Linear Response Functions

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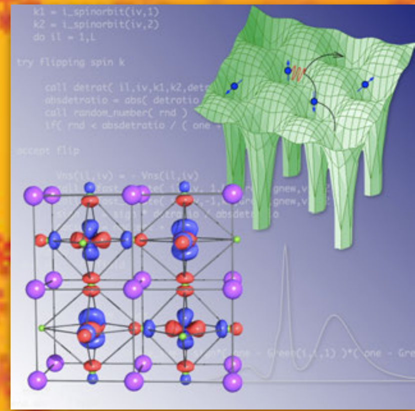
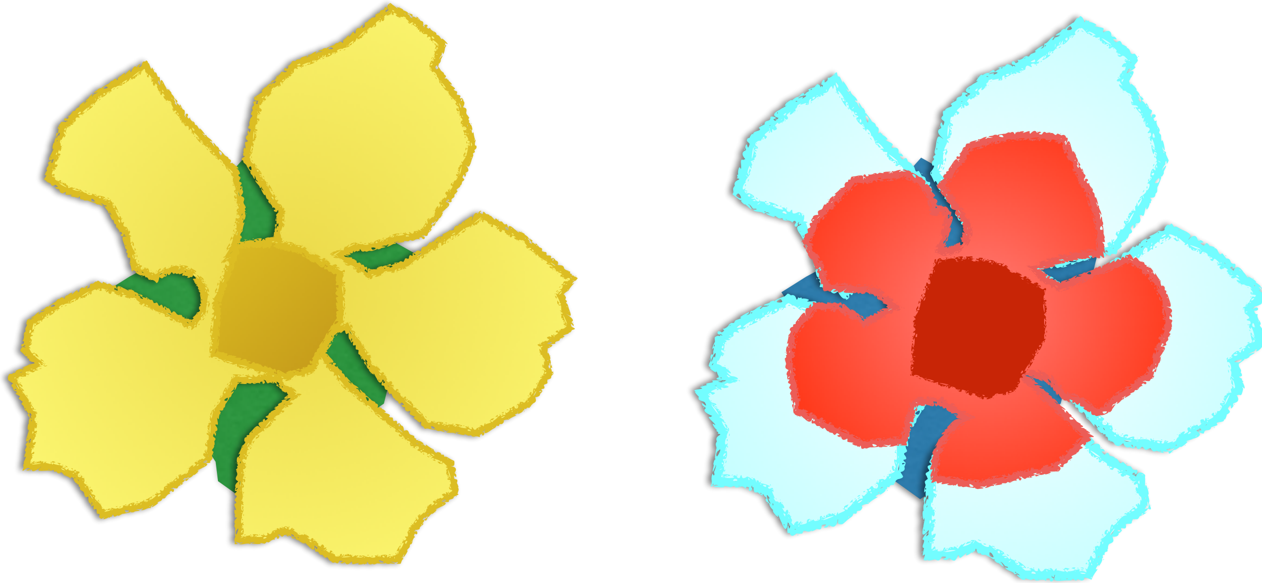


Autumn School on Correlated Electrons

DMFT at 25: Infinite Dimensions

15 – 19 September 2014 at Forschungszentrum Jülich

introduction



$$\chi(\boldsymbol{q};\omega)$$

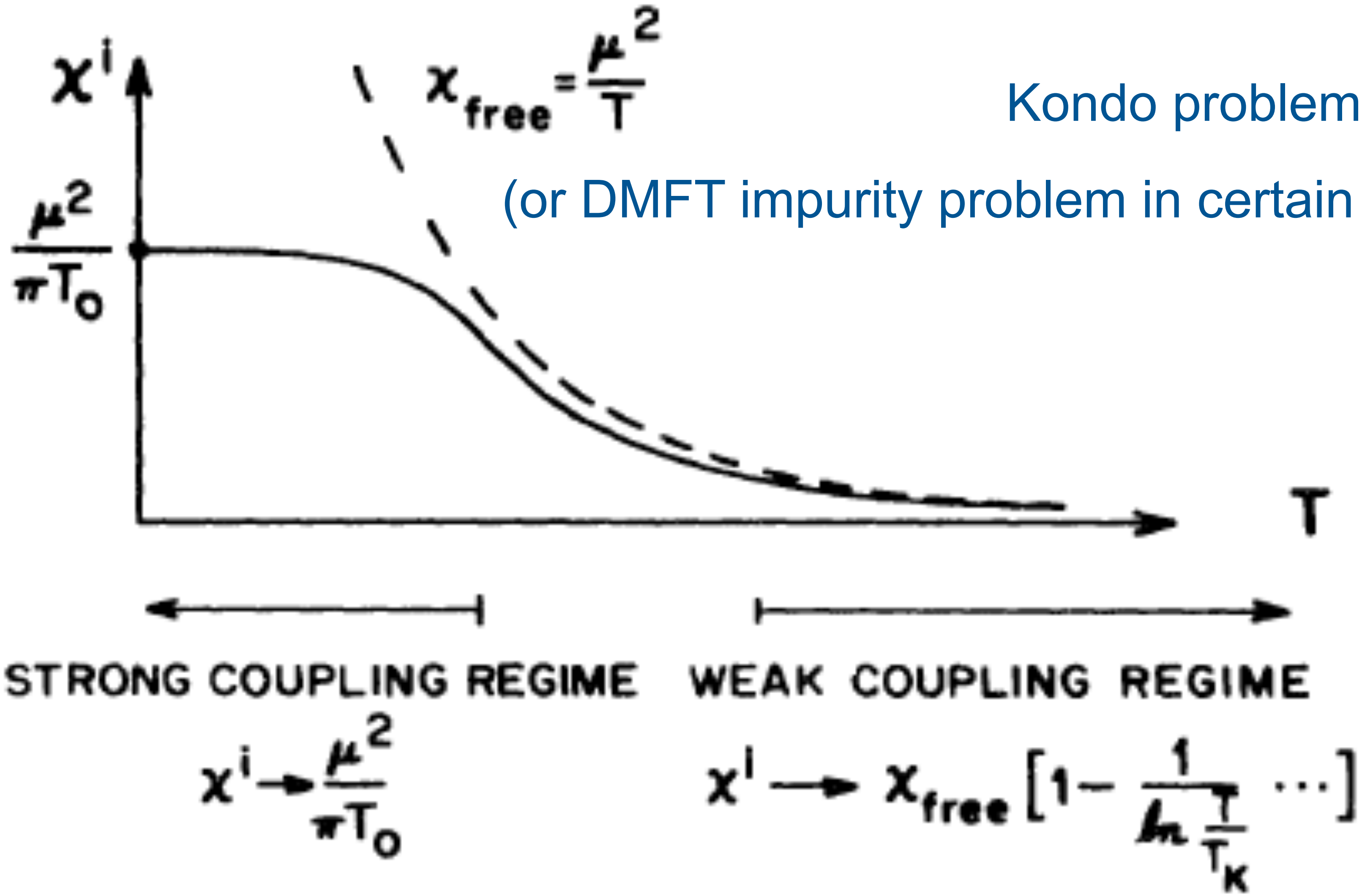
response functions

introduction

linear magnetic susceptibility

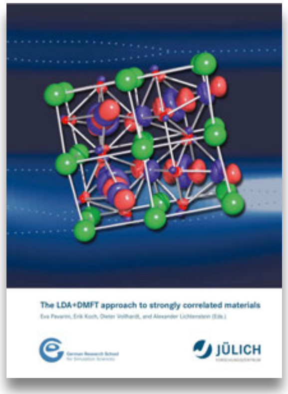
Kondo problem

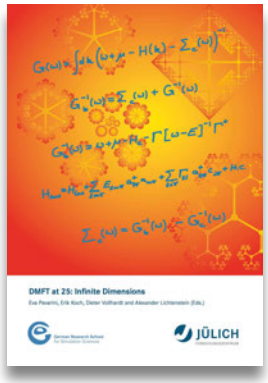
(or DMFT impurity problem in certain regime)



scheme of the lecture

- introduction: what is all about
  - theoretical models
  - the many-body problem
  - the LDA+DMFT approach
- basics of linear response theory
  - definitions & properties
  - Kramers-Kronig relations
  - fluctuation-dissipation theorem
- the dynamical susceptibility
  - one-particle Green functions
  - two-particle Green functions
  - generalized susceptibility
- the dynamical susceptibility in LDA+DMFT
  - the bubble term
  - the Bethe-Salpeter equation
  - local-vertex approximation
  - local susceptibility
- example: one-band Hubbard model





theoretical models

theoretical models

what do we mean by *system* or *material*?

what is “gold”?

(figure from wikipedia)

we have in mind an *idealized* object: thermodynamic limit, ideal crystal,…

what do we want to know about it?

- its *general* properties
- we want to understand *cooperative phenomena*: color, metallicity, … (or superconductivity, ferromagnetism, antiferromagnetism,…)
- identify *elementary entities*
- the latter depend on energy scale (*electron* vs *localized spins*)
- theory describing ideal object: model Hamiltonian
- gold is not iron: material-specific Hamiltonian

material-specific theory

at first sight easy, the interactions are all known …

electronic Hamiltonian (BO first approximation)

$$\begin{aligned}\hat{H}_e &= -\frac{1}{2}\sum_i \nabla_i^2 + \frac{1}{2}\sum_{i\neq i'}\frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|} - \sum_{i\alpha}\frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|} + \frac{1}{2}\sum_{\alpha\neq\alpha'}\frac{Z_\alpha Z_{\alpha'}}{|\mathbf{R}_\alpha - \mathbf{R}_{\alpha'}|}\\ &= \hat{T}_e + \hat{V}_{ee} + \hat{V}_{en} + \hat{V}_{nn}\end{aligned}$$

lattice Hamiltonian

$$\begin{aligned}\hat{H}_n &= -\sum_\alpha \frac{1}{2M_\alpha}\nabla_\alpha^2 + \varepsilon(\{\boldsymbol{R}_\alpha\})\\ &= \hat{T}_n + \hat{U}_n,\end{aligned}$$

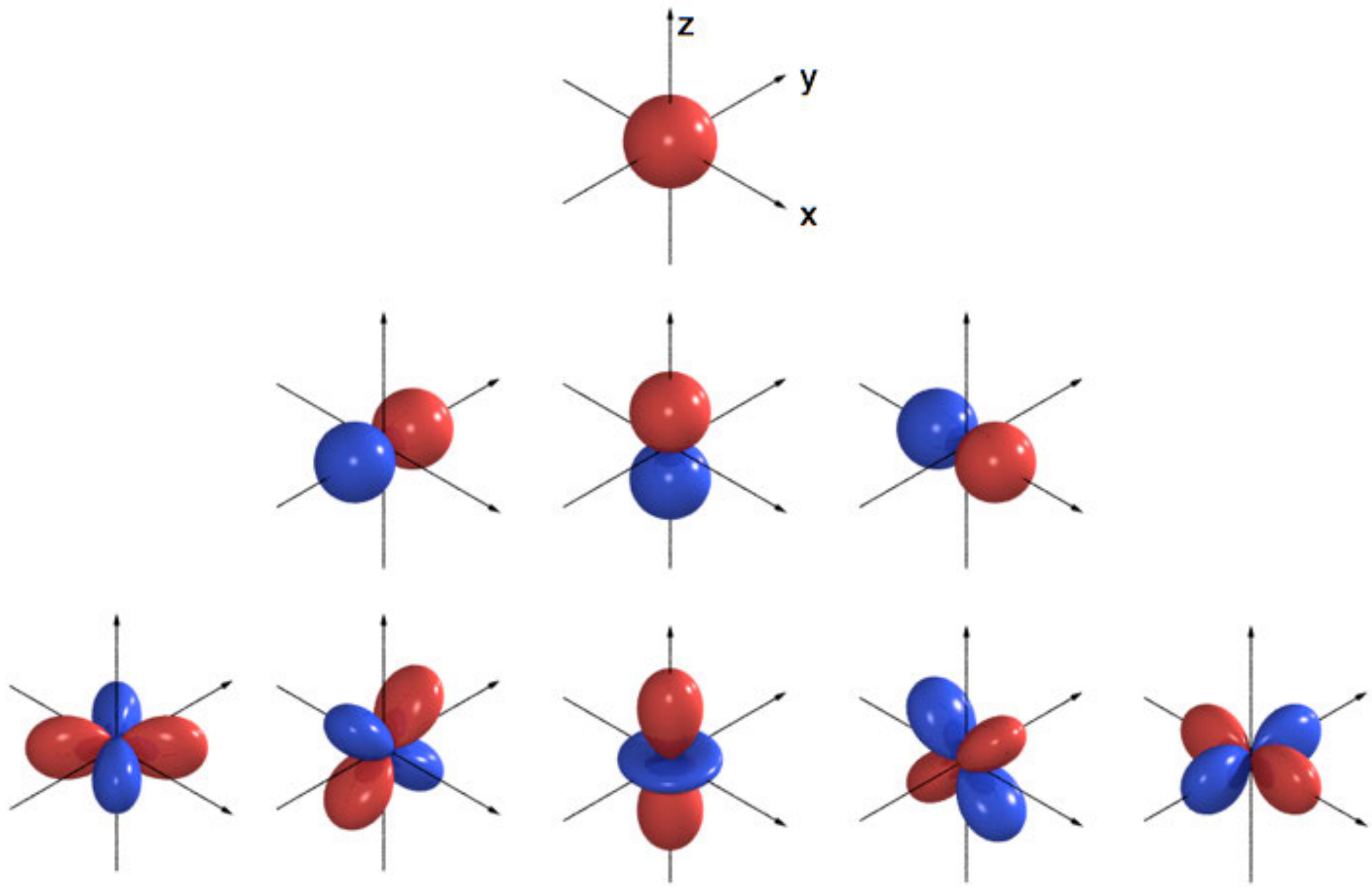
if crystal structure known we can concentrate on electrons

material-specific Hamiltonian

interactions are all known …

we choose a complete one-electron basis

for example choose **atomic** functions



material-specific Hamiltonian

… and write the Hamiltonian in second quantization

(atomic function: here neglect overlap)

$$H_e^{\mathrm{NR}} = -\sum_{ii'\sigma}\sum_{mm'} t^{i,i'}_{m,m'} c^\dagger_{im\sigma} c_{i'm'\sigma} + \frac{1}{2}\sum_{ii'jj'}\sum_{\sigma\sigma'}\sum_{mm'}\sum_{\tilde{m}\tilde{m}'} U^{iji'j'}_{mm'\tilde{m}\tilde{m}'} c^\dagger_{im\sigma} c^\dagger_{jm'\sigma'} c_{j'\tilde{m}'\sigma'} c_{i'\tilde{m}\sigma}$$

one-electron terms: hopping integrals + crystal field

$$t^{i,i'}_{m,m'} = -\int d\boldsymbol{r}\, \overline{\psi_{im\sigma}}(\boldsymbol{r}) \left[-\frac{1}{2}\nabla^2 + v_{\mathrm{R}}(\boldsymbol{r})\right] \psi_{i'm'\sigma}(\boldsymbol{r})$$

two-electron terms: Coulomb interaction tensor

$$U^{iji'j'}_{mm'\tilde{m}\tilde{m}'} = \int d\boldsymbol{r}_1 \int d\boldsymbol{r}_2\, \frac{\overline{\psi_{im\sigma}}(\boldsymbol{r}_1)\overline{\psi_{jm'\sigma'}}(\boldsymbol{r}_2)\psi_{j'\tilde{m}'\sigma'}(\boldsymbol{r}_2)\psi_{i'\tilde{m}\sigma}(\boldsymbol{r}_1)}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|}$$

to make progress we have to solve it

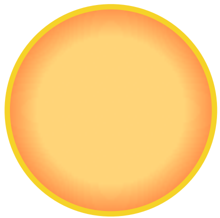
the many-body problem

the problem is known, but no exact solution :(

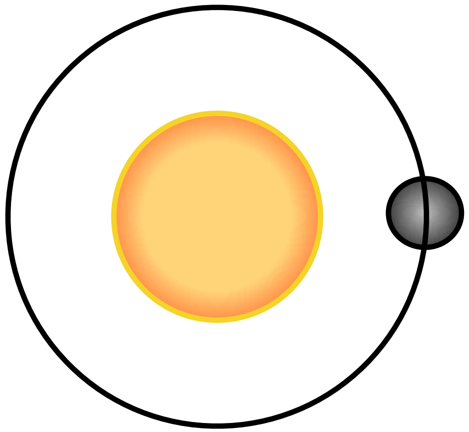
$$H\Psi = E\Psi$$

do we need it?

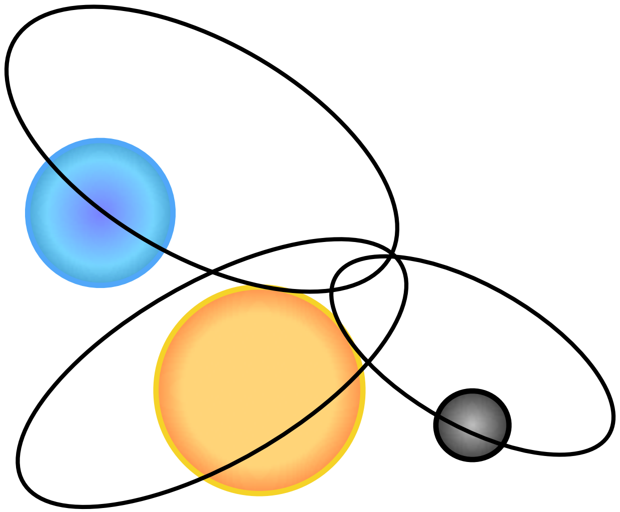
classical N-body problem



one body: no interactions



two-body: analytically solvable problem



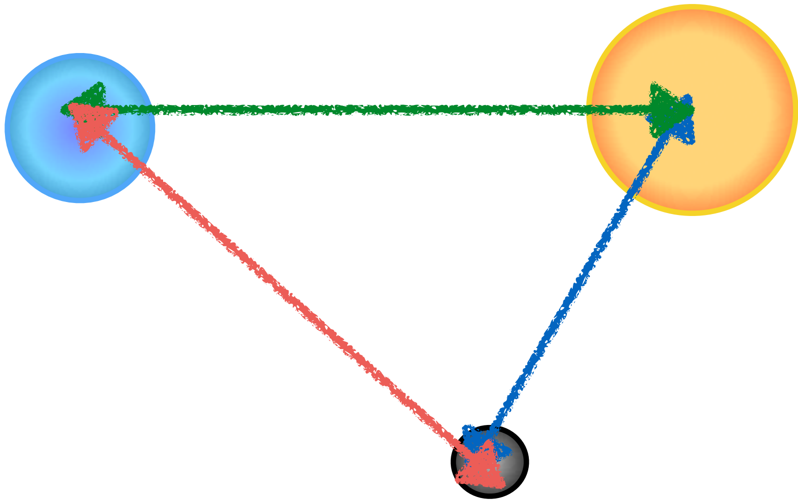
three-body: chaotic behavior possible

solution very difficult

correlations

many objects with simple two-body interactions

can give rise to a very complex system



the end of the n-body problem?

The Solution of the n-body Problem*

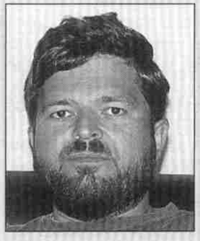
Florin Diacu

or papers or learned about at formal presentations. We often don't know a reference, have no idea who proved that result, how, and when. Usually a colleague mentioned it at some conference dinner, during a coffee-break, or in a friendly discussion in our Department. It is striking, it sticks to our mind, and after a while it is part of our mathematical heritage—we just know it. Then we tell it further under similar circumstances, and so the wheel turns on. We will call this component of our knowledge *folk-mathematics*.

Without denying the positive role folk-mathematics plays in spreading information, we must admit that results gathered through it are sometimes misleading or misunderstood. A typical example is the *Cantor set*. Everybody knows that the middle-third Cantor set has zero Lebesgue measure, and many believe that the middle-fifth analogue has positive measure. Intuitively this sounds plausible: if we remove each time a smaller segment, the remaining quantity should be larger. Unfortunately, the intuition leads us astray this time. For any

*Dedicated to Philip Holmes, for his deep mathematics, for his warm and candid poetry, and for the immense intellectual joy he has instilled in me during the time our book took shape.

Florin Diacu



Florin Diacu obtained his Diploma in Mathematics at the University of Bucharest, got his Ph.D. in Heidelberg, taught in Dortmund, and was a postdoctoral fellow at the Centre de Recherches Mathématiques in Montréal. Since 1991 he has been a professor at the University of Victoria, in British Columbia, Canada. His main research interests are in *celestial mechanics* and *dynamical systems*. His forthcoming book *Celestial Encounters—The Origins of Chaos and Stability*, written with Philip Holmes of Princeton University, describes the historical background, the people, and the ideas that led to the birth and development of the theory of dynamical systems. It will be published in 1996 by Princeton University Press.

Sundman's method failed to apply to the n-body problem for $n > 3$. It took about 7 decades until the general case was solved. In 1991, a Chinese student, Quidong (Don) Wang, published a beautiful paper [Wa], [D1], in which he provided a convergent power series solution of the n-body problem. He omitted only the case of solutions leading to singularities—collisions in particular. (To understand the complications raised by solutions with singularities, see [D2].)

Did this mean the end of the n-body problem? Was this old question—unsuccessfully attacked by the greatest mathematicians of the last 3 centuries—merely solved by a student in a moment of rare inspiration? Though he provided a solution as defined in sophomore textbooks, does this imply that we know everything about gravitating bodies, about the motion of planets and stars? Paradoxically, we do not; in fact we know nothing more than before having this solution.

K.F. Sundman (n=3)

Q. Wang (generalization)

exact solution does not help

The following section deals with this apparent paradox.

The Foundations of Mathematics

What Sundman and Wang did is in accord with the way solutions of initial value problems are defined; everything is apparently all right; but there is a problem, a big one: these series solutions, though convergent on the whole real axis, have very slow convergence. One would have to sum up millions of terms to determine the motion of the particles for insignificantly short intervals of time. The round-off errors make these series unusable in numerical work. From the theoretical point of view, these solutions add nothing to what was previously known about the n-body problem.

ing the fundamentals of differential equations theory, the structure on which a significant part of modern science and technology is based. Do we have an answer to this last challenge?

References

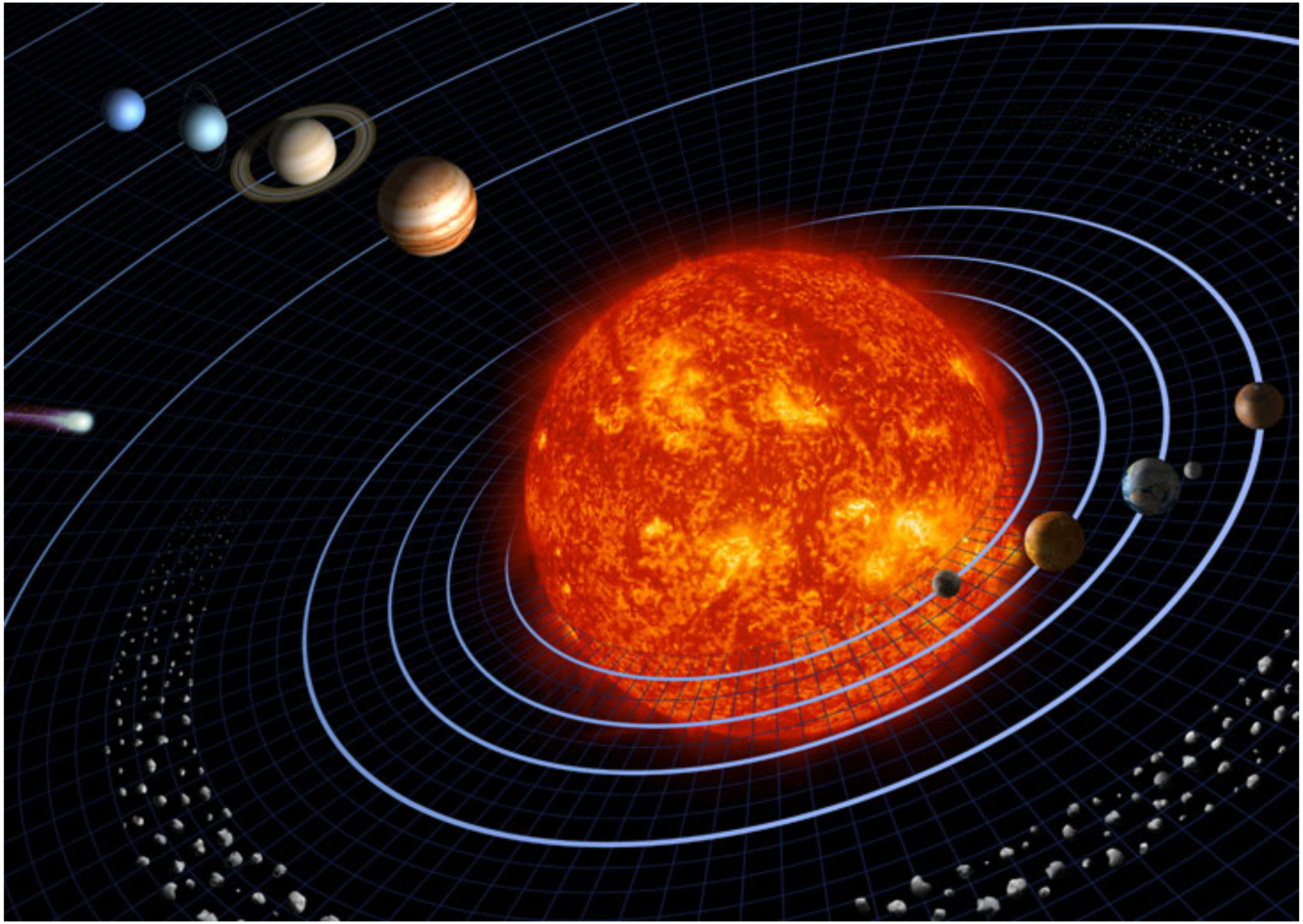
[A] K.G. Andersson, Poincaré's discovery of homoclinic points, *Archive for History of Exact Sciences* 48 (1994), 133–147.

