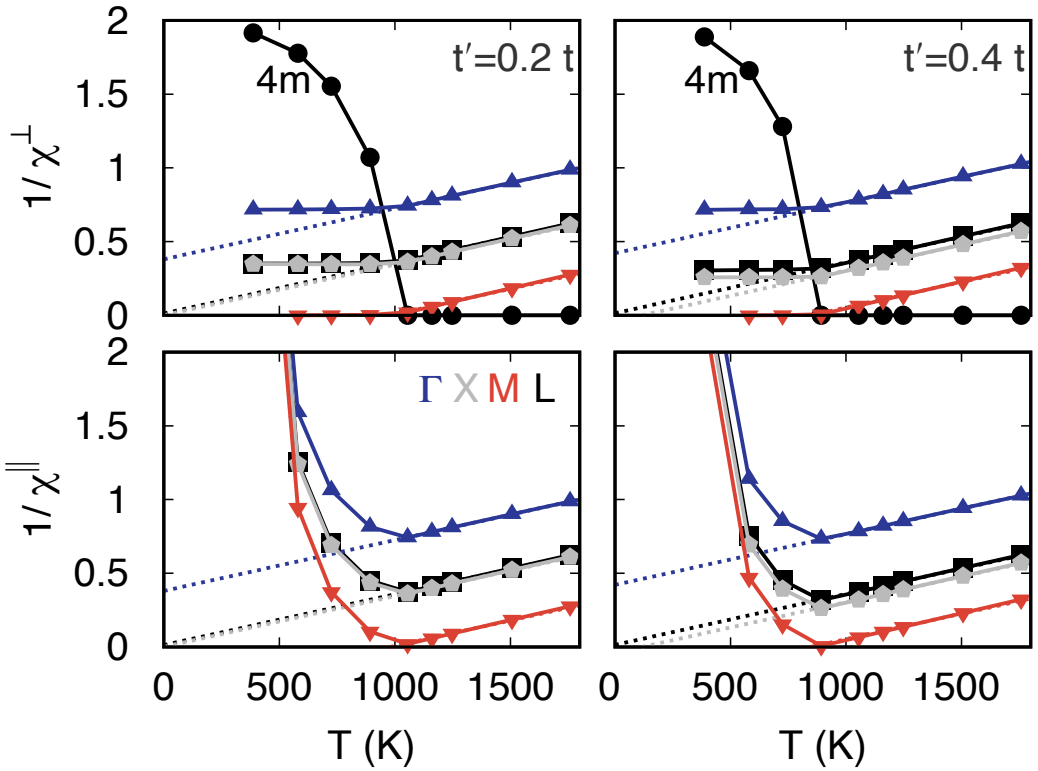
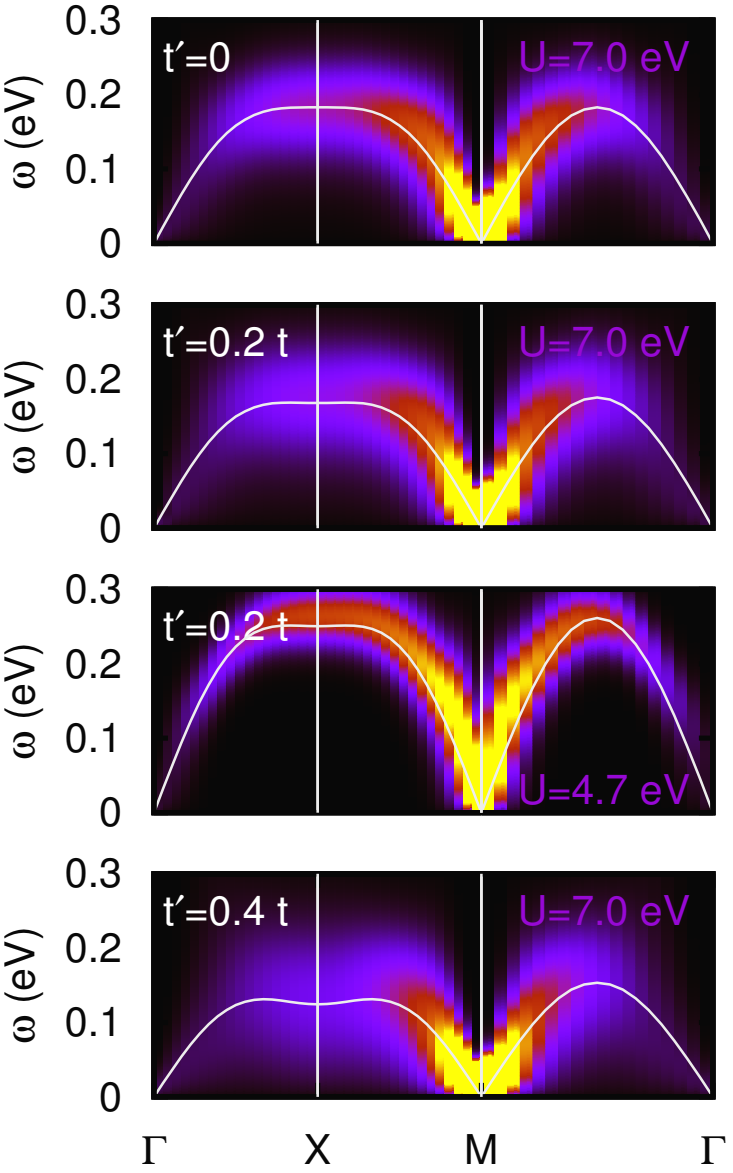
half filling (x=0)