[BG] J. Barrow-Green, Oscar II's prize competition and the error in Poincaré's memoir on the three body problem, *Archive for History of Exact Sciences* 48 (1994), 107–131.

[B] J. Bernoulli, *Opera Omnia*, vol. I, Georg Olms Verlagsbuchhandlung, Hildesheim, 1968.

[Bi] G. Bisconcini, Sur le problème des trois corps, *Acta Mathematica* 30 (1906), 49–92.

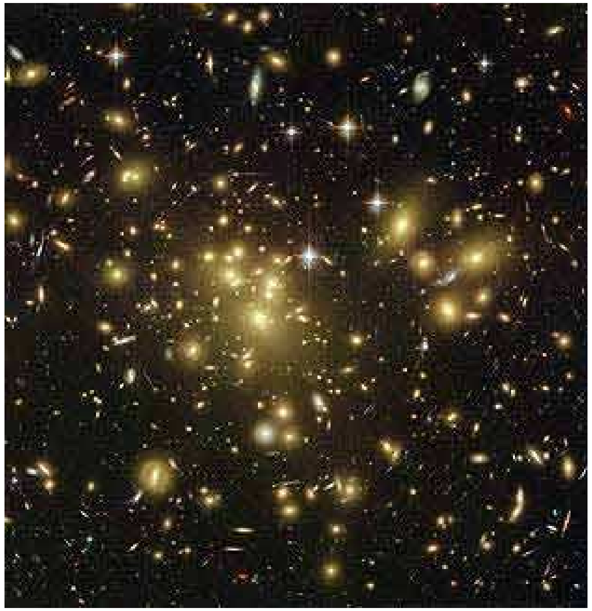
emergent behavior



(from NASA website)

a single iron atom

26 electrons, 78 arguments,
10^{78} values
10 X 10 X 10 grid



(from NASA website)

$$\Psi_0(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_{26})$$

do we need the exact solution?

no.

too many details.

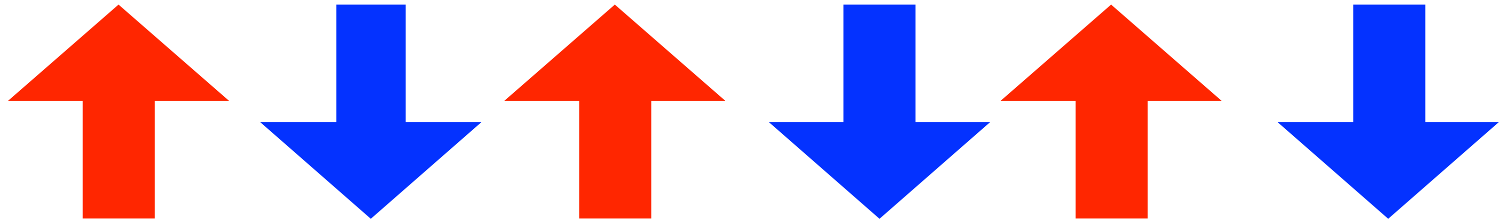
we need answers to interesting questions

- its *general* properties
- we want to understand *cooperative phenomena*: color, metallicity, …
  (or superconductivity, ferromagnetism, antiferromagnetism,…)
- identify *elementary entities*
- the latter depend on energy scale (*electron* vs *localized spins*)
- theory describing ideal object: model Hamiltonian
- gold is not iron: material-specific Hamiltonian

a solid-state example: antiferromagnetism

prediction: Néel (1932)

from mean-field theory



experiment: Shull and Smart (1949)

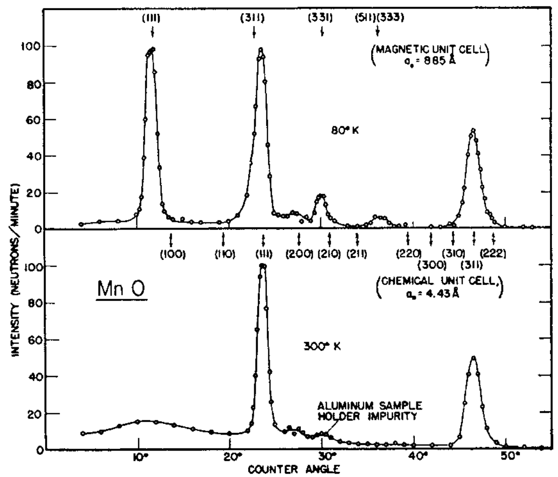
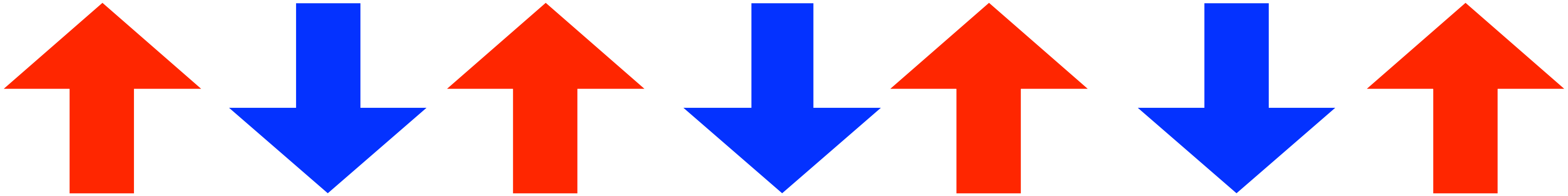


FIG. 1. Neutron diffraction patterns for MnO at room temperature and at 80°K.

but the theory was wrong…

Bethe: ground state of linear Heisenberg chain has S=0

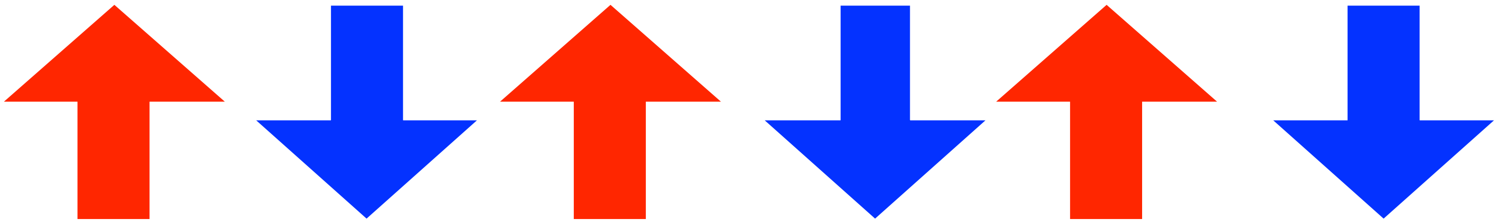
static mean-field ground state is wrong



Anderson: broken symmetry & quantum fluctuations

after we understand the mechanism everything is simpler…

simple (*wrong*) method sufficient



static mean-field solution

the *standard* model

density-functional theory

state-of the art approach; works for a large class of systems

shifts the focus from the wavefunction to the electronic density

$$\Psi_0(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_{26}) \rightarrow n(\mathbf{r})$$

exact (T=0) in principle, but only approximate functionals in practice

(LDA,GGA….)

density-functional theory

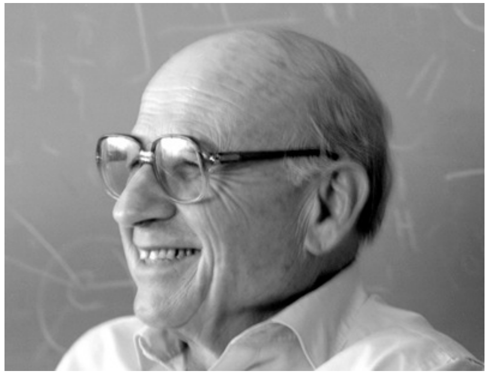
$$\hat{H} = -\frac{1}{2}\sum_i \nabla_i^2 + \frac{1}{2}\sum_{i\neq i'} \frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|} - \sum_{i,\alpha} \frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|} - \sum_\alpha \frac{1}{2M_\alpha}\nabla_\alpha^2 + \frac{1}{2}\sum_{\alpha\neq\alpha'} \frac{Z_\alpha Z_{\alpha'}}{|\mathbf{R}_\alpha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

Kohn-Sham Hamiltonian

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

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

(in practice: LDA,GGA,…)



Walter Kohn

Nobel Prize in Chemistry (1998)

Kohn-Sham equations

understand and predict properties of solids, molecules, biological systems, geological systems...

strongly correlated systems

….those for which DFT (LDA) fails….

….LDA effective potential not enough….

….Coulomb average effects not enough….

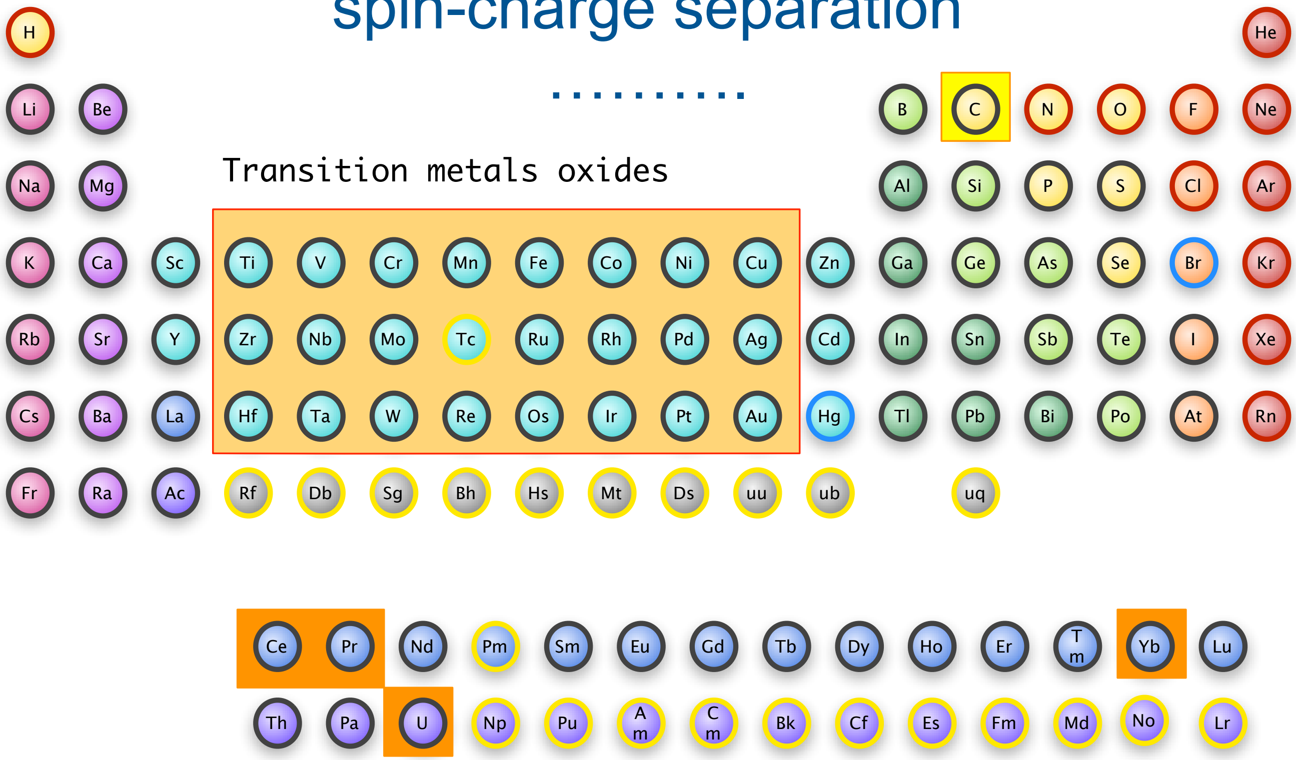
strongly correlated systems

how do we recognize them?

anomalous phenomena

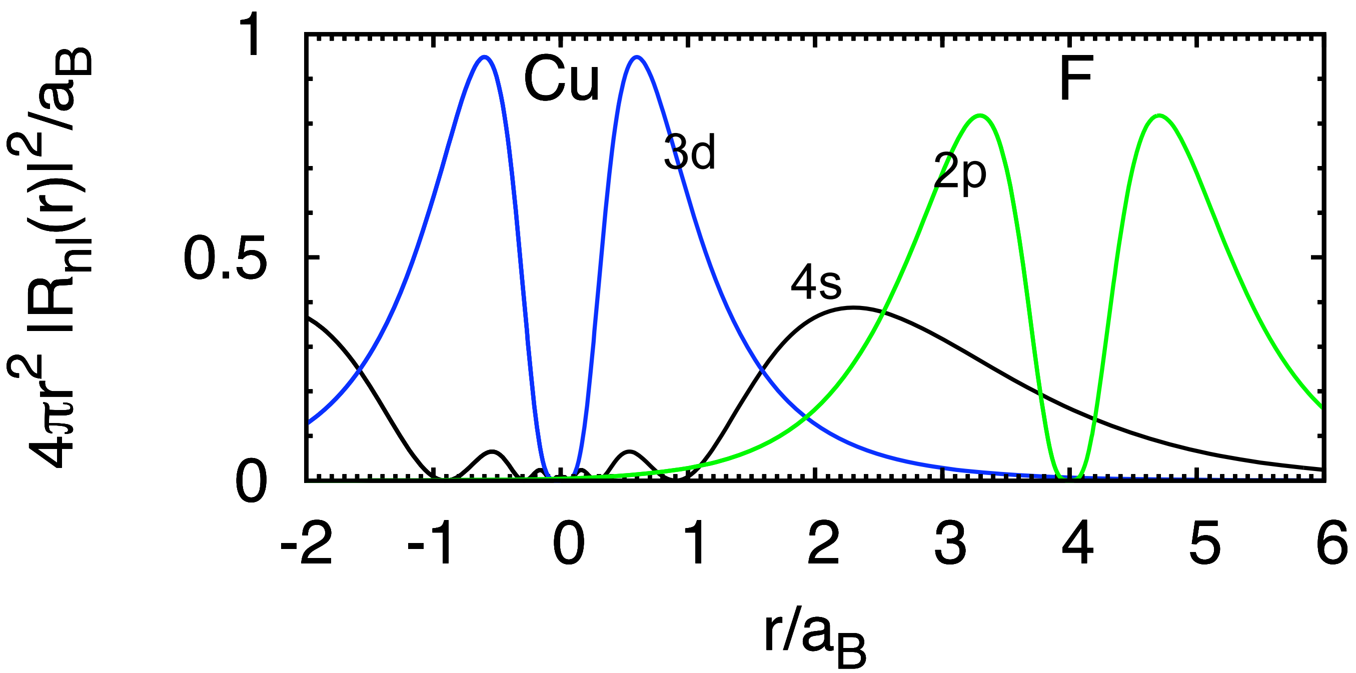
Mott insulators
heavy-Fermions
unconventional superconductivity
spin-charge separation

....



localized electrons

partiallty filled localized *d* and *f* shell; atomic physics plays important role



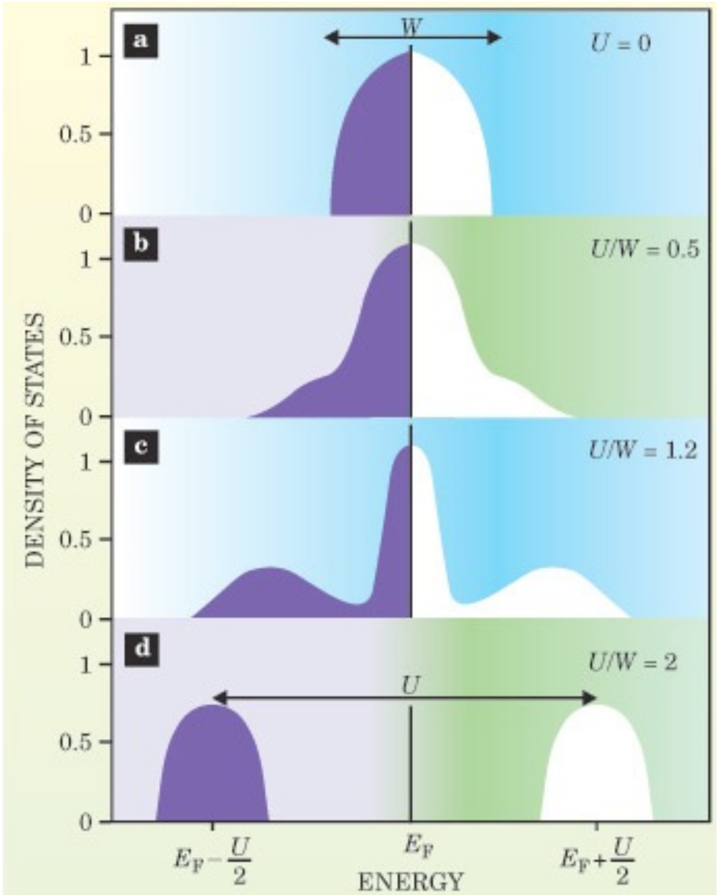
$$\psi_{nlm}(\rho,\theta,\phi) = R_{nl}(\rho) Y_l^m(\theta,\phi)$$

$$R_{nl}(\rho) = \sqrt{\left(\frac{2Z}{n}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3}} e^{-\rho/n} \left(\frac{2\rho}{n}\right)^l L_{n-l-1}^{2l+1}\left(\frac{2\rho}{n}\right)$$

(hydrogen-like atom: Appendix B)

JÜLICH FORSCHUNGSZENTRUM

metal-insulator transition



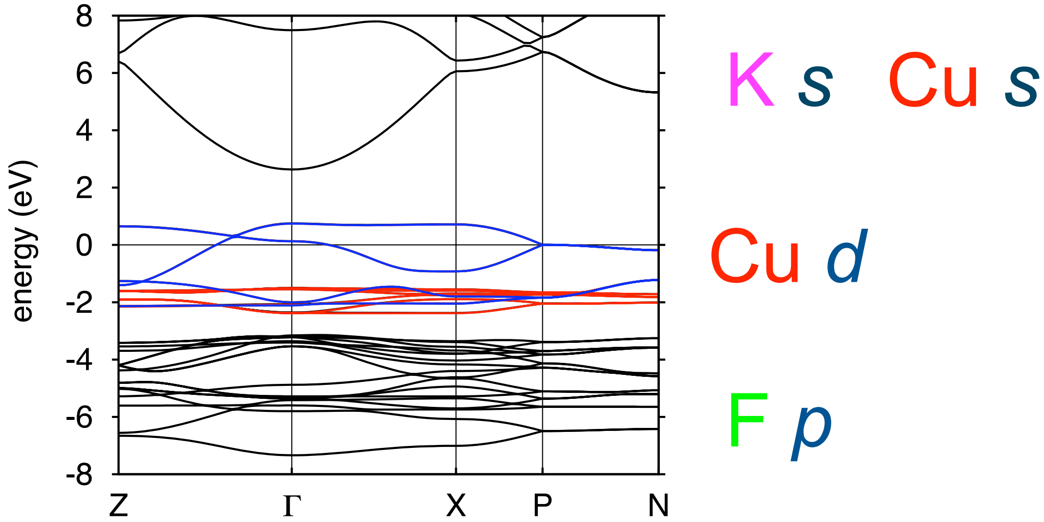
G. Koltiar and D. Vollhardt, Physics Today **57,** 53 (2004)

not explained by mean-field, Hartree-Fock, perturbation theory, Fermi-liquid, DFT, etc.…

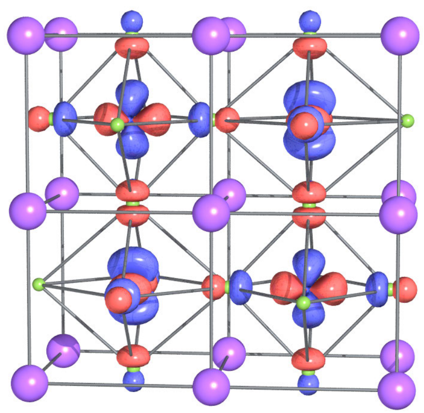
a Mott insulator

an example: $KCuF_3$

LDA or GGA, or simple functional calculation



(odd number of electrons)



in real life: large gap orbitally ordered insulator

magnetic only below 40 K

it not a quantitative failure, but qualitative one

we can start from LDA, however

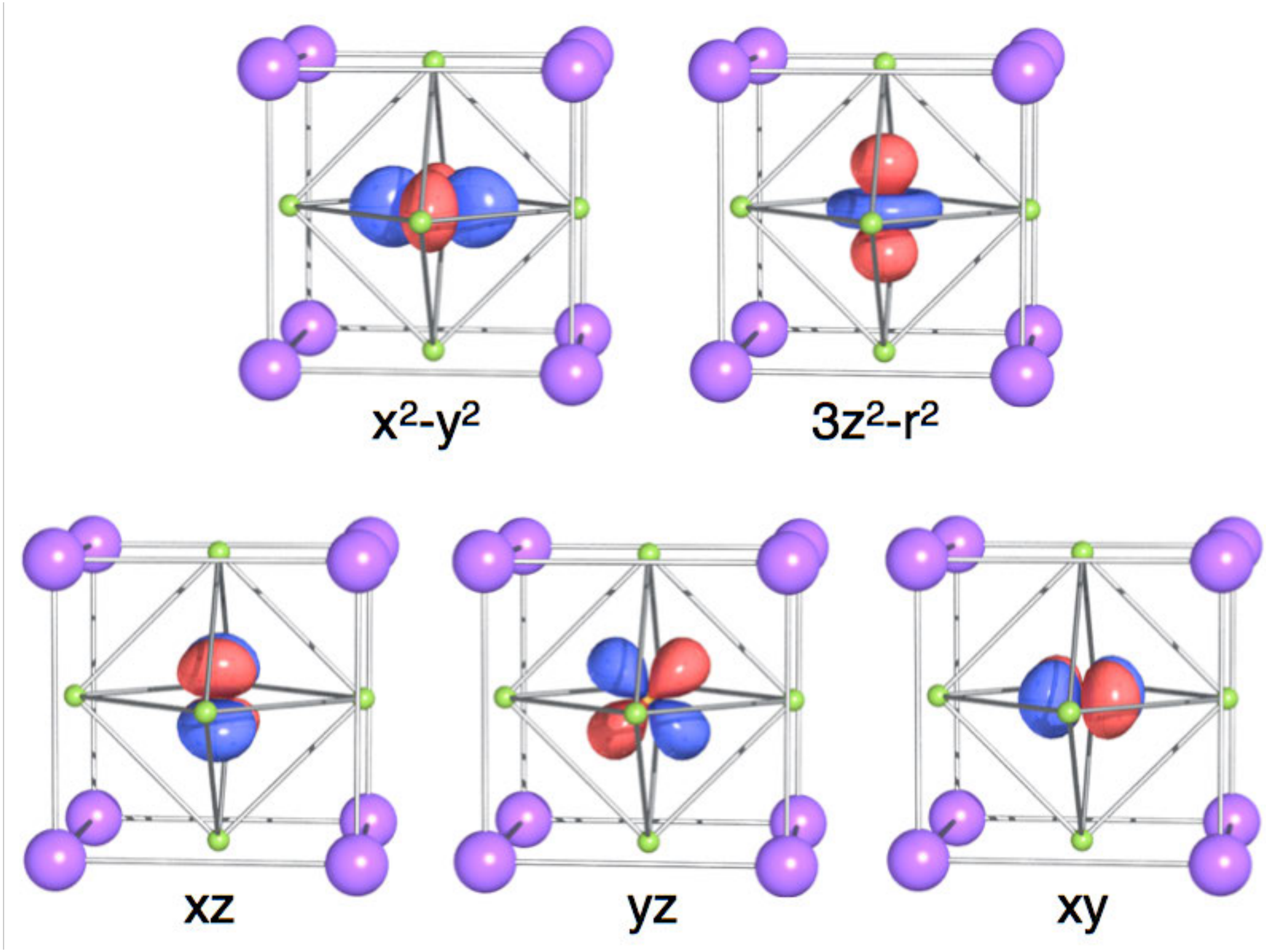
correlation effects can be see as correction of DFT (LDA)

we can build one-electron basis from DFT

for example localized Wannier functions

$$\psi_{in\sigma}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{R}_i\cdot\mathbf{k}}\ \psi_{n\mathbf{k}\sigma}(\mathbf{r})$$

ab-initio Wannier functions



realistic models from DFT(LDA)

basis functions

$$\psi_{in\sigma}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{R}_i \cdot \mathbf{k}} \, \psi_{n\mathbf{k}\sigma}(\mathbf{r})$$

localized Wannier functions
from LDA (GGA,...)