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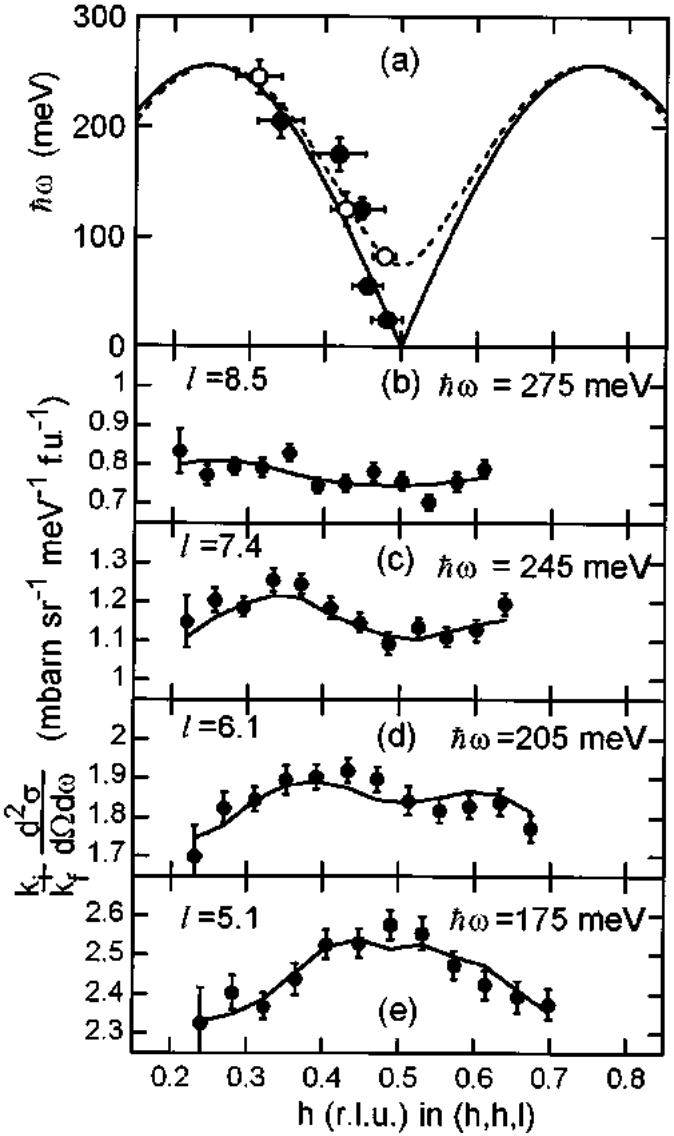
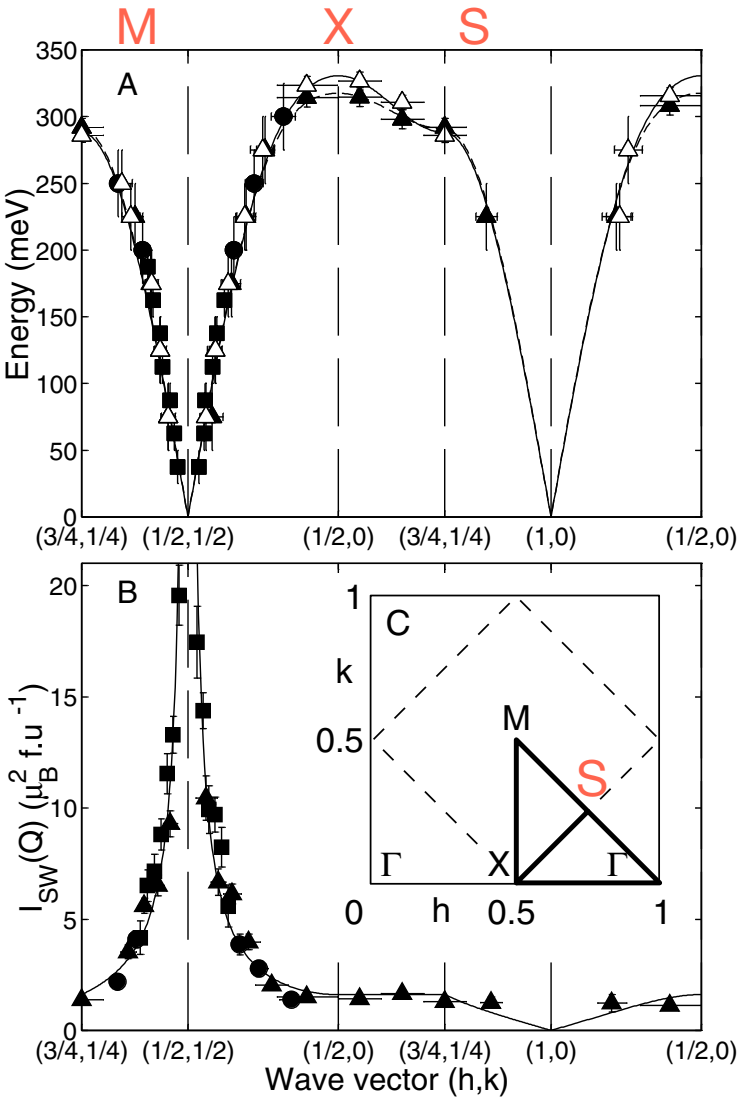
half filling

YBCO



PNS- Hayden et al PRB 54, 6905 (1996)

LSCO



INS — Coldea et al PRL 86, 5377 (2001)

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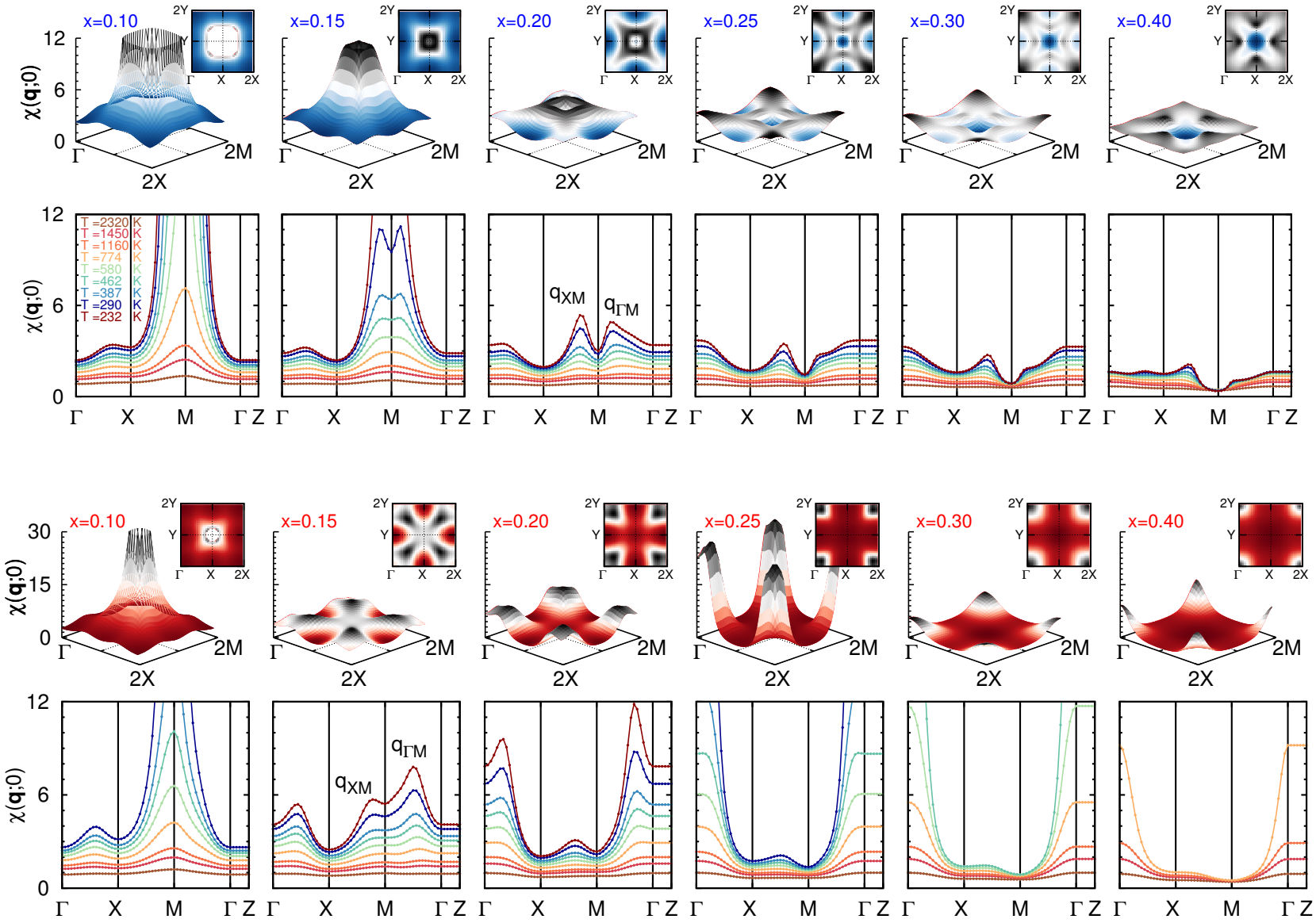
increasing x, finite **q**

t'/t=0.2

t'/t=0.4



Properties that change as superconductivity disappears at high-doping concentrations in $La_{2-x}Sr_xCuO_4$