Hamiltonian

$$\hat{H}_e = \hat{H}^{\mathrm{LDA}} + \hat{U} - \hat{H}_{\mathrm{DC}}$$

$$\hat{H}^{\mathrm{LDA}} = -\sum_{\sigma} \sum_{in,i'n'} t^{i,i'}_{n,n'} c^{\dagger}_{in\sigma} c_{i'n'\sigma}$$

LDA Hamiltonian

$$t^{i,i'}_{n,n'} = -\int d\mathbf{r}\, \overline{\psi}_{in\sigma}(\mathbf{r}) [-\frac{1}{2}\nabla^2 + v_{\mathrm{R}}(r)] \psi_{i'n'\sigma}(\mathbf{r})$$

Coulomb and double counting

$$\hat{H}_e = \hat{H}^{\mathrm{LDA}} + \hat{U} - \hat{H}_{\mathrm{DC}}$$

$$\hat{U} = \frac{1}{2} \sum_{ii'jj'} \sum_{\sigma\sigma'} \sum_{nn'pp'} U^{iji'j'}_{np\,n'p'} c^{\dagger}_{in\sigma} c^{\dagger}_{jp\sigma'} c_{j'p'\sigma'} c_{i'n'\sigma}$$

bare Coulomb integrals

$$\begin{aligned} \hat{U} = \frac{1}{2} U^{iji'j'}_{np\,n'p'} &= \langle in\sigma\; jp\sigma' | \hat{U} | i'n'\sigma\; j'p'\sigma' \rangle \\ &= \int d\mathbf{r}_1 \int d\mathbf{r}_2\, \overline{\psi}_{in\sigma}(\mathbf{r}_1) \overline{\psi}_{jp\sigma'}(\mathbf{r}_2) \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \psi_{j'p'\sigma'}(\mathbf{r}_2) \psi_{i'n'\sigma}(\mathbf{r}_1) \end{aligned}$$

$\hat{H}_{\mathrm{DC}}$ long range Hartree and mean-field exchange-correlation already are well described by LDA (GGA,..)

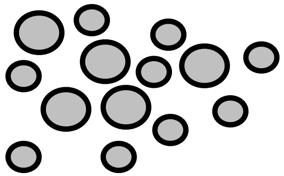
difference U-H_{DC} short range!

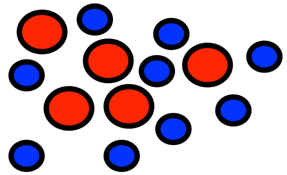
if it would be long range perhaps *not so strongly correlated*…

light and heavy electrons

electrons

light (weakly correlated): LDA (GGA,..)





heavy(strongly correlated): U

$$\hat{H}_e = \hat{H}^{\text{LDA}} + \hat{U}^l - \hat{H}^l_{\text{DC}}$$

eg. *l* shell

$$\hat{U}^l - \hat{H}^l_{\text{DC}}$$

short-range correction to LDA

local or almost local

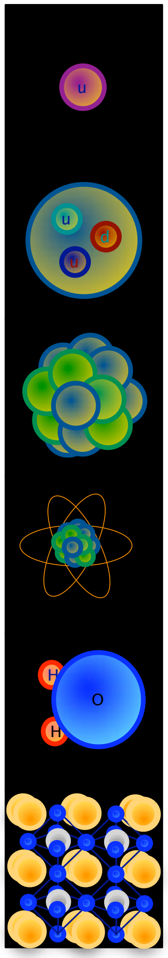
for a *l* shell, the local Coulomb interaction is

$$\hat{U}^l = \frac{1}{2} \sum_i \sum_{\sigma\sigma'} \sum_{m_\alpha m'_\alpha} \sum_{m_\beta m'_\beta} U_{m_\alpha m_\beta m'_\alpha m'_\beta} c^\dagger_{i m_\alpha \sigma} c^\dagger_{i m_\beta \sigma'} c_{i m'_\beta \sigma'} c_{i m'_\alpha \sigma}$$

screening? cRPA, cLDA, …. various approximations to be put to a test

from LDA to minimal models

energy scales



10^9 eV — quarks

proton

10^7 eV

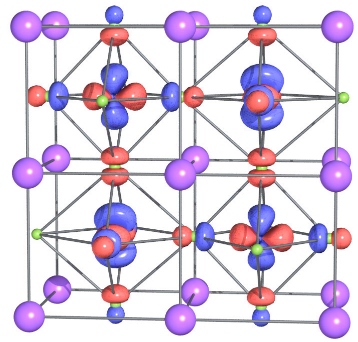
nucleus

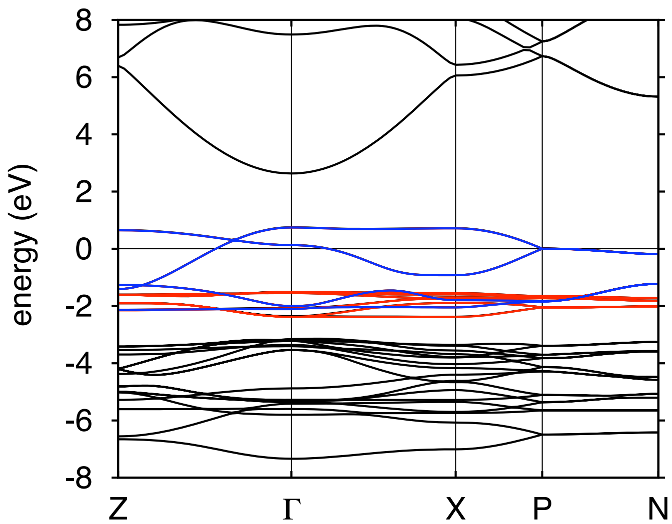
10^5 eV — atom

molecule

10^3 eV

crystal





K *s* Cu *s*

Cu *d*

F *p*

simple low-energy models

typical model

generalized Hubbard model

$$\hat{H}_e = \hat{H}^{\mathrm{LDA}} + \hat{H}_U^l - \hat{H}_{\mathrm{DC}}^l$$

$$\hat{H}^{\mathrm{LDA}} = -\sum_{ii'} \sum_{\sigma} \sum_{m_\alpha m'_\alpha} t^{i,i'}_{m_\alpha, m'_\alpha} c^\dagger_{i m_\alpha \sigma} c_{i' m'_\alpha \sigma} = \sum_{\boldsymbol{k}} \sum_{\sigma} \sum_{m_\alpha m'_\alpha} \left[H^{\mathrm{LDA}}_{\boldsymbol{k}} \right]_{m_\alpha, m'_\alpha} c^\dagger_{\boldsymbol{k} m_\alpha \sigma} c_{\boldsymbol{k} m'_\alpha \sigma}$$

$$\hat{H}_U^l = \frac{1}{2} \sum_{i} \sum_{\sigma\sigma'} \sum_{m_\alpha m'_\alpha} \sum_{m_\beta m'_\beta} U_{m_\alpha m_\beta m'_\alpha m'_\beta} c^\dagger_{i m_\alpha \sigma} c^\dagger_{i m_\beta \sigma'} c_{i m'_\beta \sigma'} c_{i m'_\alpha \sigma}$$

one-band Hubbard model

$$\hat{H}_{\text{Hubbard}} = \underbrace{-\sum_{ii'}\sum_{\sigma} t_{1,1}^{i,i'} c_{i\sigma}^{\dagger} c_{i'\sigma}}_{\hat{H}_0} + \underbrace{\varepsilon_d \sum_{i\sigma} n_{i\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}}_{\hat{H}_U}$$

$$\begin{cases} \varepsilon_d & = & -t_{1,1}^{i,i} \\ t & = & t_{1,1}^{\langle i,i' \rangle} \\ U & = & U_{1111}^{iiii} \end{cases}$$

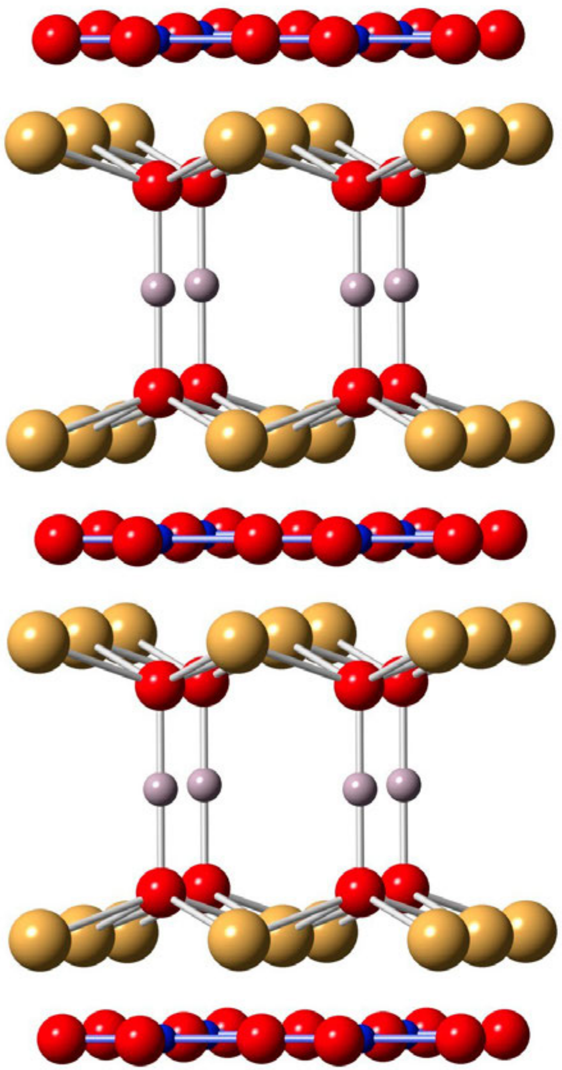
half filling

t=0: N_s atoms, insulator

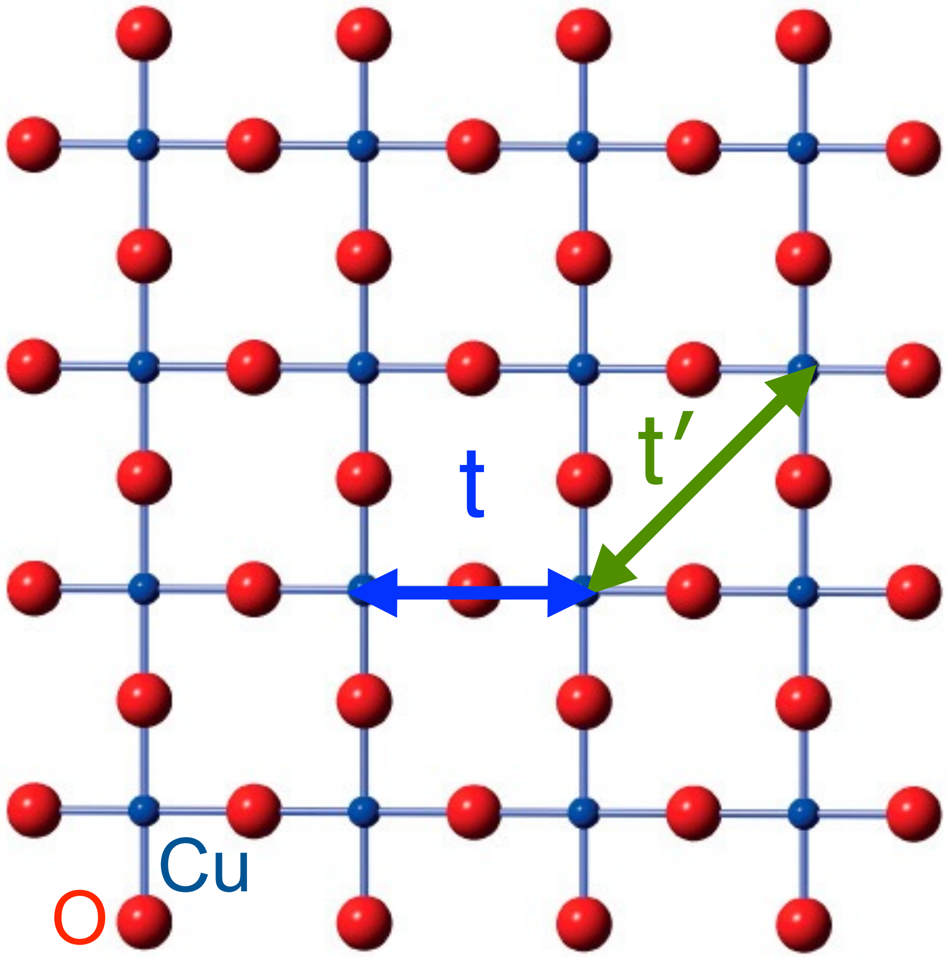
U=0: half-filled band, metal

model for high-temperature superconducting cuprates

high-T_c superconducting cuprates



$HgBa_2CuO_4$



CuO_2 planes

high-T_c superconducting cuprates

VOLUME 87, NUMBER 4 PHYSICAL REVIEW LETTERS 23 JULY 2001

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

E. Pavarini, I. Dasgupta,* T. Saha-Dasgupta,† O. Jepsen, and O. K. Andersen
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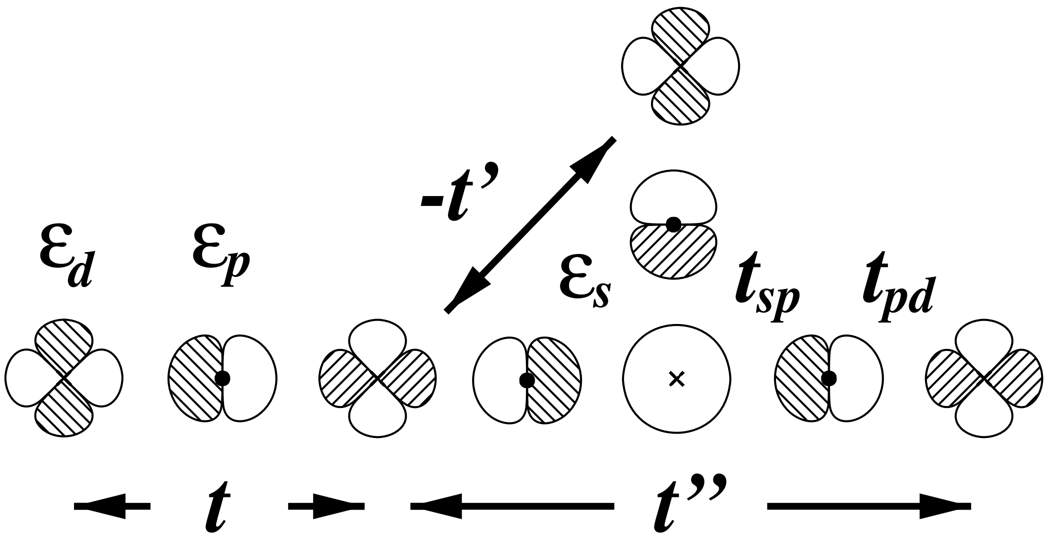
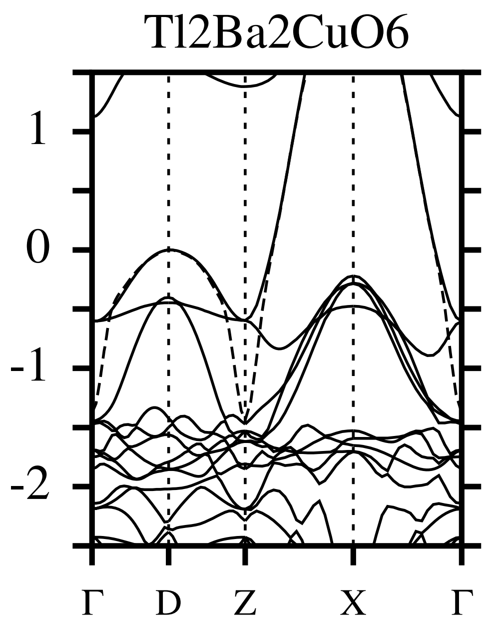
(Received 4 December 2000; published 10 July 2001)

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 $4s$, apical-oxygen $2p_z$, and farther orbitals. Materials with higher $T_{c\,\mathrm{max}}$ have larger hopping ranges and axial orbitals more localized in the CuO_2 layers.





parameters for high-T_c superconductors

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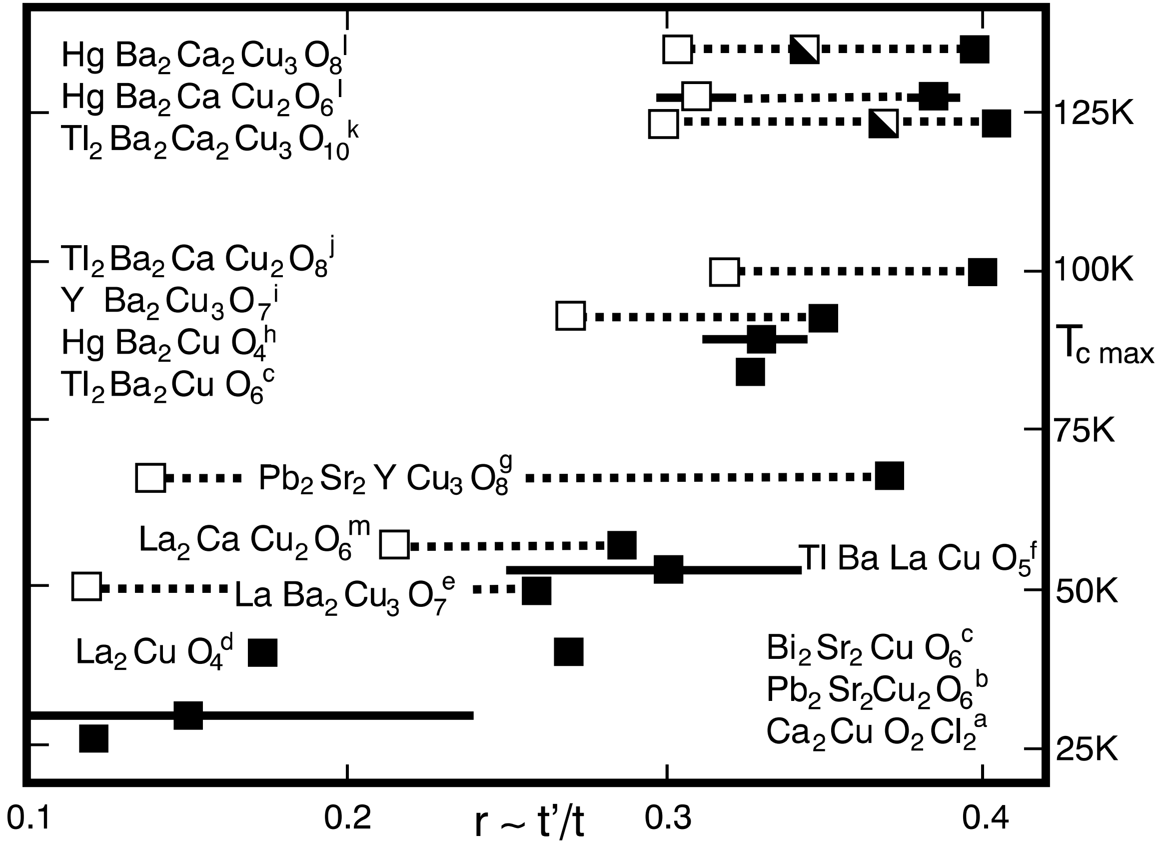


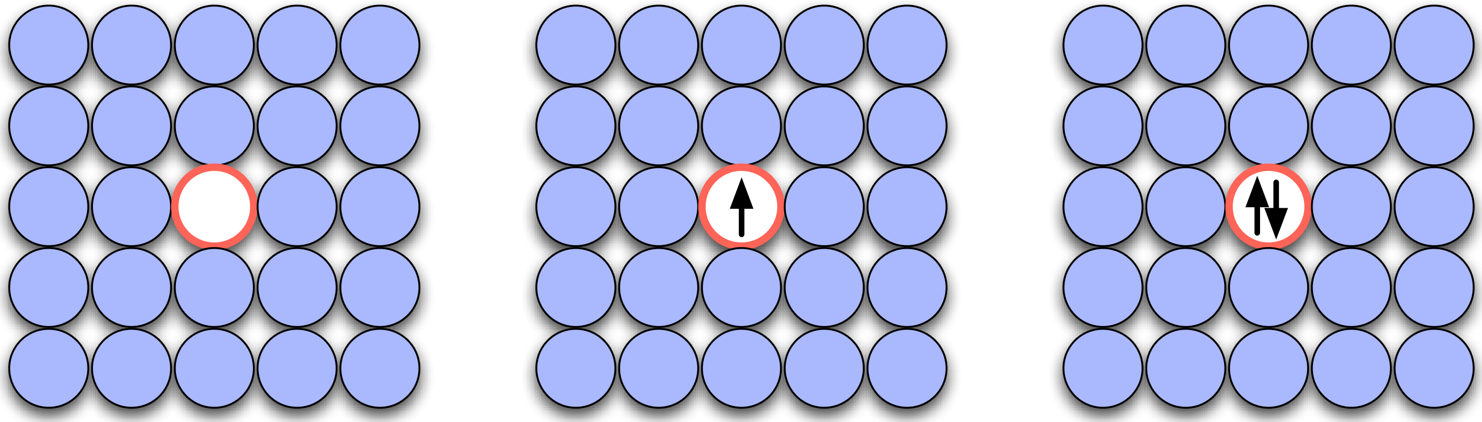
we still need a solution method

… should describe at least Mott physics ..
… should be flexible, work for all models of Hubbard type ..

NB: flexible alone is not enough
e.g.: very flexible: HF, or LDA; however, no Mott transition

DMFT

stat-of-the art approach for Hubbard-like models



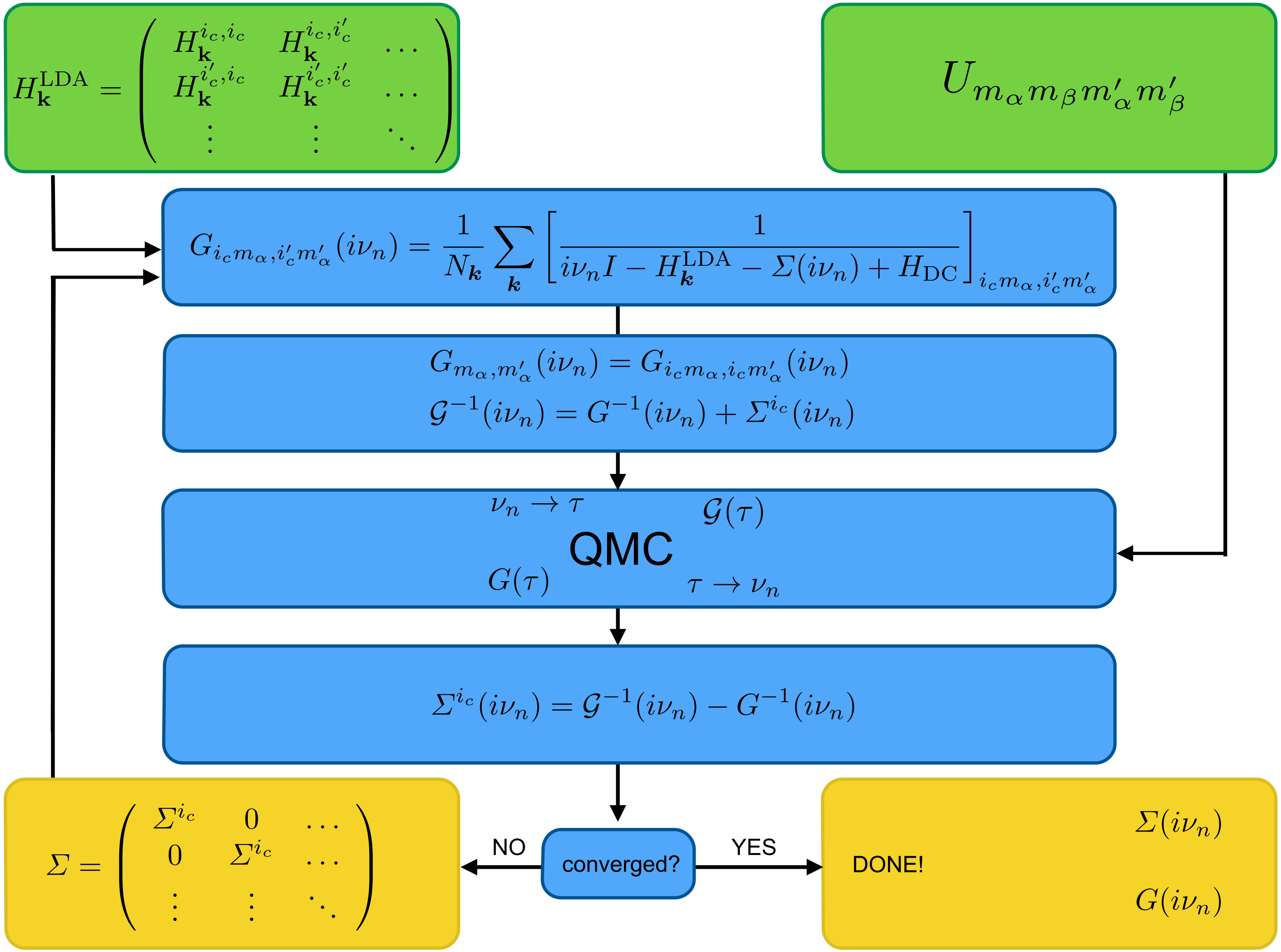
$$G_0{}^{-1} - G^{-1} = \Sigma(\omega)$$

dynamics captured   self-energy local

exact in infinite dimensions

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

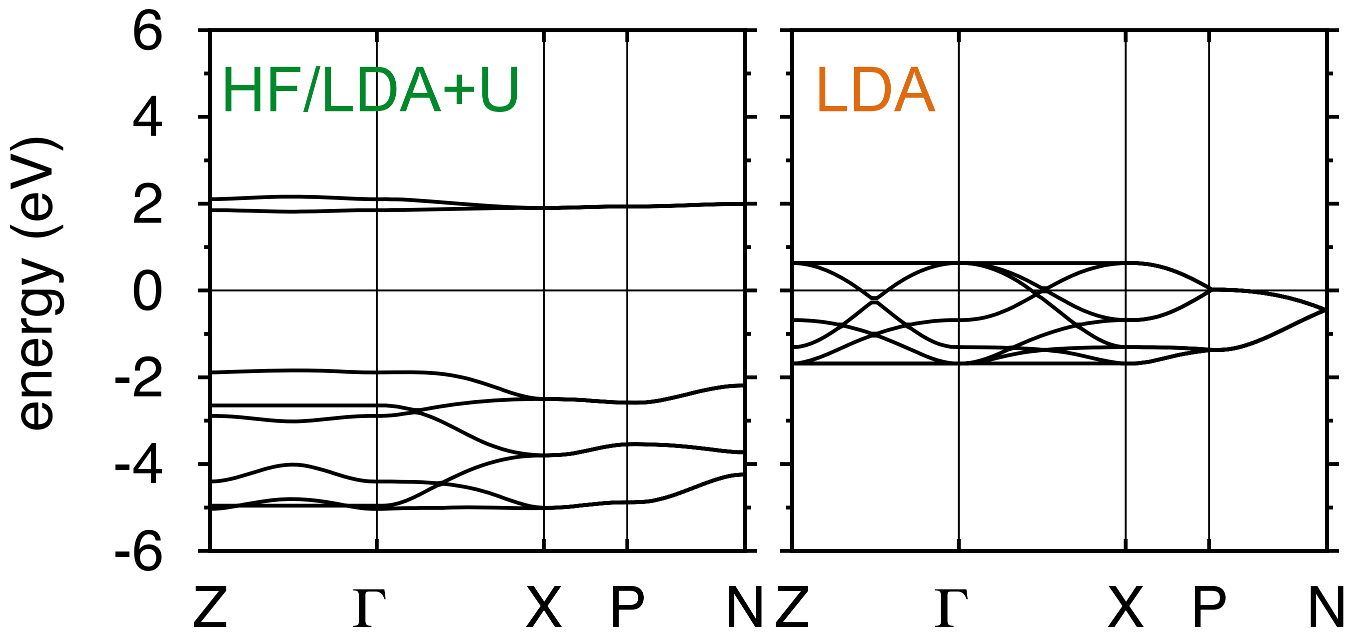
LDA+DMFT



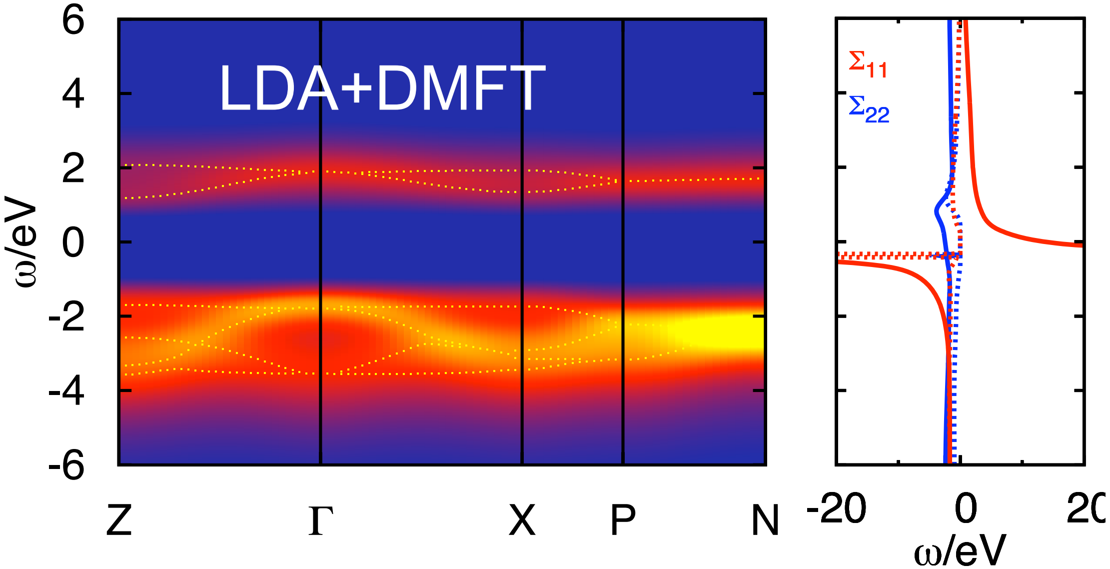
$H_{\mathbf{k}}^{\mathrm{LDA}} = \begin{pmatrix} H_{\mathbf{k}}^{i_c,i_c} & H_{\mathbf{k}}^{i_c,i'_c} & \cdots \\ H_{\mathbf{k}}^{i'_c,i_c} & H_{\mathbf{k}}^{i'_c,i'_c} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$
$U_{m_\alpha m_\beta m'_\alpha m'_\beta}$
$G_{i_c m_\alpha, i'_c m'_\alpha}(i\nu_n) = \frac{1}{N_{\boldsymbol{k}}} \sum_{\boldsymbol{k}} \left[\frac{1}{i\nu_n I - H_{\boldsymbol{k}}^{\mathrm{LDA}} - \Sigma(i\nu_n) + H_{\mathrm{DC}}} \right]_{i_c m_\alpha, i'_c m'_\alpha}$
$G_{m_\alpha, m'_\alpha}(i\nu_n) = G_{i_c m_\alpha, i_c m'_\alpha}(i\nu_n)$
$\mathcal{G}^{-1}(i\nu_n) = G^{-1}(i\nu_n) + \Sigma^{i_c}(i\nu_n)$
$\nu_n \to \tau$
$\mathcal{G}(\tau)$
QMC
$G(\tau)$
$\tau \to \nu_n$
$\Sigma^{i_c}(i\nu_n) = \mathcal{G}^{-1}(i\nu_n) - G^{-1}(i\nu_n)$
$\Sigma = \begin{pmatrix} \Sigma^{i_c} & 0 & \cdots \\ 0 & \Sigma^{i_c} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$
NO
converged?
YES
DONE!
$\Sigma(i\nu_n)$
$G(i\nu_n)$

$KCuF_3$: various types of solutions

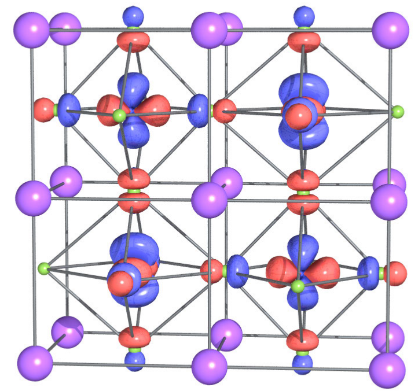
insulating & AFM



non-magnetic & metallic



orbital ordering in paramagnetic phase



early successes: details matter

mechanism of Mott transition in the series explained

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

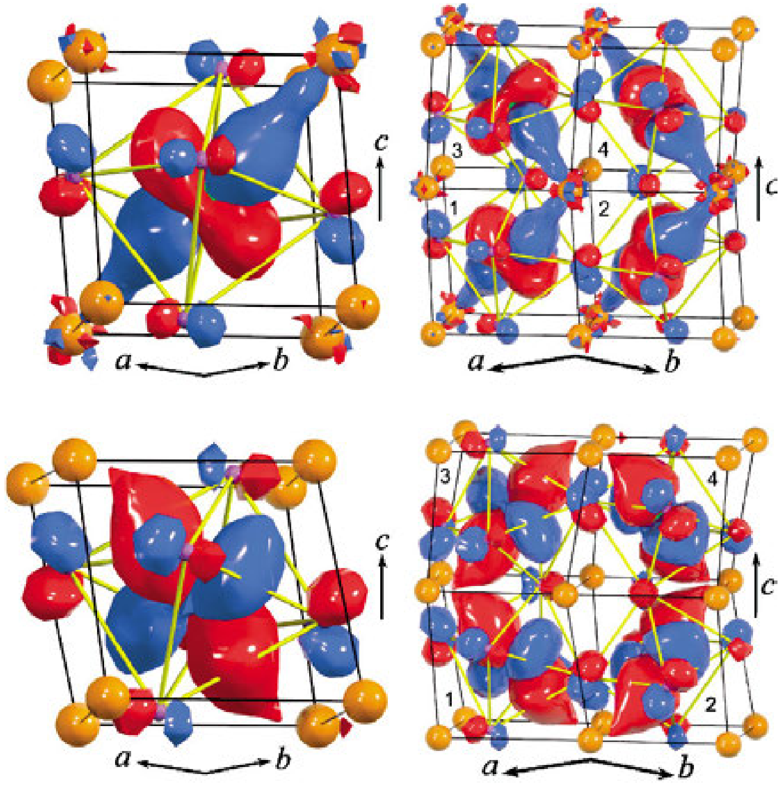
Mott Transition and Suppression of Orbital Fluctuations in Orthorhombic $3d^1$ Perovskites

E. Pavarini,[1] S. Biermann,[2] A. Poteryaev,[3] A. I. Lichtenstein,[3] A. Georges,[2] and O. K. Andersen[4]

$t_{2g}{}^1$

Δ=200-300 meV

LDA+DMFT 770 K



a small crystal field plays a key role

spectral functions

(one-electron Green function)

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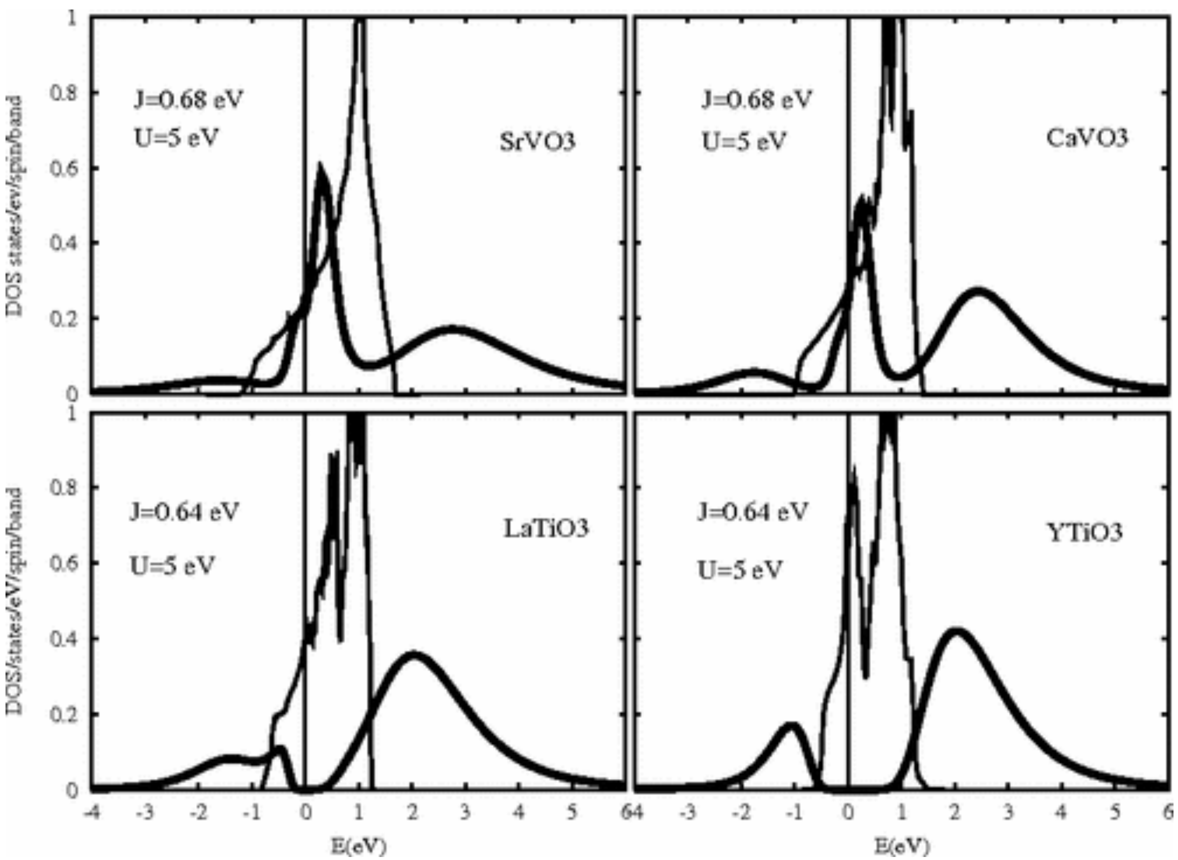

what about linear response functions?

Hubbard Model in Infinite Dimensions: A Quantum Monte Carlo Study

M. Jarrell

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(Received 5 December 1991)

An essentially exact solution of the infinite-dimensional Hubbard model is made possible by a new self-consistent Monte Carlo procedure. Near half filling antiferromagnetism and a pseudogap in the single-particle density of states are found for sufficiently large values of the intrasite Coulomb interaction. At half filling the antiferromagnetic transition temperature obtains its largest value when the intrasite Coulomb interaction $U \approx 3$.

PACS numbers: 75.10.Jm, 71.10.+x, 75.10.Lp, 75.30.Kz

problem:

$$\mathcal{G}^0(i\omega_n) = G'_{ii}(i\omega_n) = G^0_{ii}(i\omega_n) + \sum_k G^0_{ik}(i\omega_n)\Sigma'_k(i\omega_n)G'_{ki}(i\omega_n)\,, \quad (2)$$

where

$$\Sigma'_k(i\omega_n) = \begin{cases} 0, & \text{if } i=k, \\ \Sigma(i\omega_n), & \text{otherwise.} \end{cases} \quad (3)$$

The prime indicates that the self-energy is set to zero on site i. This spatial dependence of Σ'_k is necessary to avoid overcounting of diagrams, since the Green's function $\mathcal{G}$ is calculated to all orders in U by the QMC process. The diagrammatic equation shown in Fig. 2 is the same as that needed to solve the Anderson impurity problem. Thus, given $\mathcal{G}^0$, I may solve for $\mathcal{G}$ with the QMC algorithm of Hirsch and Fye [7]. The Green's function calculated in this process may then be inverted to yield a new estimate for $\Sigma(i\omega_n)$,

$$\mathcal{G}(i\omega_n)^{-1} = \mathcal{G}^0(i\omega_n)^{-1} - \Sigma(i\omega_n)\,. \quad (4)$$

Thus the QMC procedure and Eqs. (2) and (4) constitute a set of self-consistent equations for the lattice self-energy Σ which essentially reduce the problem to a self-consistently embedded Anderson impurity problem [8].

A variety of two-particle properties may also be calculated with this procedure [9], since, using similar arguments applied to the self-energy, one may argue that the irreducible vertex function is also local. For example, the static magnetic susceptibility matrix

$$\chi_{ij}(i\omega_n,i\omega_m) = \chi^0_{ij}(i\omega_n)\delta_{nm} + T\sum_{p,k}\chi^0_{ik}(i\omega_n)\Gamma(i\omega_n,i\omega_p) \times\chi_{kj}(i\omega_p,i\omega_m)\,, \quad (5)$$

where $\omega_n = (2n+1)\pi T$. This is related to the static susceptibilities by

$$\chi_{\mathbf{q}} = \frac{T}{N}\sum_{n,m,i,j} e^{-i\mathbf{q}\cdot\mathbf{R}_{ij}}\chi_{ij}(i\omega_n,i\omega_m)\,. \quad (6)$$

The noninteracting part is

$$\chi^0_{\mathbf{q}}(i\omega_n) = \frac{1}{N}\sum_{\mathbf{k}} G_{\mathbf{k}}(i\omega_n)G_{\mathbf{k}+\mathbf{q}}(i\omega_n)\,, \quad (7)$$

where $G_{\mathbf{k}}(i\omega_n) = 1/[i\omega_n - \epsilon - \epsilon_{\mathbf{k}} - \Sigma(i\omega_n)]$. Equation (7) may readily be evaluated in the ferromagnetic $[\mathbf{q} = (0,0,0,\dots)]$ and antiferromagnetic $[\mathbf{q} = (\pi,\pi,\pi,\dots)]$ limits, in which it may be reexpressed as an integral over the Gaussian density of states. The function Γ is the local irreducible vertex function which may be calculated in the QMC procedure by solving

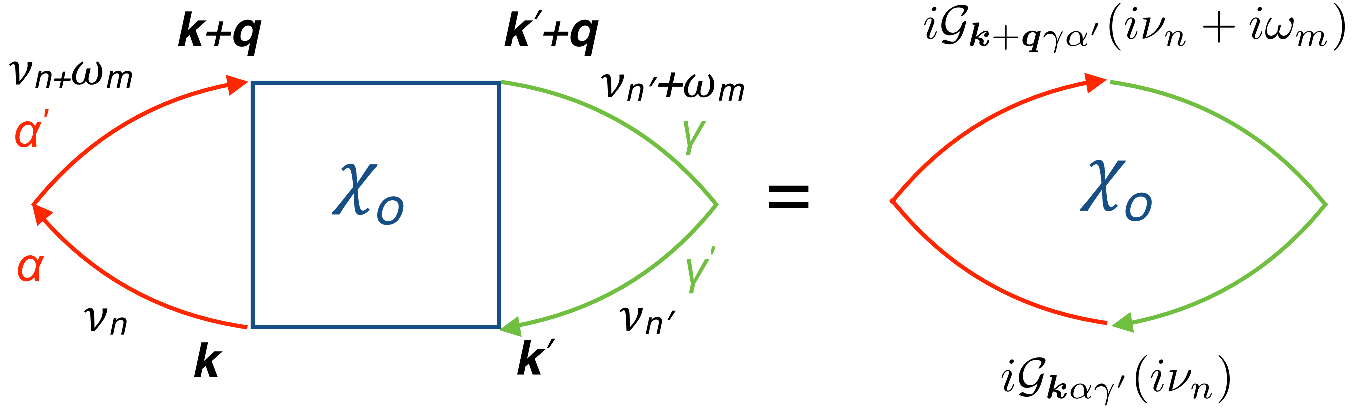
$$\chi_{ii}(i\omega_n,i\omega_m) = \mathcal{G}(i\omega_n)^2\delta_{nm} - T\sum_p \mathcal{G}(i\omega_n)^2\Gamma(i\omega_n,i\omega_p) \times\chi_{ii}(i\omega_p,i\omega_m)\,. \quad (8)$$

Here χ_{ii} is the opposite-spin two-particle Green's function,

$$\chi_{ii}(i\omega_n,i\omega_m) = -T^2\int_0^\beta d\tau_1\int_0^\beta d\tau_2\int_0^\beta d\tau_3\int_0^\beta d\tau_4 e^{-i\omega_m(\tau_1-\tau_2)}e^{-i\omega_n(\tau_3-\tau_4)}\langle T_\tau C_{i,\uparrow}(\tau_4)C^\dagger_{i,\downarrow}(\tau_3)C_{i,\downarrow}(\tau_2)C^\dagger_{i,\uparrow}(\tau_1)\rangle \quad (9)$$

non-interacting case

Wick's theorem holds



$$[\chi_0(\boldsymbol{q}; i\omega_m)]_{\boldsymbol{k}L_\alpha,\boldsymbol{k}'L_\gamma} = -\beta N_{\boldsymbol{k}} \mathcal{G}_{\boldsymbol{k}\alpha\gamma'}(i\nu_n) \mathcal{G}_{\boldsymbol{k}'+\boldsymbol{q}\alpha'\gamma}(i\nu_{n'} + i\omega_m) \delta_{n,n'} \delta_{\boldsymbol{k},\boldsymbol{k}'}$$

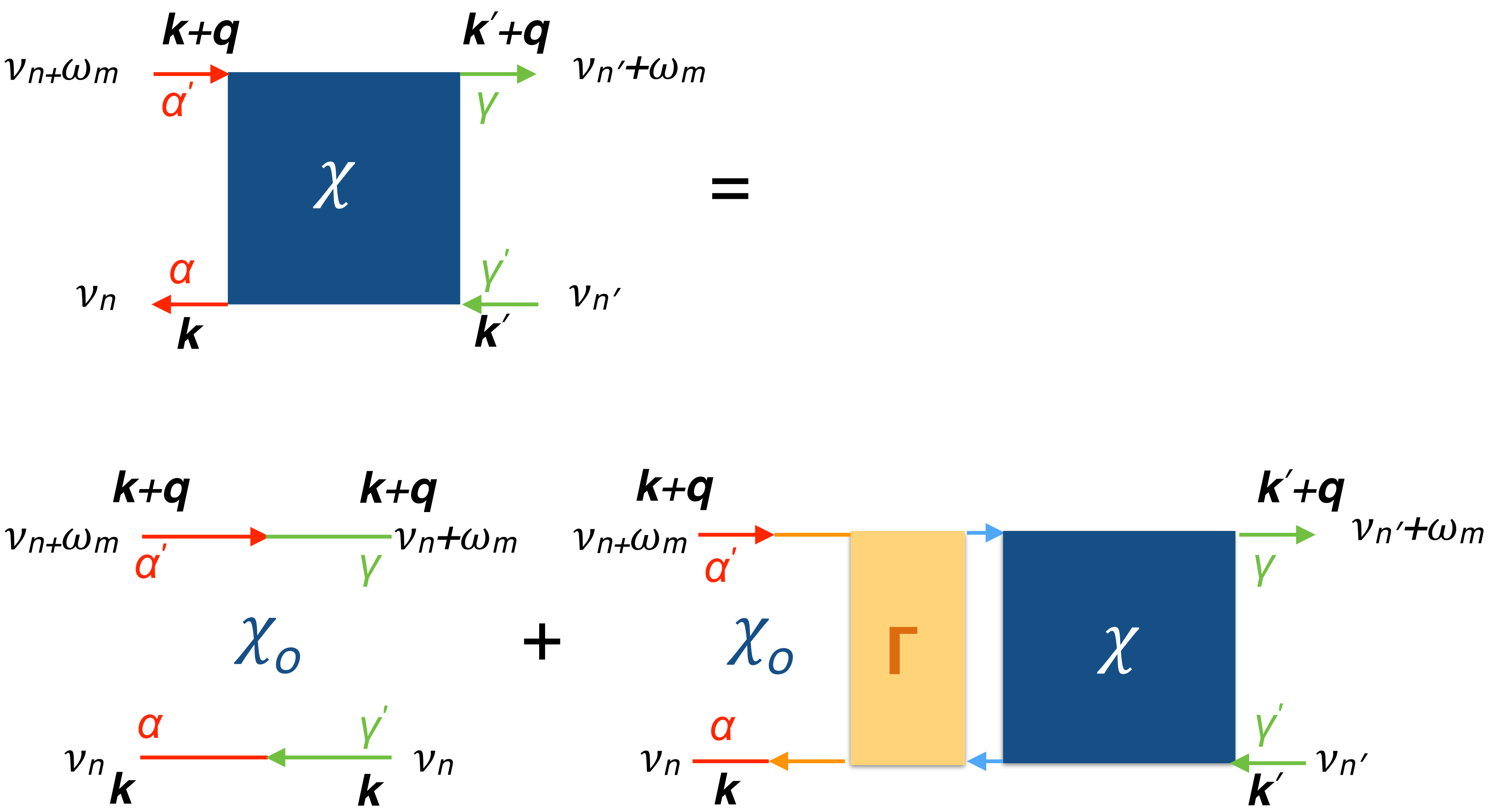
generalized susceptibility in LDA+DMFT

replace non-interacting *G* with G^{DMFT}

G^{DMFT} is the Green function obtained via DMFT

$$[\chi_0(\boldsymbol{q};i\omega_m)]_{L_\alpha,L_\gamma} = -\beta\delta_{nn'}\frac{1}{N_{\boldsymbol{k}}}\sum_{\boldsymbol{k}} G^{\mathrm{DMFT}}_{\alpha\gamma'}(\boldsymbol{k};i\nu_n)G^{\mathrm{DMFT}}_{\alpha'\gamma}(\boldsymbol{k}+\boldsymbol{q};i\nu_n+i\omega_m)$$

Bethe-Salpeter equation



local-vertex approximation

vertex in BS equation local in infinite dimensions
approximation for real materials

$$[\chi(\boldsymbol{q};i\omega_m)]_{L_\alpha,L_\gamma} = [\chi_0(\boldsymbol{q};\omega_m) + \chi_0(\boldsymbol{q};i\omega_m)\boxed{\Gamma(i\omega_m)}\chi(\boldsymbol{q};i\omega_m)]_{L_\alpha,L_\gamma}$$

define local susceptibilities

$$[\chi_0(i\omega_m)]_{L_\alpha^{ic},L_\gamma^{ic}} = \frac{1}{N_{\boldsymbol{q}}}\sum_{\boldsymbol{q}}[\chi_0(\boldsymbol{q};i\omega_m)]_{L_\alpha^{ic},L_\gamma^{ic}} \,,$$

$$[\chi(i\omega_m)]_{L_\alpha^{ic},L_\gamma^{ic}} = \frac{1}{N_{\boldsymbol{q}}}\sum_{\boldsymbol{q}}[\chi(\boldsymbol{q};i\omega_m)]_{L_\alpha^{ic},L_\gamma^{ic}}$$

local-vertex approximation

assume that local BS equation
is also valid for the local susceptibility

$$\boxed{[\Gamma(i\omega_m)]_{L_\alpha,L_\gamma}} = \left[\chi_0^{-1}(i\omega_m)\right]_{L_\alpha,L_\gamma} - \left[\chi^{-1}(i\omega_m)\right]_{L_\alpha,L_\gamma}$$

local susceptibility: from quantum impurity solver

insert vertex in BS equation

$$[\chi(\boldsymbol{q};i\omega_m)]_{L_\alpha,L_\gamma} = [\chi_0(\boldsymbol{q};\omega_m) + \chi_0(\boldsymbol{q};i\omega_m)\boxed{\Gamma(i\omega_m)}\chi(\boldsymbol{q};i\omega_m)]_{L_\alpha,L_\gamma}$$

q-dependence here from non-interacting part

Hubbard Model in Infinite Dimensions: A Quantum Monte Carlo Study

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An essentially exact solution of the infinite-dimensional Hubbard model is made possible by a new self-consistent Monte Carlo procedure. Near half filling antiferromagnetism and a pseudogap in the single-particle density of states are found for sufficiently large values of the intrasite Coulomb interaction. At half filling the antiferromagnetic transition temperature obtains its largest value when the intrasite Coulomb interaction $U \approx 3$.