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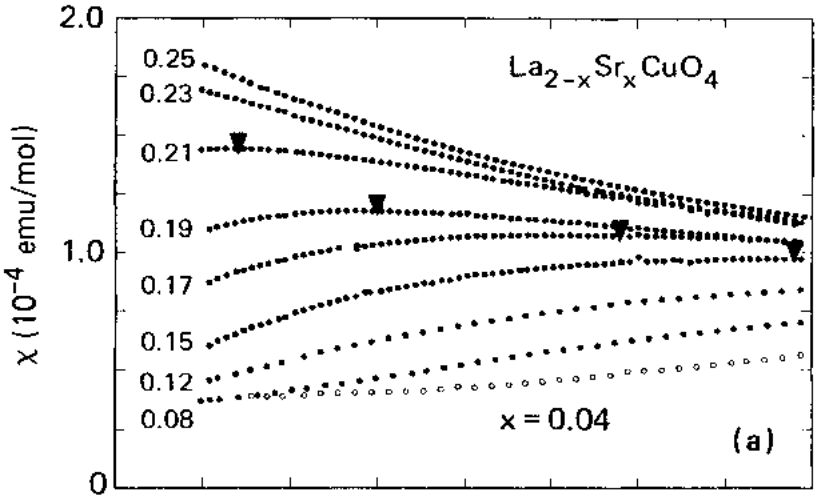
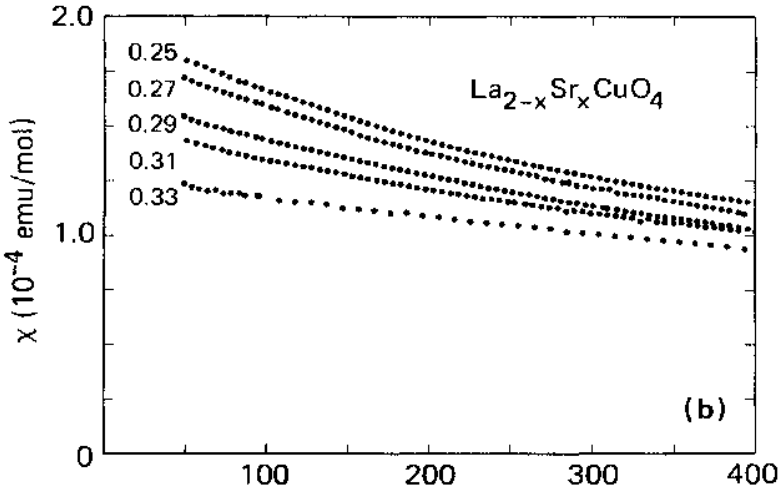
(Received 10 May 1989)





search for ferromagnetism

PNAS

Direct search for a ferromagnetic phase in a heavily overdoped nonsuperconducting copper oxide

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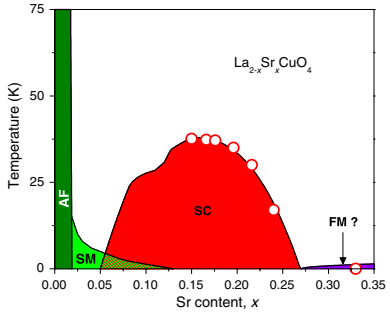
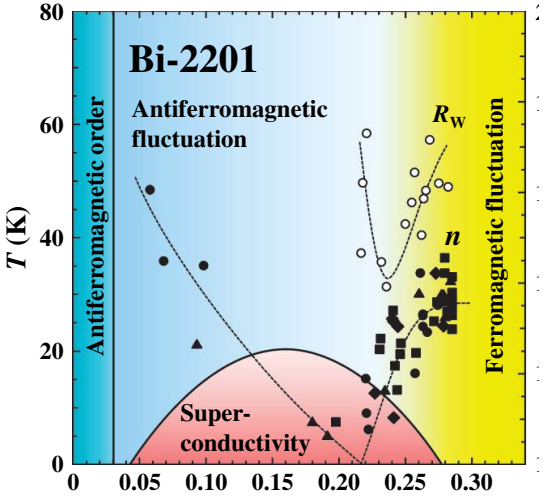
Edited by Zachary Fisk, University of California, Irvine, CA, and approved August 12, 2010 (received for review May 25, 2010)

The doping of charge carriers into the CuO_2 planes of copper oxide Mott insulators causes a gradual destruction of antiferromagnetism and the emergence of high-temperature superconductivity. Optimal superconductivity is achieved at a doping concentration *p* beyond which further increases in doping cause a weakening and eventual disappearance of superconductivity. A potential explanation for this demise is that ferromagnetic fluctuations compete with superconductivity in the overdoped regime. In this case, a ferromagnetic phase at very low temperatures is predicted to exist beyond the doping concentration at which superconductivity disappears. Here we report on a direct examination of this scenario in overdoped $La_{2-x}Sr_xCuO_4$ using the technique of muon spin relaxation. We detect the onset of static magnetic moments of electronic origin at low temperature in the heavily overdoped nonsuperconducting region. However, the magnetism does not exist in a commensurate long-range ordered state. Instead it appears as a





PHYSICAL REVIEW LETTERS **121,** 057002 (2018)