PACS numbers: 75.10.Jm, 71.10.+x, 75.10.Lp, 75.30.Kz

Hirsch-Fye QMC

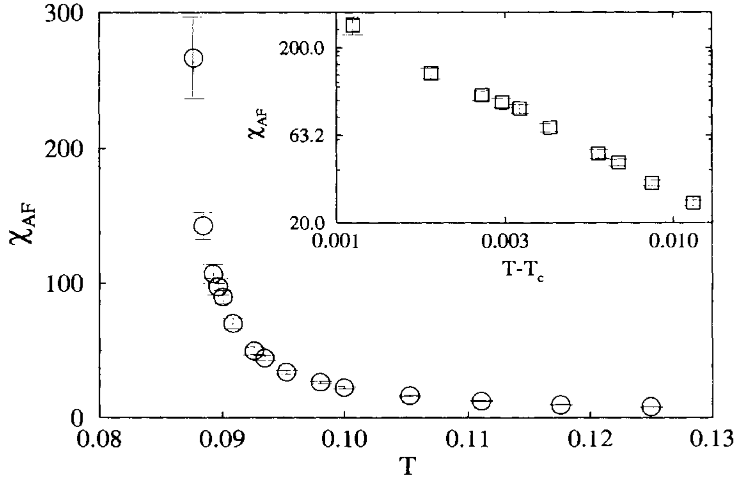
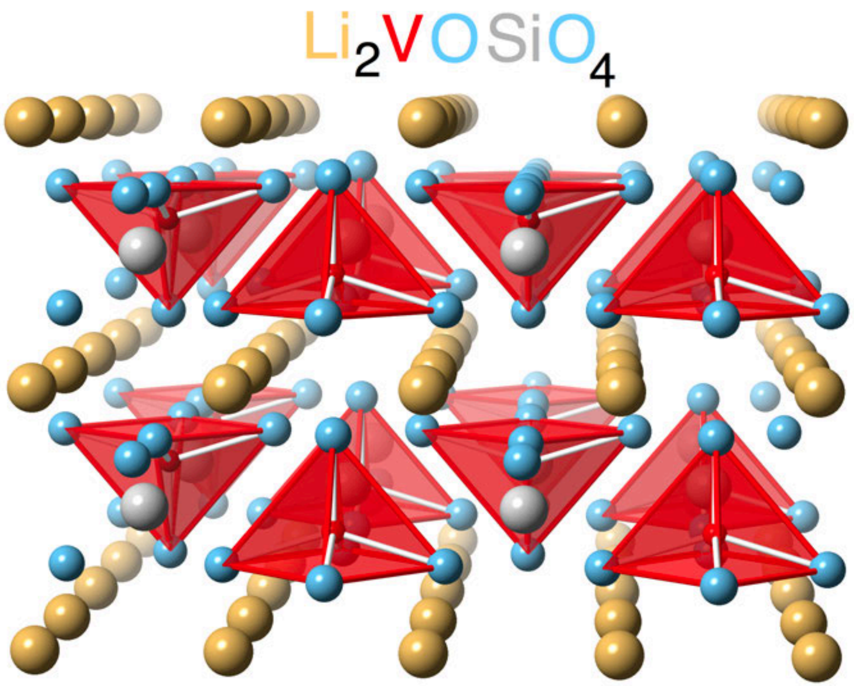
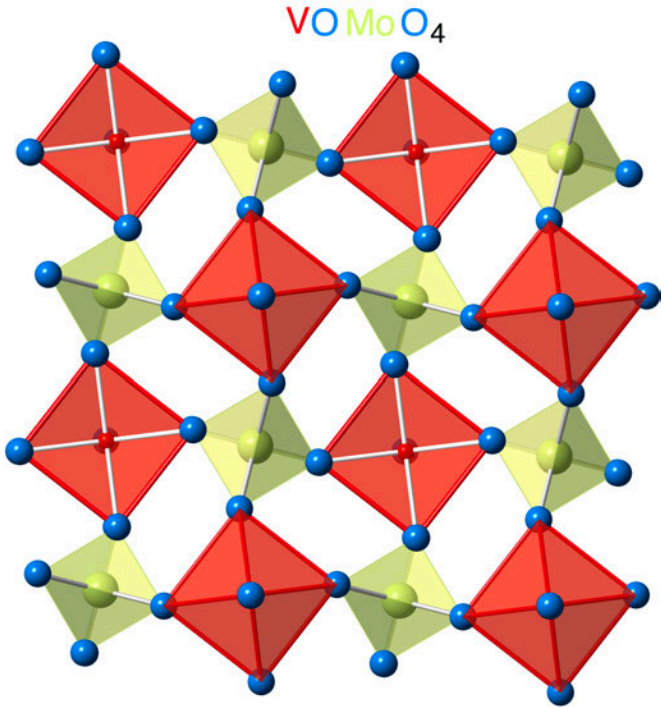


FIG. 3. Antiferromagnetic susceptibility $\chi_{AF}(T)$ vs temperature T when $U=1.5$ and $\epsilon=0.0$. The logarithmic scaling behavior is shown in the inset. The data close to the transition fit the form $\chi_{AF} \propto |T-T_c|^{\nu}$ with $T_c=0.0866\pm0.0003$ and $\nu=-0.99\pm0.05$. The points at $U=0$ reflect exactly known limits.

Li_2VOSiO_4 vs $VOMoO_4$

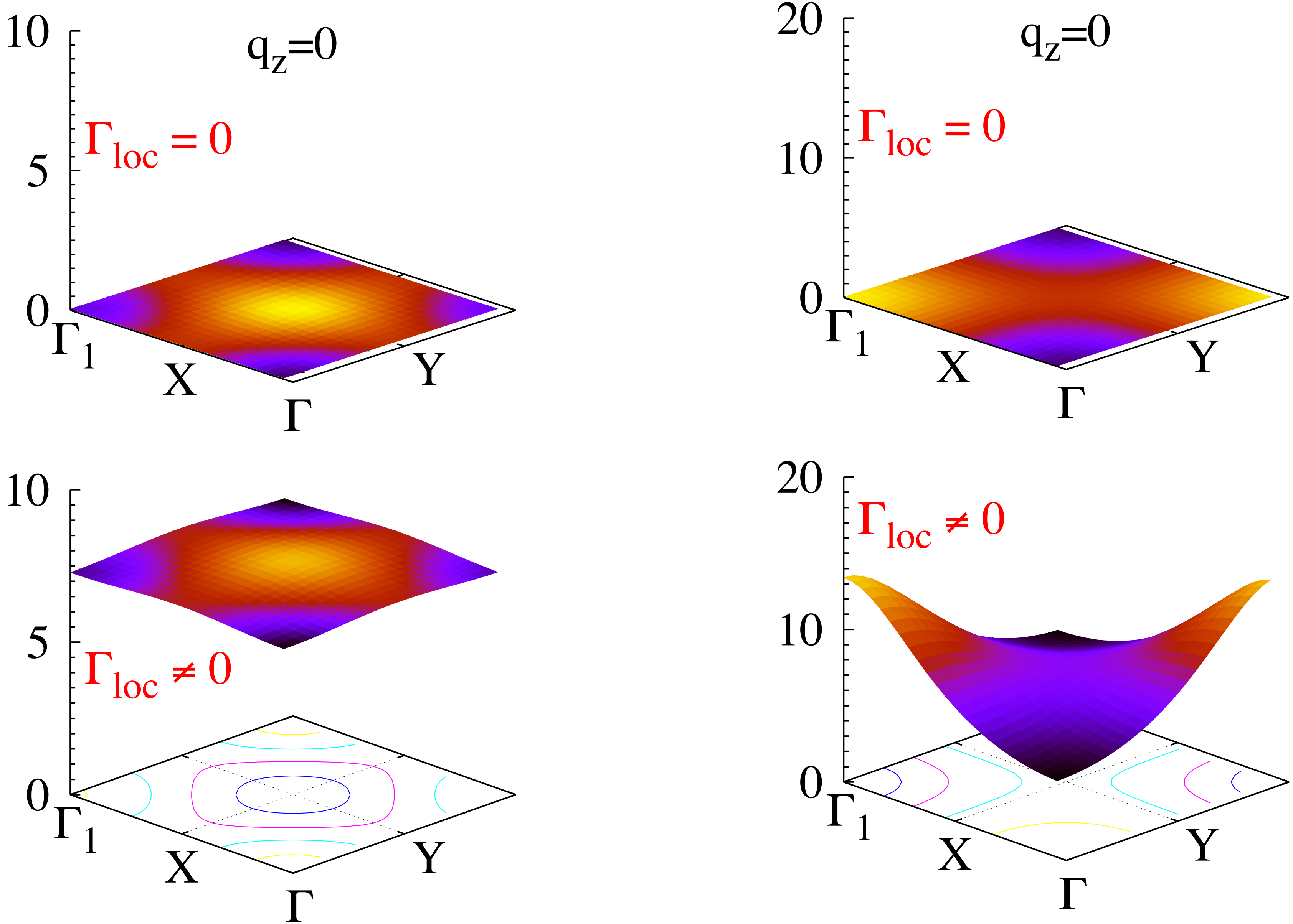
poster Amin Kiani





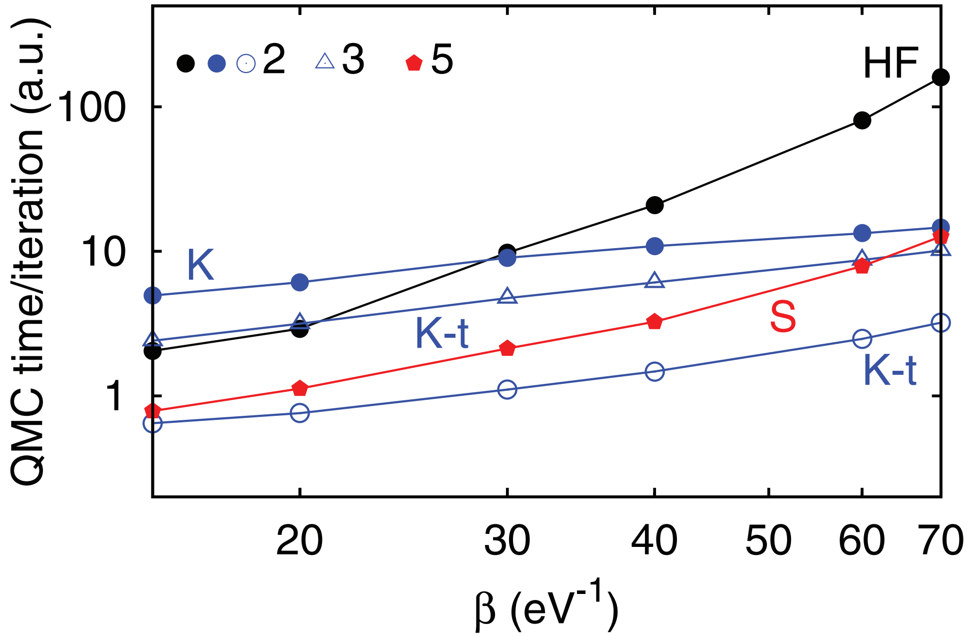
Li_2VOSiO_4 vs $VOMoO_4$

poster Amin Kiani



CT-QMC solver

(performance of our general code on BlueGene)



t_{2g} full self-energy matrix

full Coulomb matrix

can include:

full self-energy matrix in spin-orbital space

full Coulomb matrix

spin-orbit

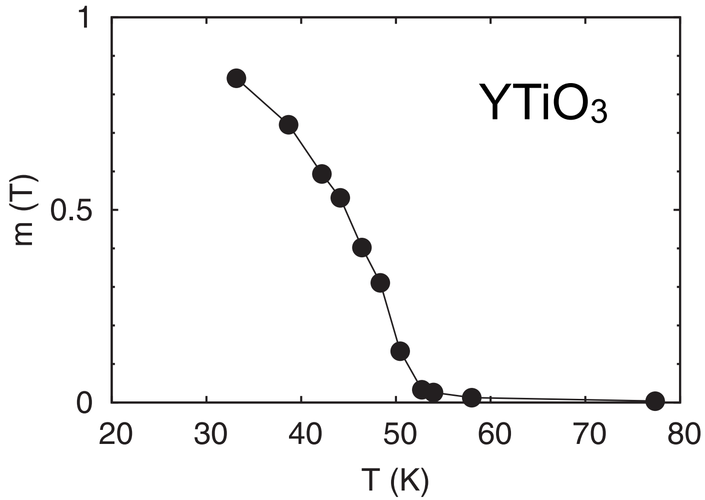


FIG. 3. Ferromagnetic spin polarization as a function of temperature in YTiO$_3$. The plot shows a transition at the critical temperature $T_C \sim 50$ K, slightly overestimating the experimental value $T_C \sim 30$ K, as one might expect from a mean-field calculations.

Phys. Rev. B **87**, 195141

linear-response theory

we need some definitions

a **small** space- and time-dependent perturbation *H_1*

$$\hat{H} \quad \rightarrow \hat{H} + \int d\boldsymbol{r}\, \hat{H}_1(\boldsymbol{r};t) + \ldots$$

$$\hat{H}_1(\boldsymbol{r};t) \quad = -\sum_\nu \hat{O}_\nu(\boldsymbol{r};t) h_\nu(\boldsymbol{r};t),$$

$$\hat{O}_\nu(\boldsymbol{r};t) = e^{i(\hat{H}-\mu\hat{N})t}\hat{O}_\nu(\boldsymbol{r})e^{-i(\hat{H}-\mu\hat{N})t},$$

$$Z = \mathrm{Tr}\, e^{-\beta(\hat{H}-\mu\hat{N})}$$

partition function

$\beta=1/k_BT$

$$\langle\hat{A}\rangle_0 = \frac{1}{Z}\mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\hat{A}\right]$$

expectation value

$$\Delta\hat{A}(\boldsymbol{r};t) = \hat{A}(\boldsymbol{r};t) - \langle\hat{A}(\boldsymbol{r})\rangle_0$$

difference wrt unperturbed equilibrium case

linear response theory

a **small** space- and time-dependent perturbation H_1

$$\begin{aligned}\hat{H} &\to \hat{H} + \int d\boldsymbol{r}\ \hat{H}_1(\boldsymbol{r};t) + \dots \\ \hat{H}_1(\boldsymbol{r};t) &= -\sum_\nu \hat{O}_\nu(\boldsymbol{r};t) h_\nu(\boldsymbol{r};t),\end{aligned}$$

property of the system **external field**

linear effect on some property *P*

$$\langle \hat{P}_\nu(\boldsymbol{r};t)\rangle = \langle \hat{P}_\nu(\boldsymbol{r})\rangle_0 + \langle \delta\hat{P}_\nu(\boldsymbol{r};t)\rangle_0,$$

$$\langle \delta\hat{P}_\nu(\boldsymbol{r};t)\rangle_0 = -i \int d\boldsymbol{r}' \int_{-\infty}^{t} dt' \left\langle \boxed{\left[\Delta\hat{P}_\nu(\boldsymbol{r};t), \Delta\hat{H}_1(\boldsymbol{r}';t')\right]} \right\rangle_0 .$$

term to calculate

linear response function

replacing *H₁* with its expression

$$\langle \delta \hat{P}_\nu(\boldsymbol{r};t)\rangle_0 = i \sum_{\nu'} \int d\boldsymbol{r}' \int_{-\infty}^{t} dt' \left\langle \left[\Delta\hat{P}_\nu(\boldsymbol{r};t), \Delta\hat{O}_{\nu'}(\boldsymbol{r}';t') \right] \right\rangle_0 h_{\nu'}(\boldsymbol{r}';t')$$

linear response

linear response function

$$\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\boldsymbol{r},\boldsymbol{r}';t,t') = i \left\langle \left[\Delta\hat{P}_\nu(\boldsymbol{r};t), \Delta\hat{O}_{\nu'}(\boldsymbol{r}';t') \right] \right\rangle_0 \Theta(t-t')$$

$$\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\boldsymbol{r},\boldsymbol{r}';t,t') \equiv \lim_{h_{\nu'}\to 0} \frac{\partial \langle \hat{P}_\nu(\boldsymbol{r};t)\rangle}{\partial h_{\nu'}(\boldsymbol{r}';t')}.$$

now recognize the correlation function

$$\mathcal{S}_{\hat{P}_\nu \hat{O}_{\nu'}}(\boldsymbol{r},\boldsymbol{r}';t,t') = \langle \Delta\hat{P}_\nu(\boldsymbol{r};t)\Delta\hat{O}_{\nu'}(\boldsymbol{r}';t')\rangle_0$$

..and it is retarded…

a perturbation has only effects **after** it has been switched on

effect perturbation

$$\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\boldsymbol{r}, \boldsymbol{r}'; t, t') = i \left\langle \left[\Delta\hat{P}_\nu(\boldsymbol{r}; t), \Delta\hat{O}_{\nu'}(\boldsymbol{r}'; t') \right] \right\rangle_0 \Theta(t - t').$$

effect only after perturbation

$$\Theta(t - t') = \begin{cases} 1 & \text{if} \quad t - t' > 0 \\ 0 & \text{if} \quad t - t' < 0. \end{cases}$$

Fourier transform

often it is better to work in Fourier space

for system with time and space translation invariance

$$\langle \delta \hat{P}_\nu(\boldsymbol{q};\omega)\rangle_0 = \sum_{\nu'} \chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\boldsymbol{q};\omega) h_{\nu'}(\boldsymbol{q};\omega)$$

ideal crystal

rewrite operators in second quantization

$$\Delta\hat{P}_\nu(\boldsymbol{r}) = \Phi^\dagger(\boldsymbol{r})\Delta\hat{\mathcal{P}}_\nu\,\Phi(\boldsymbol{r})$$

operator

$$\Delta\hat{P}_\nu(\boldsymbol{r}) = \sum_{ii'}\sum_{\alpha\alpha'} \underbrace{\overline{\psi_{i\alpha'}}(\boldsymbol{r})\psi_{i'\alpha}(\boldsymbol{r})}_{\rho^{i,i'}_{\alpha'\alpha}(\boldsymbol{r})}\ \underbrace{c^\dagger_{i\alpha'}\ [\Delta\hat{\mathcal{P}}_\nu]_{\alpha\alpha'}\ c_{i'\alpha}}_{\Delta\hat{\mathcal{P}}^{i,i'}_{\nu,\alpha\alpha'}} = \sum_{ii'}\sum_{\alpha\alpha'} \boxed{\rho^{i,i'}_{\alpha'\alpha}(\boldsymbol{r})}\,\boxed{\Delta\hat{\mathcal{P}}^{i,i'}_{\nu,\alpha\alpha'}}$$

weight

if we use a localized one-electron basis

$$\Delta\hat{P}_\nu(\boldsymbol{r}) \sim \sum_{i}\sum_{\alpha\alpha'} \boxed{\rho^{i,i}_{\alpha'\alpha}(\boldsymbol{r})}\,\Delta\hat{\mathcal{P}}^{i}_{\nu,\alpha\alpha'}$$

example: magnetic susceptibility

$$\hat{M}_z(\boldsymbol{r}) \sim -g\mu_B \sum_i \sum_{m_\alpha m'_\alpha} \rho_{m_\alpha m'_\alpha}(\boldsymbol{r}) \, \frac{1}{2} \sum_{\sigma\sigma'} c^\dagger_{im_\alpha\sigma} \, [\Delta \hat{M}_z]_{\sigma\sigma'} \, c_{im'_\alpha\sigma'},$$

$$[\Delta \hat{M}_z]_{\sigma\sigma'} = \langle \sigma | \hat{\sigma}_z | \sigma' \rangle$$

one-band case, e.g., one-band Hubbard model

$$\langle \delta \hat{M}_z(\boldsymbol{q};\omega)\rangle_0 \sim (g\mu_B)^2 |\rho(\boldsymbol{q})|^2 \sum_{ii'} e^{-i\boldsymbol{q}\cdot(\boldsymbol{T}_i - \boldsymbol{T}_{i'})} \sum_{\sigma\sigma'} \sigma\sigma' \chi^{\sigma\sigma\sigma'\sigma'}_{\hat{S}^i_z \hat{S}^{i'}_z}(\omega) \, h_z(\boldsymbol{q};\omega)$$

$$= (g\mu_B)^2 |\boxed{\rho(\boldsymbol{q})}|^2 \boxed{\chi_{\hat{S}_z\hat{S}_z}(\boldsymbol{q};\omega)} \boxed{h_z(\boldsymbol{q};\omega),}$$

magnetic field

example: magnetic susceptibility

system with partially filled 3d shells, i.e., localized magnetic moments

$$\langle \delta \hat{M}_z(\boldsymbol{q};\omega)\rangle_0 \sim (g\mu_B)^2 |\rho_s(\boldsymbol{q})|^2 \sum_{ii'} e^{-i\boldsymbol{q}\cdot(\boldsymbol{T}_i - \boldsymbol{T}_{i'})} \sum_{\sigma\sigma'} \sigma\sigma' \chi^{\sigma\sigma\sigma'\sigma'}_{\hat{S}^i_z \hat{S}^{i'}_z}(\omega) h_z(\boldsymbol{q};\omega)$$

$$= (g\mu_B)^2 |\boxed{\rho_s(\boldsymbol{q})}|^2 \boxed{\chi_{\hat{S}_z\hat{S}_z}(\boldsymbol{q};\omega)} h_z(\boldsymbol{q};\omega).$$

atomic form factor (neutron scattering)	spin susceptibility

question: where do localized magnetic moments come from ?

$$\chi_{\hat{S}_z\hat{S}_z}(\boldsymbol{q};\omega) = i \int dt\; e^{i\omega t} \boxed{\left\langle \left[\hat{S}_z(\boldsymbol{q};t), \hat{S}_z(-\boldsymbol{q};0) \right] \right\rangle_0} \Theta(t).$$

localized magnetic moments

atomic physics (+ crystal field)

more details: see, e.g., my lecture of last year

many electron atoms

$$H_e^{\mathrm{NR}} = -\frac{1}{2}\sum_i \nabla_i^2 - \sum_i \frac{Z}{r_i} + \sum_{i>j} \frac{1}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}$$

one shell, 2nd quantization

$$H_e^{\mathrm{NR}} = \varepsilon_{nl} \sum_{m\sigma} c^\dagger_{m\sigma} c_{m\sigma} + \frac{1}{2}\sum_{\sigma\sigma'} \sum_{m\tilde{m}m'\tilde{m}'} U^l_{mm'\tilde{m}\tilde{m}'} c^\dagger_{m\sigma} c^\dagger_{m'\sigma'} c_{\tilde{m}'\sigma'} c_{\tilde{m}\sigma}$$

kinetic+central potential

Coulomb interaction

$$U^{iji'j'}_{mm'\tilde{m}\tilde{m}'} = \int d\boldsymbol{r}_1 \int d\boldsymbol{r}_2 \, \frac{\overline{\psi_{im\sigma}}(\boldsymbol{r}_1)\overline{\psi_{jm'\sigma'}}(\boldsymbol{r}_2)\psi_{j'\tilde{m}'\sigma'}(\boldsymbol{r}_2)\psi_{i'\tilde{m}\sigma}(\boldsymbol{r}_1)}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|}$$

many electron atoms

does the atom/ion carry a magnetic moment?

total spin **S** and total angular momentum **L**

filled shells

S=L=0

partially filled shell: **magnetic ions**

1. Hund's rule max S

origin: Coulomb repulsion

direct term: the same for all N electron states

$$U_{\rm avg} = \frac{1}{(2l+1)^2} \sum_{mm'} U^l_{mm'mm'}$$

exchange term: 1. Hund's rule

$$U_{\rm avg} - J_{\rm avg} = \frac{1}{2l(2l+1)} \sum_{mm'} \left(U^l_{mm'mm'} - U^l_{mm'm'm}\right)$$

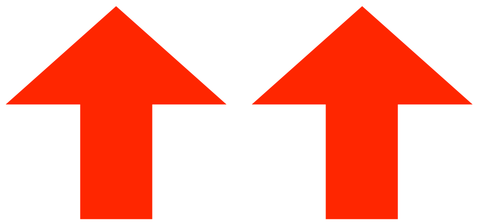
Coulomb exchange

C atom, p shell

$$
\begin{aligned}
J^p_{m,m'} &= U^p_{mm'm'm} \\
&= \int d\boldsymbol{r}_1 \int d\boldsymbol{r}_2 \, \frac{\overline{\psi_{im\sigma}}(\boldsymbol{r}_1)\overline{\psi_{im'\sigma}}(\boldsymbol{r}_2)\psi_{im\sigma}(\boldsymbol{r}_2)\psi_{im'\sigma}(\boldsymbol{r}_1)}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|} \\
&= \int d\boldsymbol{r}_1 \int d\boldsymbol{r}_2 \, \frac{\phi_{imm'\sigma}(\boldsymbol{r}_1)\overline{\phi_{imm'\sigma}}(\boldsymbol{r}_2)}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|} = \frac{1}{V}\sum_{\boldsymbol{k}} \frac{4\pi}{k^2} \left|\phi_{imm'\sigma}(\boldsymbol{k})\right|^2 ,
\end{aligned}
$$

positive, hence ferromagnetic

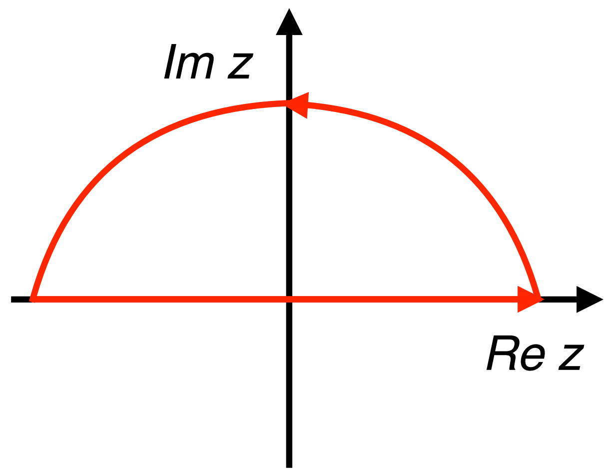
$$
-\frac{1}{2}\sum_{\sigma}\sum_{m\neq m'} J^p_{m,m'} c^\dagger_{m\sigma} c_{m\sigma} c^\dagger_{m'\sigma} c_{m'\sigma} = -\frac{1}{2}\sum_{m\neq m'} 2J^p_{m,m'}\left[S^m_z S^{m'}_z + \frac{1}{4} n_m n'_m\right]
$$



analytic properties of $X(\boldsymbol{q};\omega)$

$\{\Psi_n^N\}$ *N*: number of electrons

n: eigenvalue



$$
\begin{aligned}
P_\nu^{nm}(\boldsymbol{q}) &= \langle \Psi_n^N | \Delta\hat{P}_\nu(\boldsymbol{q};0)|\Psi_m^N\rangle, \\
O_{\nu'}^{mn}(\boldsymbol{q}) &= \langle \Psi_m^N | \Delta\hat{O}_{\nu'}(\boldsymbol{q};0)|\Psi_n^N\rangle
\end{aligned}
$$

$$
\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\boldsymbol{q};\omega) = \frac{1}{Z}\sum_{nm}\frac{e^{-\beta(E_n^N-\mu N)} - e^{-\beta(E_m^N-\mu N)}}{E_m^N - E_n^N - \omega - i\delta} P_\nu^{nm}(\boldsymbol{q}) O_{\nu'}^{mn}(-\boldsymbol{q})
$$