Development of Ferromagnetic Fluctuations in Heavily Overdoped $(Bi,Pb)_2Sr_2CuO_{6+\delta}$ Copper Oxides

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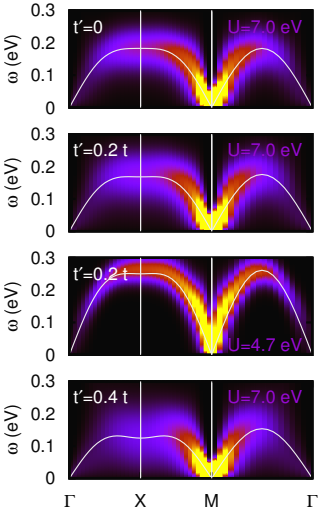
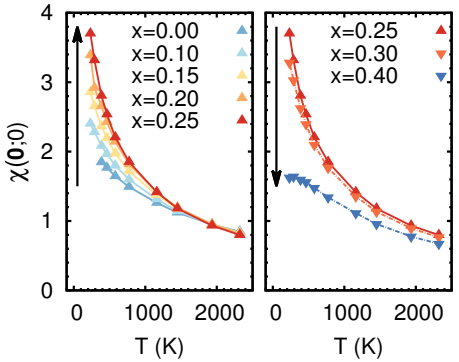
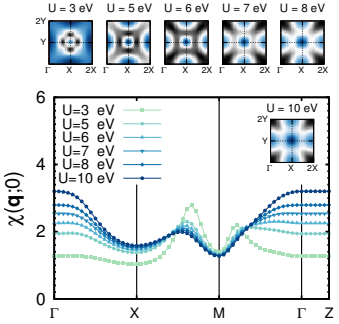
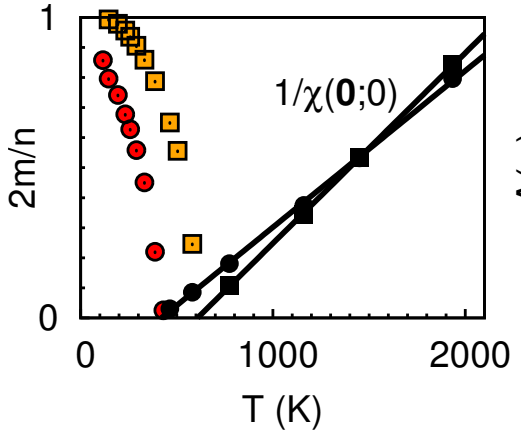
magnetic response very sensitive to t'/t

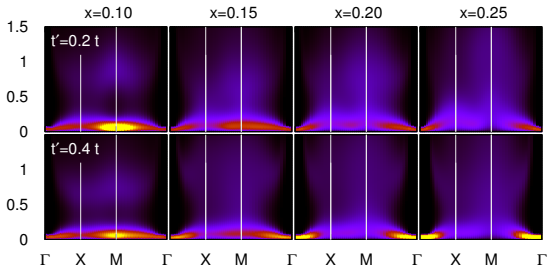
- spin waves
- q=0 behavior
- scaling
- ferromagnetism



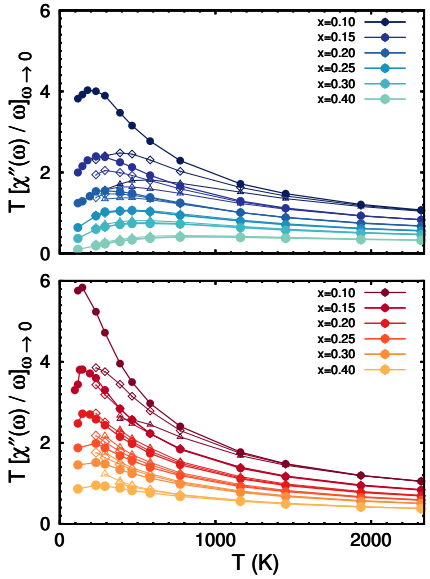








- resonant mode



but not sufficient alone !

PRB **103**, 075136 (2021)

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GCS
Gauss Centre for Supercomputing

thank you!