δ>0 analytic in the upper part of the complex plane

Hermitian operators

if the operators are Hermitian

symmetry properties

$$\mathrm{Re}\left[\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\boldsymbol{q};\omega)\right] = \mathrm{Re}\left[\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(-\boldsymbol{q};-\omega)\right],$$

even

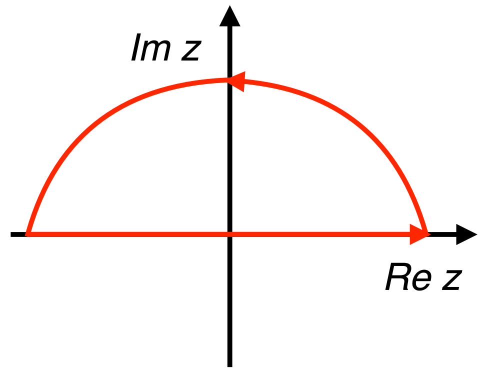
$$\mathrm{Im}\left[\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\boldsymbol{q};\omega)\right] = -\mathrm{Im}\left[\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(-\boldsymbol{q};-\omega)\right].$$

odd

Kramers-Kronig relations

analytic function in upper part complex plane + fast decaying

$$I_{\mathcal{C}} = \oint_{\mathcal{C}} \frac{\chi(\boldsymbol{q}; z)}{z - \omega + i\,\delta}\, dz = 0$$



$$\mathrm{Re}\,[\chi(\boldsymbol{q};\omega)] - \mathrm{Re}\,[\chi(\boldsymbol{q};\infty)] \quad = \quad \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{+\infty} \frac{\mathrm{Im}\,[\chi(\boldsymbol{q};\omega')]}{\omega' - \omega} d\omega',$$

$$\mathrm{Im}\,[\chi(\boldsymbol{q};\omega)] \quad = \quad -\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{+\infty} \frac{\mathrm{Re}\,[\chi(\boldsymbol{q};\omega')] - \mathrm{Re}\,[\chi(\boldsymbol{q};\infty)]}{\omega' - \omega} d\omega'.$$

thermodynamic sum-rule

let us take the static (ω=0) limit

$$\mathrm{Re}\left[\chi(\boldsymbol{q};\omega=0)\right]-\mathrm{Re}\left[\chi(\boldsymbol{q};\infty)\right]=\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{+\infty}\frac{\mathrm{Im}\left[\chi(\boldsymbol{q};\omega')\right]}{\omega'}d\omega'$$

let us take in addition the uniform (***q***=0) limit

$$\chi_{\nu\nu'}(\mathbf{0};0)=\lim_{h_{\nu'}\to 0}\frac{\partial\langle P_\nu\rangle}{\partial h_{\nu'}}$$

response to a uniform and static perturbation

Thomas-Reich-Kuhn sum-rule

if O $\propto$ P$^+$

$$\frac{2}{\pi}\int_0^\infty \omega\,\mathrm{Im}\left[\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\boldsymbol{q};\omega)\right] d\omega = \left\langle \left[[\hat{P}_\nu, \hat{H}], \hat{O}_{\nu'} \right] \right\rangle_0$$

to proof it use a complete basis of eigenvectors
+ invariance of trace under cyclic permutations

also known as *f*-sum rule

detailed-balance

$$\mathcal{S}_{\hat{P}_\nu \hat{O}_{\nu'}}(\boldsymbol{q};t) = \Big\langle \Delta\hat{P}_\nu(\boldsymbol{q};t)\Delta\hat{O}_{\nu'}(-\boldsymbol{q}) \Big\rangle_0$$

$$\begin{aligned}
\mathcal{S}_{\hat{P}_\nu \hat{O}_{\nu'}}(\boldsymbol{q};\omega) &= \int_{-\infty}^{\infty} dt\, e^{i\omega t} \langle \Delta\hat{P}_\nu(\boldsymbol{q};t)\Delta\hat{O}_{\nu'}(-\boldsymbol{q};0)\rangle_0 \\
&= \frac{1}{Z}\sum_{nm}\int_{-\infty}^{\infty} dt\, e^{i(\omega+E_n^N-E_m^N)t} e^{-\beta(E_n^N-\mu N)} P_\nu^{nm}(\boldsymbol{q}) O_{\nu'}^{mn}(-\boldsymbol{q}) \\
&= \frac{2\pi}{Z}\sum_{nm} e^{-\beta(E_n^N-\mu N)} \boxed{P_\nu^{nm}(\boldsymbol{q}) O_{\nu'}^{mn}(-\boldsymbol{q})\ \delta(\omega - E_m^N + E_n^N)}
\end{aligned}$$

if O ∝ P⁺

Fermi's golden rule

$$\begin{aligned}
P_\nu^{nm}(\boldsymbol{q}) &= \langle \Psi_n^N | \Delta\hat{P}_\nu(\boldsymbol{q};0) | \Psi_m^N \rangle, \\
O_{\nu'}^{mn}(\boldsymbol{q}) &= \langle \Psi_m^N | \Delta\hat{O}_{\nu'}(\boldsymbol{q};0) | \Psi_n^N \rangle
\end{aligned}$$

detailed-balance

exchanging the operators and then *n* and *m*

$$\mathcal{S}_{\hat{O}_{\nu'}, \hat{P}_{\nu}}(\boldsymbol{q};\omega) = \frac{2\pi}{Z} \sum_{nm} e^{-\beta(E_m^N - \mu N)} P_{\nu}^{nm}(-\boldsymbol{q}) O_{\nu'}^{mn}(\boldsymbol{q}) \delta(\omega - E_n^N + E_m^N)$$

$$\mathcal{S}_{\hat{O}_{\nu'}, \hat{P}_{\nu}}(-\boldsymbol{q};-\omega) = e^{-\beta\omega} \mathcal{S}_{\hat{P}_{\nu}, \hat{O}_{\nu'}}(\boldsymbol{q};\omega)$$

The relation above can be understood as follows. If $\omega > 0$, the correlation function $\mathcal{S}_{\hat{P}_{\nu}, \hat{O}_{\nu'}}(\boldsymbol{q};\omega)$ describes the probability $P_{n \to m} \propto n(E_n)[1 - n(E_m)]$ that the system is excited from an initial state with energy E_n to a final state with higher energy $E_m = E_n + \omega$. Instead, $\mathcal{S}_{\hat{P}_{\nu}, \hat{O}_{\nu'}}(-\boldsymbol{q};-\omega)$, describes the probability $P_{m \to n} \propto n(E_m)[1 - n(E_n)]$ that the system goes from the initial state with energy E_m to a final state with lower energy $E_n = E_m - \omega$. The probability $P_{m \to n}$ is lower than $P_{n \to m}$ by the factor $e^{-\beta\omega}$.

fluctuation-dissipation theorem

if O ∝ P⁺

$$\mathcal{S}_{\hat{P}_\nu \hat{O}_{\nu'}}(\boldsymbol{q};\omega) = 2(1+n_B)\mathrm{Im}[\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\boldsymbol{q};\omega)], \qquad n_B(\omega) = \frac{1}{e^{\beta\omega}-1}$$

correlation function

imaginary part of the linear response function

Bose-Einstein dispersion

large temperature limit

$$\mathrm{Re}[\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\boldsymbol{q};\omega=0)] - \mathrm{Re}[\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\boldsymbol{q};\infty)] \sim \frac{1}{k_B T}\mathcal{S}_{\hat{P}_\nu \hat{O}_{\nu'}}(\boldsymbol{q};t=0)$$

Green functions

single-particle Green functions

temperature Green function

for a consistent perturbation theory at finite temperature

$$G_{\alpha\alpha'}(\boldsymbol{\tau}) = -\langle \mathcal{T} c_\alpha(\tau_1) c^\dagger_{\alpha'}(\tau_2)\rangle_0 = -\frac{1}{Z}\mathrm{Tr}\,\left[e^{-\beta(\hat{H}-\mu\hat{N})}\mathcal{T} c_\alpha(\tau_1) c^\dagger_{\alpha'}(\tau_2)\right]$$

$$0 < \tau_i < \beta \qquad\qquad o(\tau) = e^{\tau(\hat{H}-\mu\hat{N})}o\, e^{-\tau(\hat{H}-\mu\hat{N})}$$

invariance of trance under **cyclic** permutations of operators

$$G_{\alpha\alpha'}(\boldsymbol{\tau}) = \boxed{G_{\alpha\alpha'}(\tau_1-\tau_2)}$$

only **one** independent imaginary time variable

temperature Green function

using a full basis set

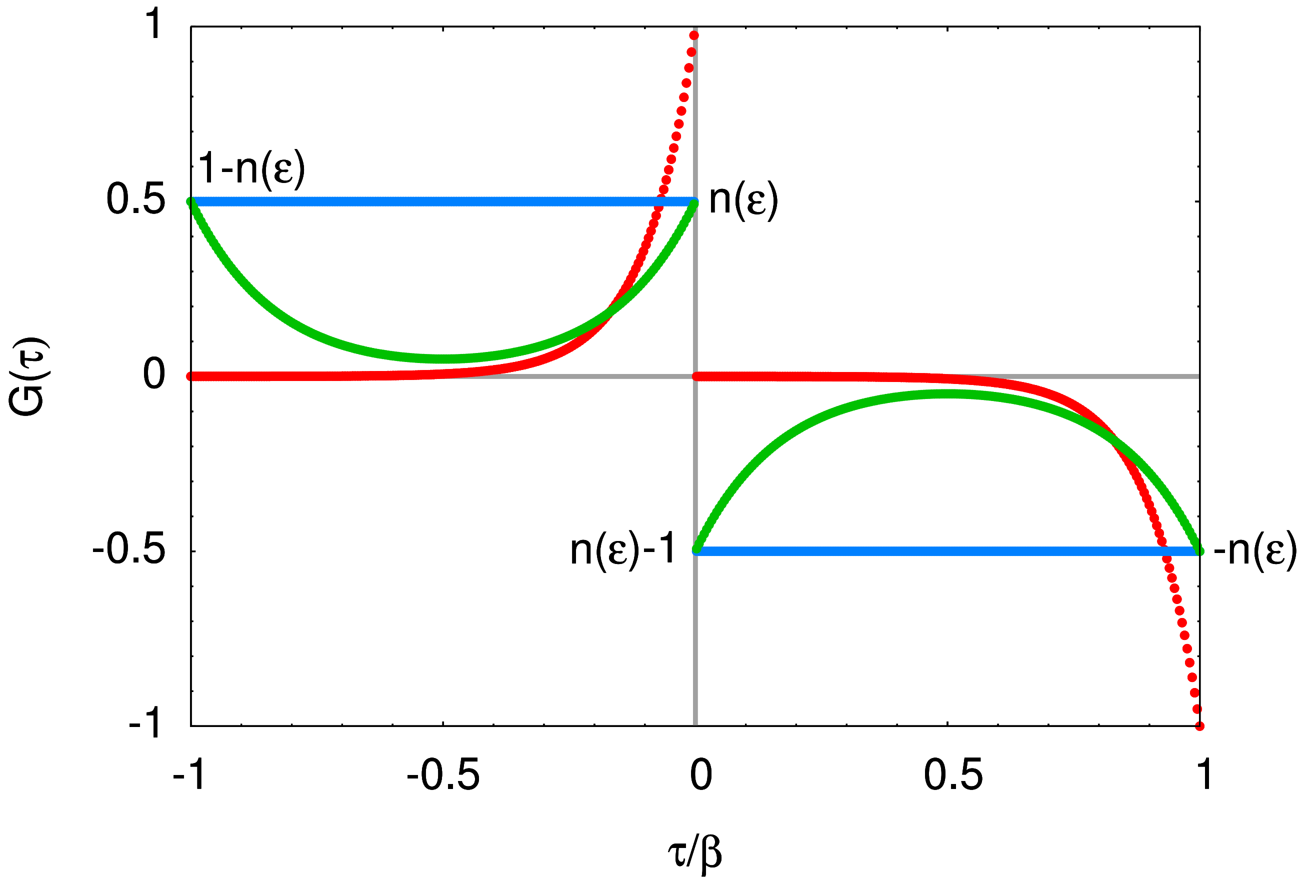
$$\boxed{G_{\alpha\alpha'}(\tau)} = \frac{1}{Z}\sum_{Nnm} \langle \Psi_n^N | c_\alpha | \Psi_m^{N+1}\rangle \langle \Psi_m^{N+1} | c_{\alpha'}^\dagger | \Psi_n^N \rangle e^{-\beta(E_n^N-\mu N)} \begin{cases} -e^{(E_n^N - E_m^{N+1}+\mu)\tau} & \tau > 0 \\ e^{-(E_n^N - E_m^{N+1}+\mu)(-\beta-\tau)} & \tau < 0 \end{cases}$$

only well defined in the interval

$$-\beta < \tau < \beta$$

and how does it look like?

anti-periodic



we can define it everywhere as

$$\tilde{G}_{\alpha\alpha'}(\tau_1 \pm n_1\beta, \tau_2 \pm n_2\beta) \equiv (-1)^{n_1+n_2} G_{\alpha\alpha'}(\tau_1, \tau_2)$$

temperature Green function

let us make it periodic with period 2β

Fourier transform

$$G_{\alpha\alpha'}(\tau) = \frac{1}{\beta}\sum_{n=-\infty}^{+\infty} e^{-i\nu_n\tau} G_{\alpha\alpha'}(i\nu_n),$$

ν_n are fermionic Matsubara frequencies

i.e., the poles of the Fermi distribution function

$$\nu_n = \pi(2n+1)/\beta$$

Fourier coefficients

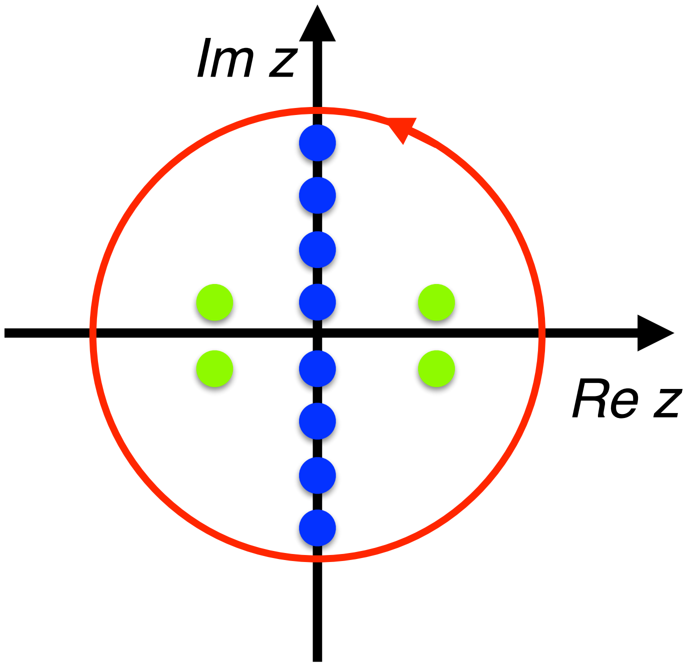
$$G_{\alpha\alpha'}(i\nu_n) = \frac{1}{2}\int_{-\beta}^{\beta} d\tau e^{i\nu_n\tau} G_{\alpha\alpha'}(\tau) = \frac{1}{2}(1-e^{-i\nu_n\beta})\int_0^{\beta} d\tau e^{i\nu_n\tau} G_{\alpha\alpha'}(\tau) = \int_0^{\beta} d\tau e^{i\nu_n\tau} G_{\alpha\alpha'}(\tau)$$

sums over Matsubara frequencies

often we have to calculate Matsubara sums

$$\sum_n f(i\nu_n)$$

how do we do this?



some of the poles of the Fermi function

possible poles of the *F* function

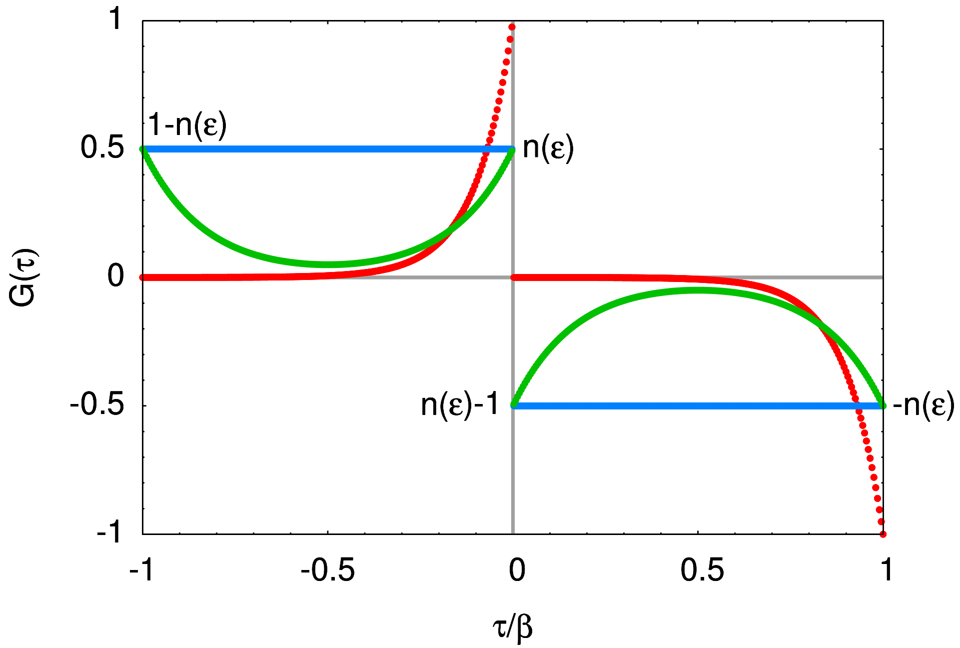
F function   Fermi function

$$I_{\mathcal{C}} = \frac{1}{2\pi i} \oint_{\mathcal{C}} \mathcal{F}_{\boldsymbol{k}\sigma}(z) n_\sigma(z) e^{z\tau} dz$$

if *F* decays fast enough, using Cauchy integral theorem

$$\frac{1}{\beta} \sum_n e^{i\nu_n \tau} \mathcal{F}_{\boldsymbol{k}\sigma}(i\nu_n) = \sum_{z_p} \mathrm{Res}\ \left[\mathcal{F}_{\boldsymbol{k}\sigma}(z_p)\right] n_\sigma(z_p) e^{z_p \tau}$$

examples



$$\frac{1}{\beta}\sum_n e^{-i\nu_n 0^-}\mathcal{G}_{\boldsymbol{k}\sigma}(i\nu_n) = \mathcal{G}_{\boldsymbol{k}\sigma}(0^-) = n_\sigma(\varepsilon_{\boldsymbol{k}}),$$

$$\frac{1}{\beta}\sum_n e^{-i\nu_n 0^+}\mathcal{G}_{\boldsymbol{k}\sigma}(i\nu_n) = \mathcal{G}_{\boldsymbol{k}\sigma}(0^+) = n_\sigma(\varepsilon_{\boldsymbol{k}}) - 1.$$

most common Matsubara FT

$g_\alpha(\nu_n;x,y)$	$g_\alpha(\tau;x,y)=\frac{1}{\beta}\sum_n e^{-i\nu_n\tau}g_\alpha(\nu_n;x,y)$
$g_a(\nu_n;x,y)=[i\nu_n-x]^{-1}$	$[n_\sigma(x)-1]e^{-x\tau}$
$g_b(\nu_n;x,y)=[i\nu_n-x]^{-2}$	$n_\sigma(x)(\tau-\beta n_\sigma(x))e^{-x(\tau-\beta)}$
$g_c(\nu_n;x,y)=[i\nu_n-x]^{-1}[i\nu_n-y]^{-1}$	$-\left[e^{-x(\tau-\beta)}n_\sigma(x)-e^{-y(\tau-\beta)}n_\sigma(y)\right][x-y]^{-1}$
$g_d(\nu_n;x,y)=[i\nu_n-x]^{-1}[i\nu_n+x]^{-1}$	$[g_a(\tau;x,y)-g_a(\tau;-x,y)]/2x$

Table 1: *Some of the most common Matsubara Fourier transforms (fermionic case). The function $n_\sigma(x)$ is the Fermi-Dirac distribution function $n_\sigma(x)=1/(1+e^{x\beta})$. The parameters x and y are real numbers. For τ we consider the interval $(0,\beta)$.*

two-particle Green-functions

two-particle Green-functions

$$\chi^{\alpha\alpha'}_{\gamma\gamma'}(\boldsymbol{\tau}) = \langle \mathcal{T} \Delta\hat{P}_{\alpha\alpha'}(\tau_1,\tau_2)\Delta\hat{O}_{\gamma\gamma'}(\tau_3,\tau_4)\rangle$$

$$\Delta\hat{P}_{\alpha\alpha'}(\tau_1,\tau_2) = c^\dagger_{\alpha'}(\tau_2)c_\alpha(\tau_1) - \langle \mathcal{T} c^\dagger_{\alpha'}(\tau_2)c_\alpha(\tau_1)\rangle,$$
$$\Delta\hat{O}_{\gamma\gamma'}(\tau_3,\tau_4) = c^\dagger_{\gamma'}(\tau_4)c_\gamma(\tau_3) - \langle \mathcal{T} c^\dagger_{\gamma'}(\tau_4)c_\gamma(\tau_3)\rangle.$$

three independent variables

$$\chi^{\alpha\alpha'}_{\gamma\gamma'}(\boldsymbol{\tau}) = \chi^{\alpha\alpha'}_{\gamma\gamma'}(\tau_{14},\tau_{24},\tau_{34},0)$$

(we can also choose τ_{12} τ_{34} τ_{23})

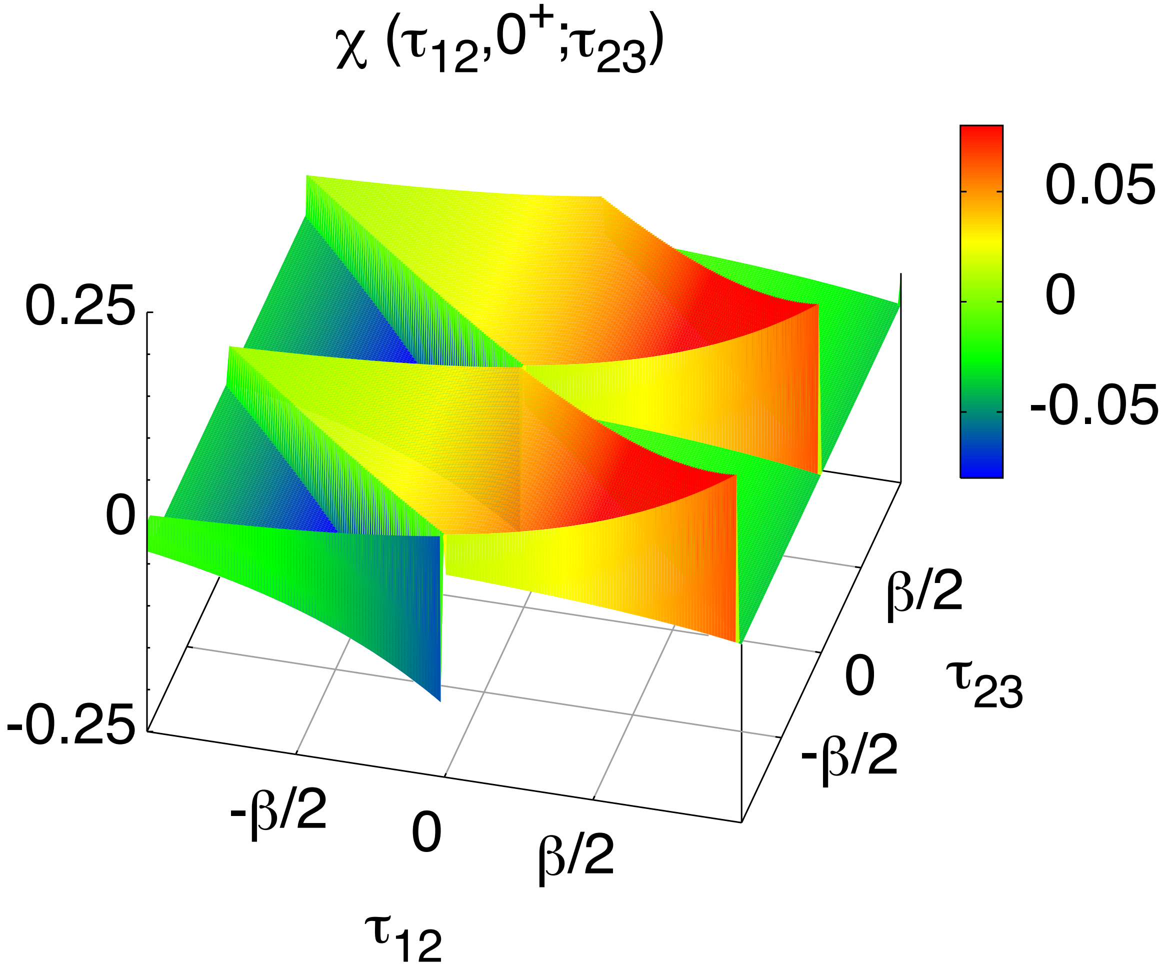
anti-periodicity

$$\chi^{\alpha\alpha'}_{\gamma\gamma'}(\tau_{14}+\beta,\tau_{24},\tau_{34},0) = -\chi^{\alpha\alpha'}_{\gamma\gamma'}(\tau_{14},\tau_{24},\tau_{34},0),$$

non-interacting example

Wick's theorem

$$\chi(\tau_{12}, 0^+; \tau_{23}) = -G_{\alpha\alpha}(\tau_{12} + \tau_{23} + 0^+)G_{\alpha\alpha}(-\tau_{23})$$



Matsubara Fourier transform

$$\chi_{\gamma\gamma'}^{\alpha\alpha'}(\boldsymbol{\nu}) = \frac{1}{16} \iiiint d\boldsymbol{\tau}\; e^{i\boldsymbol{\nu}\cdot\boldsymbol{\tau}} \chi_{\gamma\gamma'}^{\alpha\alpha'}(\boldsymbol{\tau})$$

$$\boldsymbol{\nu} = (\nu_1, \nu_2, \nu_3, \nu_4)$$

energy conservation

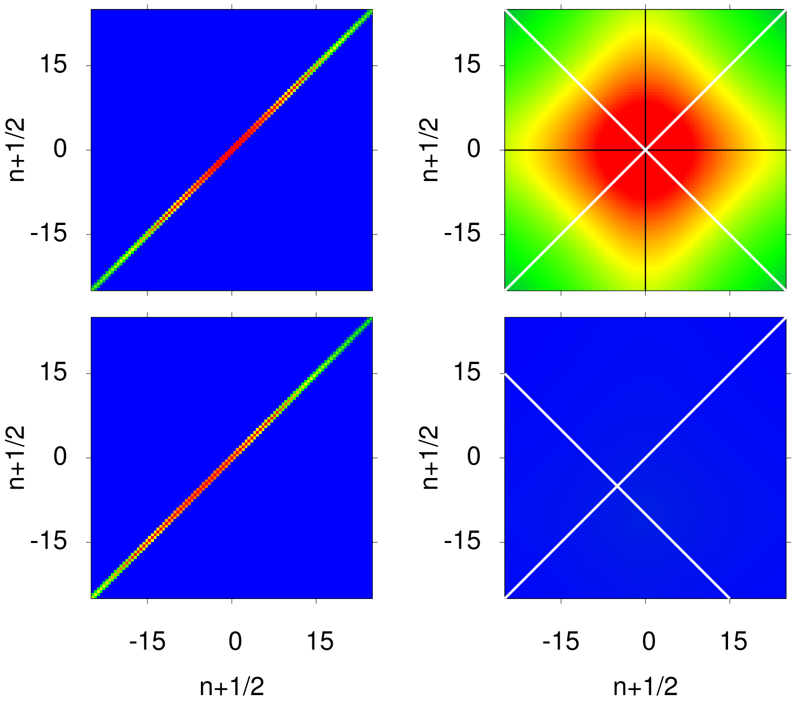
$$\boldsymbol{\nu} = (\nu_n, -\nu_n - \omega_m, \nu_{n'} + \omega_m, -\nu_{n'})$$

ω_m Bosonic frequency

symmetry lines

$$\chi^{\alpha\alpha'\gamma\gamma'}_{n,n'}(i\omega_m) = \chi^{\gamma'\gamma\alpha'\alpha}_{n',n}(i\omega_m)$$

$$\left|\chi^{\alpha\alpha'\alpha'\alpha}_{n,n'}(i\omega_m)\right| = \left|\chi^{\alpha\alpha'\alpha'\alpha}_{n',n}(i\omega_m)\right|.$$



non-interacting case

$$\chi^{\alpha\alpha'}_{\gamma\gamma'}(\boldsymbol{\tau}) = -G_{\alpha\gamma'}(\tau_{14})G_{\gamma\alpha'}(-\tau_{23})$$

from the two-particle Green-function to the susceptibility

generalized susceptibility

$$\chi_{\hat{P}^i_\nu\ \hat{O}^{i'}_{\nu'}}(\boldsymbol{\tau}) \quad = \quad \langle \mathcal{T} \Delta \hat{P}^i_\nu(\tau_1,\tau_2) \Delta \hat{O}^{i'}_{\nu'}(\tau_3,\tau_4) \rangle_0,$$

$$\hat{P}^i_\nu(\tau_1,\tau_2) \quad = \quad \sum_{\boldsymbol{\alpha}} p^\nu_{\boldsymbol{\alpha}}\, c^\dagger_{i\alpha'}(\tau_2) c_{i\alpha}(\tau_1),$$

$$\hat{O}^{i'}_{\nu'}(\tau_3,\tau_4) \quad = \quad \sum_{\boldsymbol{\gamma}} o^{\nu'}_{\boldsymbol{\gamma}}\, c^\dagger_{i'\gamma'}(\tau_4) c_{i'\gamma}(\tau_3).$$

$$v_{\boldsymbol{\alpha\gamma}} = p^\nu_{\boldsymbol{\alpha}} o^{\nu'}_{\boldsymbol{\gamma}}$$

numbers

two-particle Green function tensor

$$\chi_{\hat{P}^i_\nu\ \hat{O}^{i'}_{\nu'}}(\boldsymbol{\tau}) = \sum_{\boldsymbol{\alpha\gamma}} v_{\boldsymbol{\alpha\gamma}}\, \chi^{\boldsymbol{\alpha}_i}_{\boldsymbol{\gamma}_{i'}}(\boldsymbol{\tau}),$$

generalized susceptibility

real space   **k** space

$$\chi(\boldsymbol{q};\boldsymbol{\nu}) = \sum_{\boldsymbol{\alpha\gamma}} v_{\boldsymbol{\alpha\gamma}} \sum_{ii'} e^{i(\boldsymbol{T}_i-\boldsymbol{T}_{i'})\cdot\boldsymbol{q}} \chi^{\boldsymbol{\alpha}_i}_{\boldsymbol{\gamma}_{i'}}(\boldsymbol{\nu}) = \sum_{\boldsymbol{\alpha\gamma}} v_{\boldsymbol{\alpha\gamma}} \frac{1}{N_{\boldsymbol{k}}^2} \sum_{\boldsymbol{kk'}} \chi^{\boldsymbol{\alpha_k}}_{\boldsymbol{\gamma_{k'}}}(\boldsymbol{\nu})$$

$$= \sum_{\boldsymbol{\alpha\gamma}} v_{\boldsymbol{\alpha\gamma}} \left[\chi(\boldsymbol{q};i\omega_m)\right]_{L_\alpha,L_\gamma},$$

$$\chi_{\hat{P}_\nu\hat{O}_{\nu'}}(\boldsymbol{q};i\omega_m) = \sum_{\boldsymbol{\alpha\gamma}} v_{\boldsymbol{\alpha\gamma}} \frac{1}{\beta^2} \sum_{nn'} \left[\chi(\boldsymbol{q};\omega_m)\right]_{L_\alpha,L_\gamma}$$

matrix *L x L* $L_\alpha = n \times \alpha$

n: fermionic Matsubara frequencies

α: flavors

magnetic susceptibility

$$\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\boldsymbol{q}; i\omega_m) = \sum_{\boldsymbol{\alpha\gamma}} v_{\boldsymbol{\alpha\gamma}} \frac{1}{\beta^2} \sum_{nn'} [\chi(\boldsymbol{q}; \omega_m)]_{L_\alpha, L_\gamma} .$$

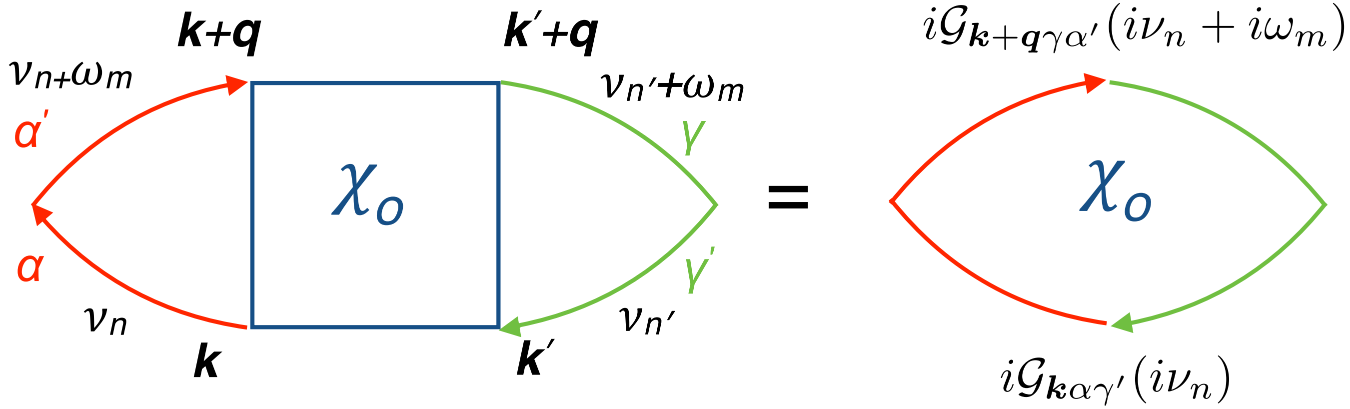
$$v_{\boldsymbol{\alpha\gamma}} = p^{\nu}_{\boldsymbol{\alpha}} o^{\nu'}_{\boldsymbol{\gamma}}$$

$$o^z_{\boldsymbol{\alpha}} = -g\mu_B \langle \sigma | \hat{\sigma}_z | \sigma \rangle, \qquad p^z_{\boldsymbol{\alpha}} = -g\mu_B \langle \sigma' | \hat{\sigma}_z | \sigma' \rangle,$$

the prefactor determines the type of response

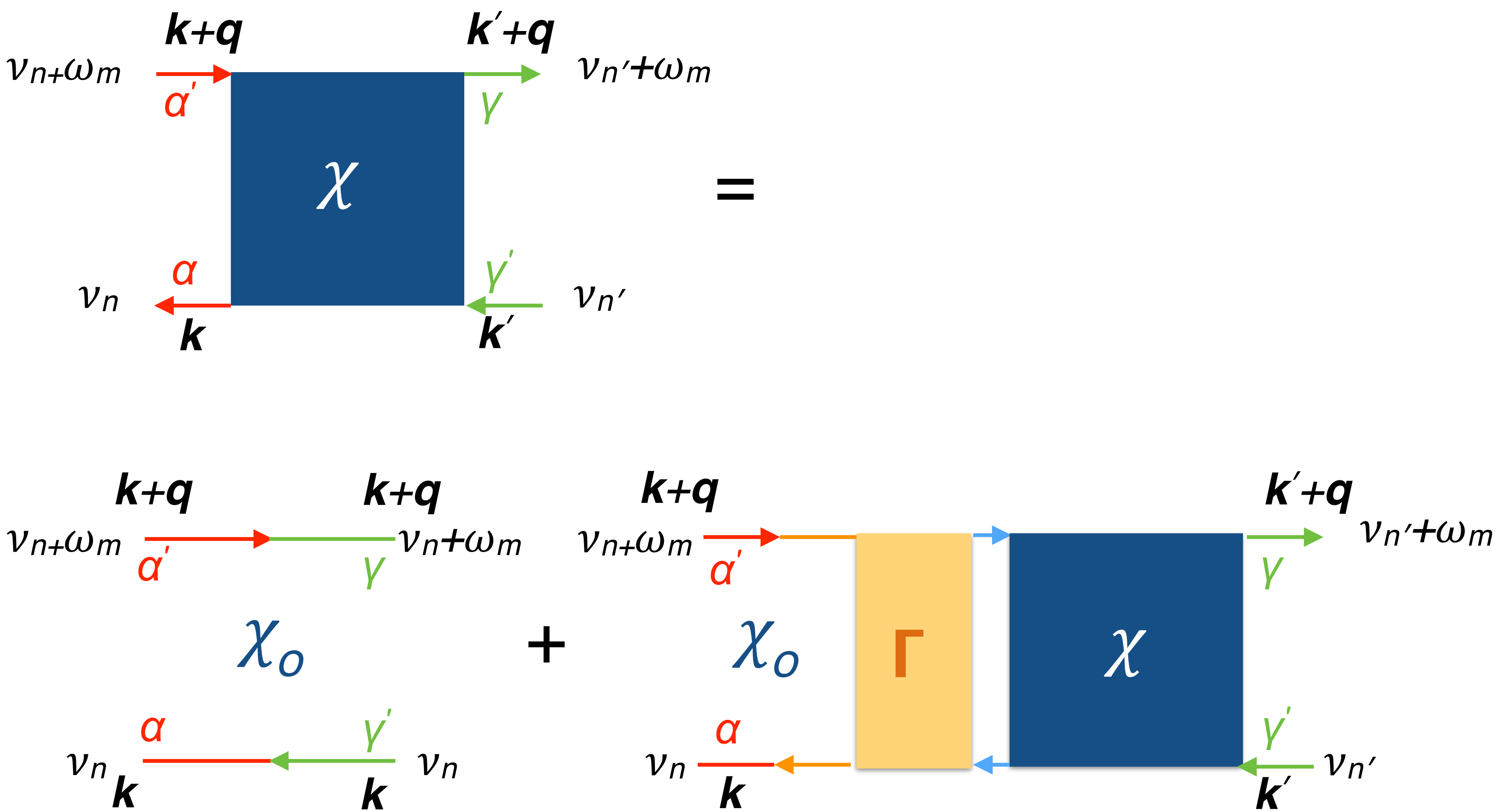
non-interacting case

Wick's theorem holds



$$[\chi_0(\boldsymbol{q};i\omega_m)]_{\boldsymbol{k}L_\alpha,\boldsymbol{k}'L_\gamma} \quad = \quad -\beta N_{\boldsymbol{k}}\mathcal{G}_{\boldsymbol{k}\alpha\gamma'}(i\nu_n)\mathcal{G}_{\boldsymbol{k}'+\boldsymbol{q}\alpha'\gamma}(i\nu_{n'}+i\omega_m)\delta_{n,n'}\delta_{\boldsymbol{k},\boldsymbol{k}'}$$

Bethe-Salpeter equation



one-band Hubbard model

magnetic response

the one-band Hubbard model

$$\hat{H}_{\text{Hubbard}} = \underbrace{-\sum_{ii'}\sum_{\sigma} t_{1,1}^{i,i'} c^{\dagger}_{i\sigma} c_{i'\sigma}}_{\hat{H}_0} \underbrace{+\, \varepsilon_d \sum_{i\sigma} n_{i\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}}_{\hat{H}_U}$$

$$\left\{ \begin{array}{ccc} \varepsilon_d & = & -t_{1,1}^{i,i} \\ t & = & t_{1,1}^{\langle i,i' \rangle} \\ U & = & U_{1111}^{iiii} \end{array} \right.$$

half filling

t=0: N_s atoms, insulator

U=0: half-filled band, metal

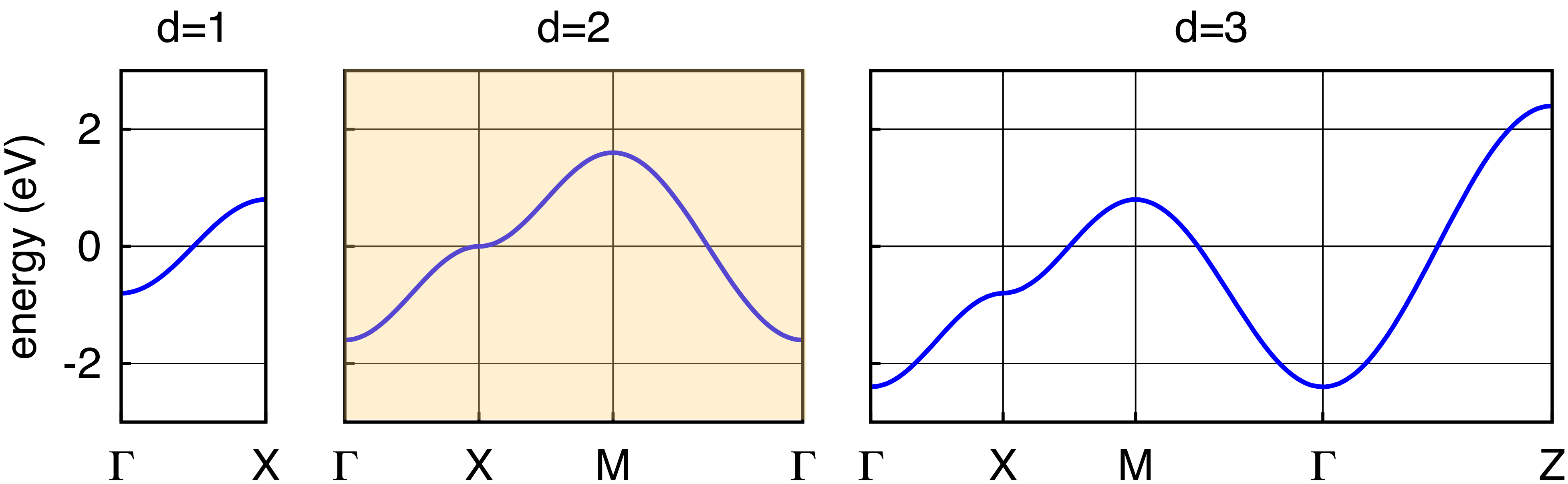
the U=0 limit

the U=0 limit

$$H_d + H_T = \sum_{\boldsymbol{k}} \sum_{\sigma} [\varepsilon_d + \varepsilon_{\boldsymbol{k}}] c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma}$$

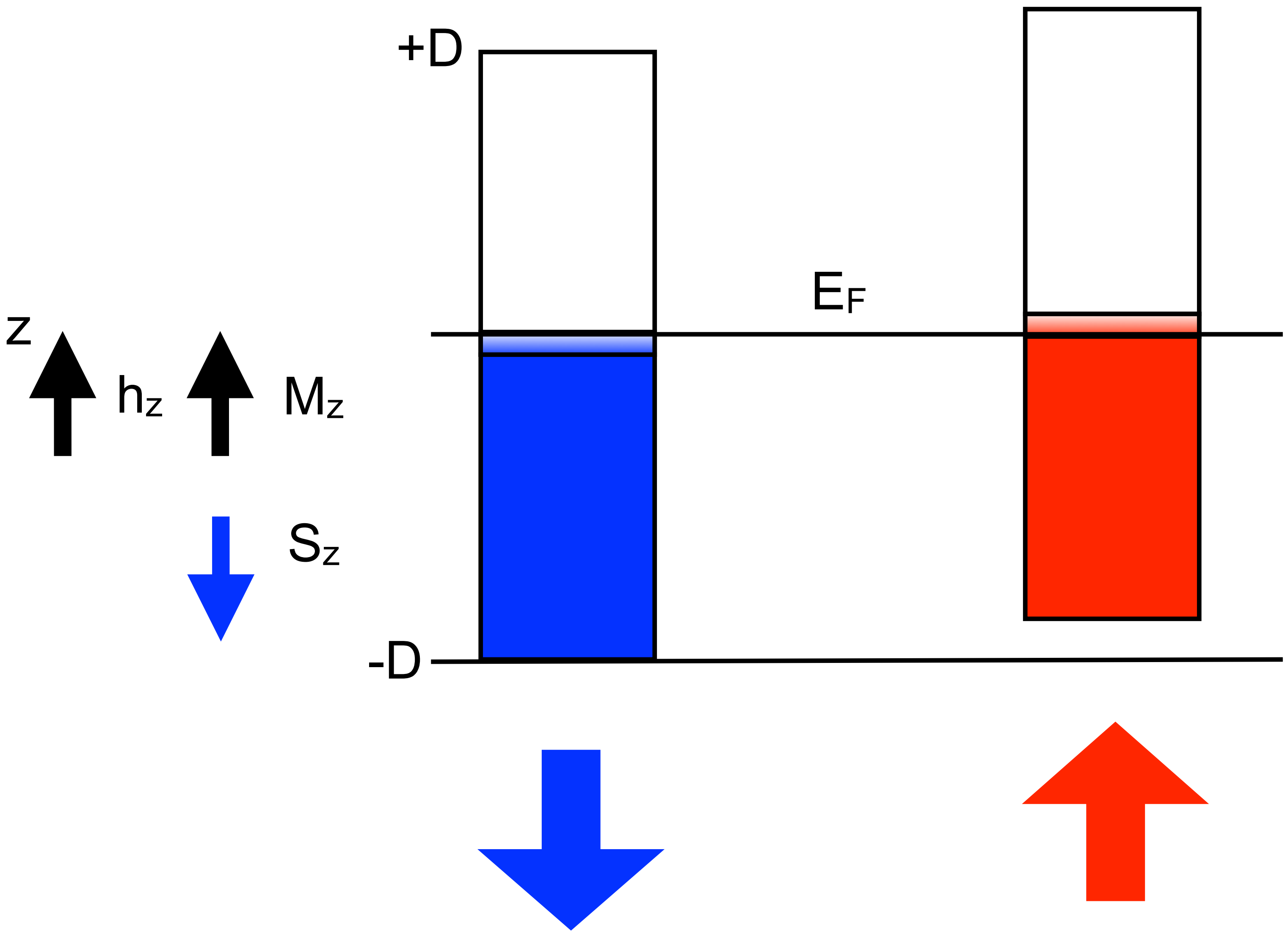
hypercubic lattice

$$\varepsilon_{\boldsymbol{k}} = -2t \sum_{\nu=1}^{d} \cos(k_{r_\nu} a)$$



Pauli paramagnetism

$$\varepsilon_{\boldsymbol{k}} \to \varepsilon_{\boldsymbol{k}\sigma} = \varepsilon_{\boldsymbol{k}} + \frac{1}{2}\sigma g \mu_B h_z$$



Pauli paramagnetism

$$M_z = -\frac{1}{2}(g\mu_B)\frac{1}{N_{\boldsymbol{k}}}\sum_{\boldsymbol{k}}\left[n_{\boldsymbol{k}\uparrow} - n_{\boldsymbol{k}\downarrow}\right] \sim \frac{1}{4}\left(g\mu_B\right)^2 \rho(\varepsilon_F) h_z$$

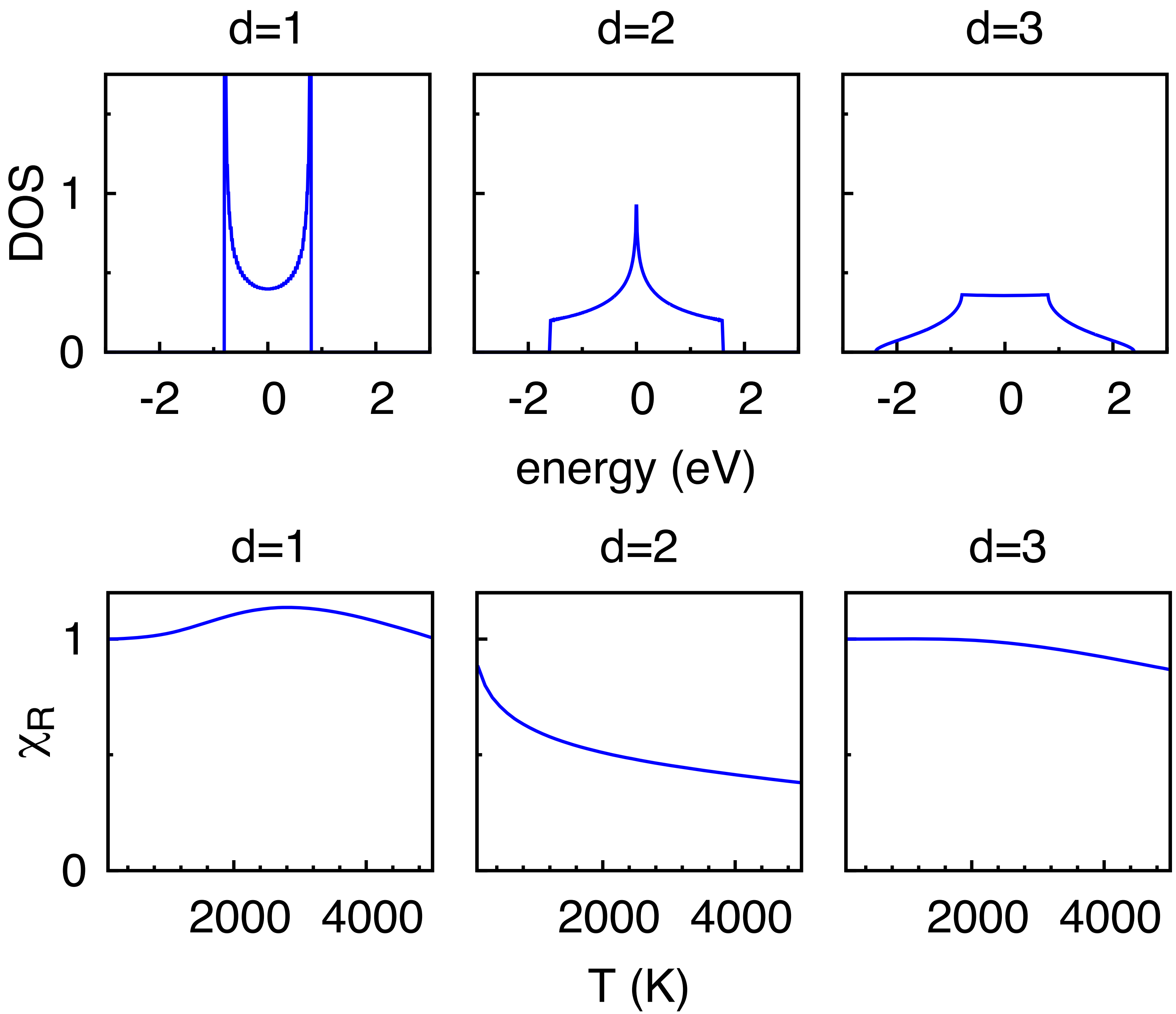
zero temperature

$$\chi^P(0) = \frac{1}{4}\left(g\mu_B\right)^2 \rho(\varepsilon_F)$$

finite temperature

$$\chi^P(T) = \frac{1}{4}\left(g\mu_B\right)^2 \int d\varepsilon \rho(\varepsilon)\left(-\frac{dn(\varepsilon)}{d\varepsilon}\right)$$

finite temperature



temperature Green function

U=0 limit

$$
\begin{aligned}
\mathcal{G}_{\boldsymbol{k}\sigma}(\tau) &= -\left\langle \mathcal{T}\left[c_{\boldsymbol{k}\sigma}(\tau)c^{\dagger}_{\boldsymbol{k}\sigma}(0)\right]\right\rangle_0 \\
&= -\left[\Theta(\tau)\left(1-n_\sigma(\varepsilon_{\boldsymbol{k}})\right)-\Theta(-\tau)n_\sigma(\varepsilon_{\boldsymbol{k}})\right]e^{-(\varepsilon_{\boldsymbol{k}}-\mu)\tau}
\end{aligned}
$$

$$
\mathcal{G}_{\boldsymbol{k}\sigma}(i\nu_n) = \frac{1}{i\nu_n - \varepsilon_{\boldsymbol{k}} + \mu}
$$

magnetic susceptibility

paramagnetic region

$$\chi_{zz}(\boldsymbol{q}; i\omega_m) = (g\mu_B)^2 \frac{1}{4}\frac{1}{\beta^2}\sum_{nn'}\sum_{\sigma}\chi_{n,n'}^{\boldsymbol{q}\sigma\sigma}(i\omega_m)$$

U=0 limit

$$\sum_{\sigma}\chi_{n,n'}^{\boldsymbol{q}\sigma\sigma}(i\omega_m) = -\beta\frac{1}{N_{\boldsymbol{k}}}\sum_{\boldsymbol{k}}\sum_{\sigma}\mathcal{G}_{\boldsymbol{k}\sigma}(i\nu_n)\mathcal{G}_{\boldsymbol{k}+\boldsymbol{q}\sigma}(i\nu_n + i\omega_m)\delta_{n,n'}$$

static case *(ω_m=0)*

$g_\alpha(\nu_n; x, y)$	$g_\alpha(\tau; x, y) = \frac{1}{\beta}\sum_n e^{-i\nu_n\tau} g_\alpha(\nu_n; x, y)$
$g_a(\nu_n; x, y) = [i\nu_n - x]^{-1}$	$[n_\sigma(x) - 1]e^{-x\tau}$
$g_b(\nu_n; x, y) = [i\nu_n - x]^{-2}$	$n_\sigma(x)(\tau - \beta n_\sigma(x))e^{-x(\tau-\beta)}$
$g_c(\nu_n; x, y) = [i\nu_n - x]^{-1}[i\nu_n - y]^{-1}$	$-\left[e^{-x(\tau-\beta)}n_\sigma(x) - e^{-y(\tau-\beta)}n_\sigma(y)\right][x-y]^{-1}$
$g_d(\nu_n; x, y) = [i\nu_n - x]^{-1}[i\nu_n + x]^{-1}$	$[g_a(\tau; x, y) - g_a(\tau; -x, y)]/2x$

U=0 limit, static case

$$\chi_{zz}(\mathbf{0};0) = \frac{1}{4}\,(g\mu_B)^2\,\rho(\varepsilon_F),$$

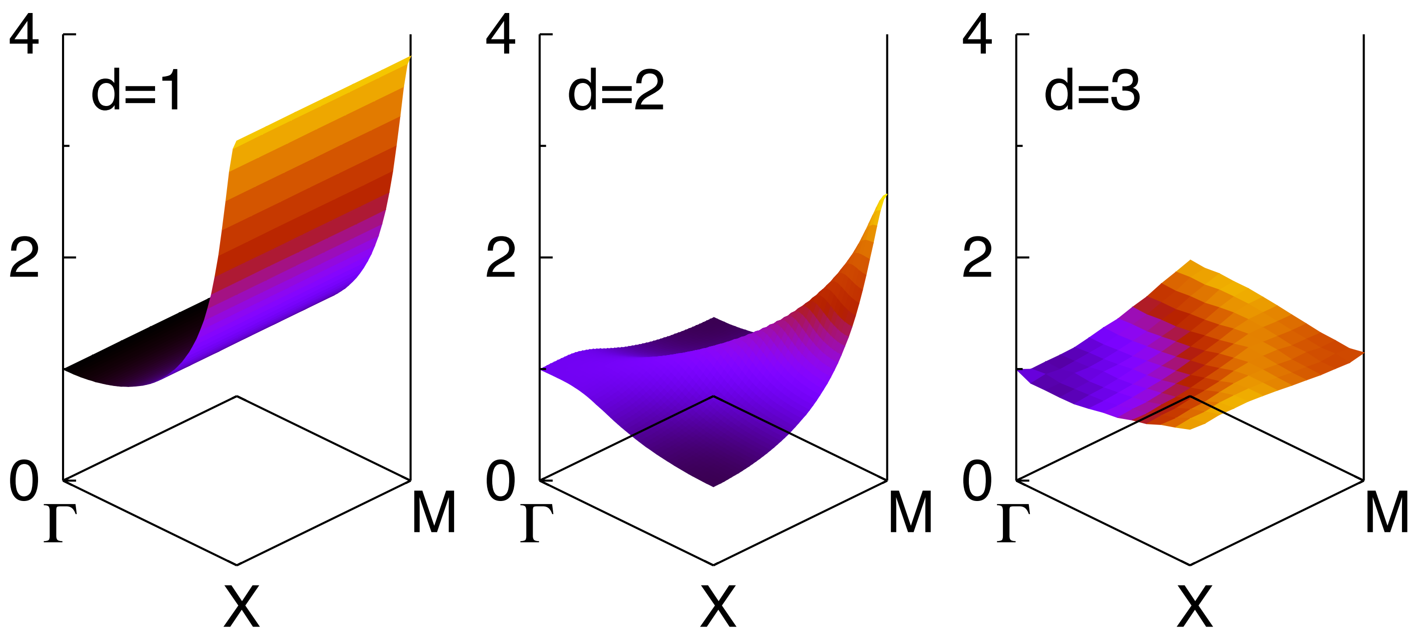
$$\rho(\varepsilon_F) = -\sum_{\sigma}\frac{1}{N_{\boldsymbol{k}}}\sum_{\boldsymbol{k}}\left.\frac{dn_{\boldsymbol{\sigma}}(\varepsilon_{\boldsymbol{k}})}{d\varepsilon_{\boldsymbol{k}}}\right|_{T=0}.$$

magnetic susceptibility

$$\varepsilon_{\boldsymbol{k}} = -2t[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)]$$

finite temperature ~ 350 K

$\chi_0(q;0)$



2-dimensional case: M point!

weakly temperature dependent

the $t=0$ limit

atomic limit (t=0) & half filling

$\vert N,S,S_z\rangle$			N	S	$E(N)$
$\vert 0,0,0\rangle$	$=$	$\vert 0\rangle$	0	0	0
$\vert 1,\frac{1}{2},\uparrow\rangle$	$=$	$c^\dagger_{i\uparrow}\vert 0\rangle$	1	$1/2$	ε_d
$\vert 1,\frac{1}{2},\downarrow\rangle$	$=$	$c^\dagger_{i\downarrow}\vert 0\rangle$	1	$1/2$	ε_d
$\vert 2,0,0\rangle$	$=$	$c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}\vert 0\rangle$	2	0	$2\varepsilon_d+U$

S=1/2

$$H_d + H_U = \varepsilon_d \sum_i n_i + U \sum_i \left[-\left(S_z^i\right)^2 + \frac{n_i^2}{4} \right]$$

emergence of the spin!

half filling: highly degenerate states, 2^{Ns} degrees of freedom

insulating behavior

magnetization

non interacting ions

uniform magnetic field h_z, Zeeman term

$$M_z = \langle M_z^i \rangle = -g\mu_B \frac{\mathrm{Tr}\,\left[e^{-g\mu_B h_z \beta S_z^i} S_z^i\right]}{\mathrm{Tr}\,\left[e^{-g\mu_B h_z \beta S_z^i}\right]} = g\mu_B S \tanh\left(g\mu_B h_z \beta S\right)$$

derivative with respect to h_z

$$\frac{\partial M_z}{\partial h_z} = \left(g\mu_B S\right)^2 \frac{1}{k_B T} \left[1 - \tanh^2\left(g\mu_B h_z \beta S\right)\right]$$

Curie susceptibility

Curie behavior

$$\chi_{zz}(\mathbf{0};0) = (g\mu_B S)^2 \frac{1}{k_B T} = \frac{C_{1/2}}{T}$$

Curie constant

$$C_{1/2} = \frac{(g\mu_B)^2 S(S+1)}{3k_B}$$

local spin as emergent entity

one-site Hubbard model

$$\chi_{zz}(\mathbf{0};0) \sim \frac{(g\mu_B)^2}{k_B T}\left\{\frac{\mathrm{Tr}\left[e^{-\beta(H_i-\mu N_i)}\ \left(S_z^i\right)^2\right]}{\mathrm{Tr}\left[e^{-\beta(H_i-\mu N_i)}\right]}-\left[\frac{\mathrm{Tr}\left[e^{-\beta(H_i-\mu N_i)}\ S_z^i\right]}{\mathrm{Tr}\left[e^{-\beta(H_i-\mu N_i)}\right]}\right]^2\right\}$$

$$= \frac{C_{1/2}}{T}\frac{e^{\beta U/2}}{1+e^{\beta U/2}}$$

$$U = E(N_i+1)+E(N_i-1)-2E(N_i)$$

infinite U limit: the spin S=1/2

only S=1/2 part of Hilbert space remains

temperature Green function

t=0 limit

$$G_\sigma(\tau) = -\frac{1}{2}\frac{1}{1+e^{\beta U/2}}\left[e^{\tau U/2} + e^{(\beta-\tau)U/2}\right]$$

$$G_\sigma(i\nu_n) = \frac{1}{2}\left[\frac{1}{i\nu_n + U/2} + \frac{1}{i\nu_n - U/2}\right]$$

magnetic susceptibility

t=0 limit

sector $\tau_1<\tau_2<\tau_3<\tau_4$

$$\chi^{i\sigma\,i\sigma}_{i\sigma' i\sigma'}(\boldsymbol{\tau}^+) = \frac{1}{2(1+e^{\beta U/2})}\left(e^{\tau_{12}U/2+\tau_{34}U/2} + \delta_{\sigma\sigma'}e^{(\beta-\tau_{12})U/2-\tau_{34}U/2}\right)$$

$$\chi_{zz}(\boldsymbol{\tau}^+) = (g\mu_B)^2\,\frac{1}{4}\frac{1}{\beta}\sum_{\sigma\sigma'}\sigma\sigma'\chi^{i\sigma\,i\sigma}_{i\sigma' i\sigma'}(\boldsymbol{\tau}) = \frac{(g\mu_B)^2}{4\beta}\frac{1}{(1+e^{\beta U/2})}e^{(\beta-\tau_{12}-\tau_{34})U/2}$$

Fourier transform

$$[\chi_{zz}]_{nn'}(i\omega_m) = \beta \frac{1}{4}(g\mu_B)^2 \sum_P \mathrm{sign}(P) f_P$$

$$f_P(i\omega_{P_1}, i\omega_{P_2}, i\omega_{P_3}) = \int_0^\beta d\tau_{14} \int_0^{\tau_{14}} d\tau_{24} \int_0^{\tau_{24}} d\tau_{34}\; e^{i\omega_{P_1}\tau_{14} + i\omega_{P_2}\tau_{24} + i\omega_{P_3}\tau_{34}} f_P(\tau_{14}, \tau_{24}, \tau_{34})$$

$$f_E(\tau_{14}, \tau_{24}, \tau_{34}) = \frac{1}{(1+e^{\beta U/2})}\; e^{\beta U/2}\; e^{-(\tau_{12}+\tau_{34})U/2} = \frac{1}{(1+e^{\beta U/2})}\; g_E(\tau_{14}, \tau_{24}, \tau_{34}$$

calculating the integral

$$I_P(x,-x,x;i\omega_{P_1},i\omega_{P_2},i\omega_{P_3}) = \int_0^\beta d\tau_{14}\int_0^{\tau_{14}} d\tau_{24}\int_0^{\tau_{24}} d\tau_{34}\; e^{i\omega_{P_1}\tau_{14}+i\omega_{P_2}\tau_{24}+i\omega_{P_3}\tau_{34}} e^{x(\tau_{14}-\tau_{24}+\tau_{34}}$$

$$= + \int_0^\beta d\tau_{14}\int_0^{\tau_{14}} d\tau\; \int_0^{\tau_{14}-\tau} d\tau'\; e^{(i\omega_{P_1}+i\omega_{P_2}+i\omega_{P_3}+x)\tau_{14}-i(\omega_{P_2}+\omega_{P_3})\tau} e^{-(i\omega_{P_3}+x)\tau'}$$

$$= + \frac{1}{i\omega_{P_3}+x}\frac{1}{-i\omega_{P_2}+x}\left[\frac{1}{i\omega_{P_1}+x}\;\frac{1}{n(x)}+\beta\delta_{\omega_{P_1}+\omega_{P_2}}\right]$$

$$+ \frac{1}{i\omega_{P_3}+x}\frac{1-\delta_{\omega_{P_2}+\omega_{P_3}}}{i(\omega_{P_2}+\omega_{P_3})}\left[\frac{1}{i\omega_{P_1}+x}-\frac{1}{i(\omega_{P_1}+\omega_{P_2}+\omega_{P_3})+x}\right]\frac{1}{n(x)}$$

$$+ \delta_{\omega_{P_2}+\omega_{P_3}}\frac{1}{i\omega_{P_3}+x}\left\{\left[\frac{1}{(i\omega_{P_1}+x)}\right]^2\frac{1}{n(x)}-\beta\left[\frac{1}{(i\omega_{P_1}+x)}\right]\frac{1-n(x)}{n(x)}\right\}.$$

magnetic susceptibility

result after Matsubara sums

$$\chi_{zz}(\boldsymbol{q};0) = (g\mu_B)^2 \frac{1}{4k_B T} \frac{e^{\beta U/2}}{1 + e^{\beta U/2}}$$

Curie-like temperature behavior

infinite U limit: emergence of spin

the small t/U limit

perturbation theory

Hubbard model

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

half filling: N=1 electrons per site

n_D = number of doubly occupied sites

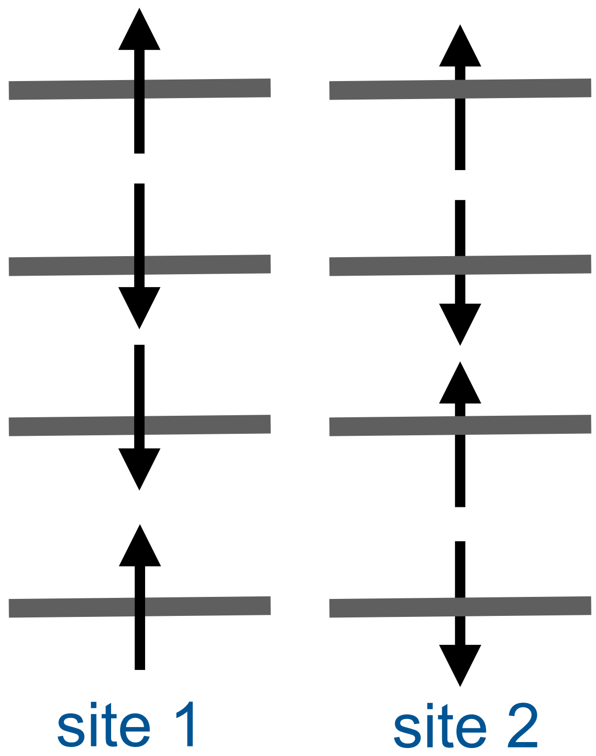
idea: divide Hilbert space into $n_D=0$ and $n_D>0$ sector

next downfold high energy $n_D>0$ sector

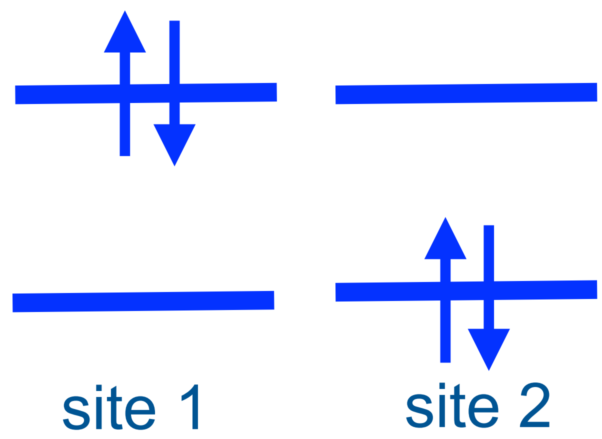
two sites

N=1 per site; N_{tot}=2

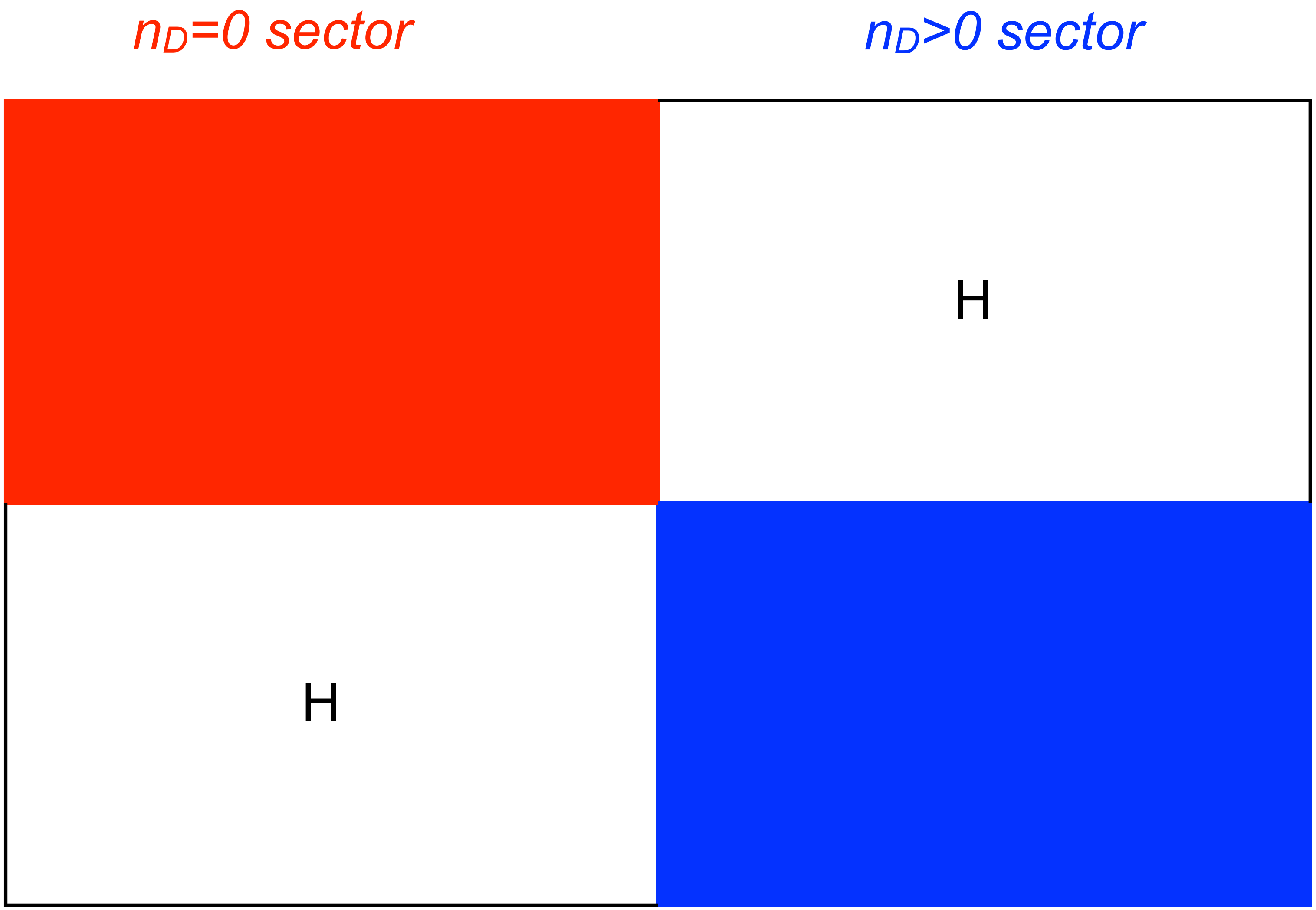
n_D=0 sector



n_D=1 sector



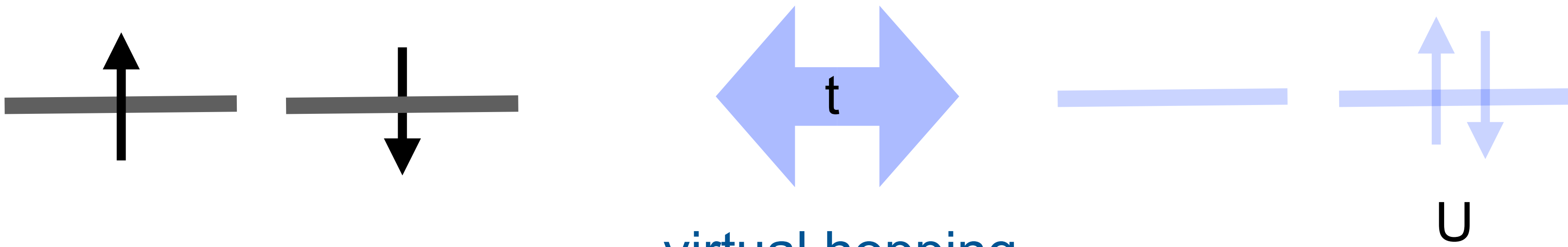
Hilbert space



next downfold high energy $n_D>0$ sector

low energy model

eliminate states with a doubly occupied site



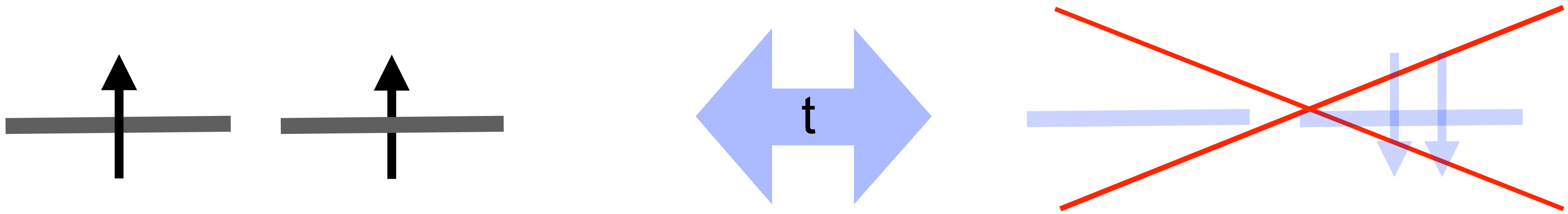
virtual hopping

energy gain

$$\Delta E_{\uparrow\downarrow} \sim -\sum_I \underbrace{\langle \uparrow, \downarrow | H_T | I \rangle}_{=t} \underbrace{\left\langle I \left| \frac{1}{E(2)+E(0)-2E(1)} \right| I \right\rangle}_{=1/U} \underbrace{\langle I | H_T | \uparrow, \downarrow \rangle}_{=t} \sim -\frac{2t^2}{U}.$$

low energy model

energy gain only for antiferromagnetic arrangement



Pauli principle

$$\frac{1}{2}\Gamma \sim (\Delta E_{\uparrow\uparrow} - \Delta E_{\uparrow\downarrow}) = \frac{1}{2}\frac{4t^2}{U}$$

$$H_S = \frac{1}{2}\Gamma \sum_{\langle ii' \rangle} \left[\boldsymbol{S}_i \cdot \boldsymbol{S}_{i'} - \frac{1}{4} n_i n_{i'} \right]$$

static mean field

$$\langle M_z^{ji} \rangle \quad = \quad -\sigma_m M_0 \cos(\boldsymbol{q} \cdot \boldsymbol{R}_j) = -g\mu_B \, m \, \cos(\boldsymbol{q} \cdot \boldsymbol{R}_j)$$

relation between critical temperature and couplings

$$k_B T_{\boldsymbol{q}} = \frac{S(S+1)}{3} \Gamma_{\boldsymbol{q}}, \quad \Gamma_{\boldsymbol{q}} = -\sum_{ij \neq 0} \Gamma^{00,ij} e^{i\boldsymbol{q}\cdot(\boldsymbol{T}_i + \boldsymbol{R}_j)}$$

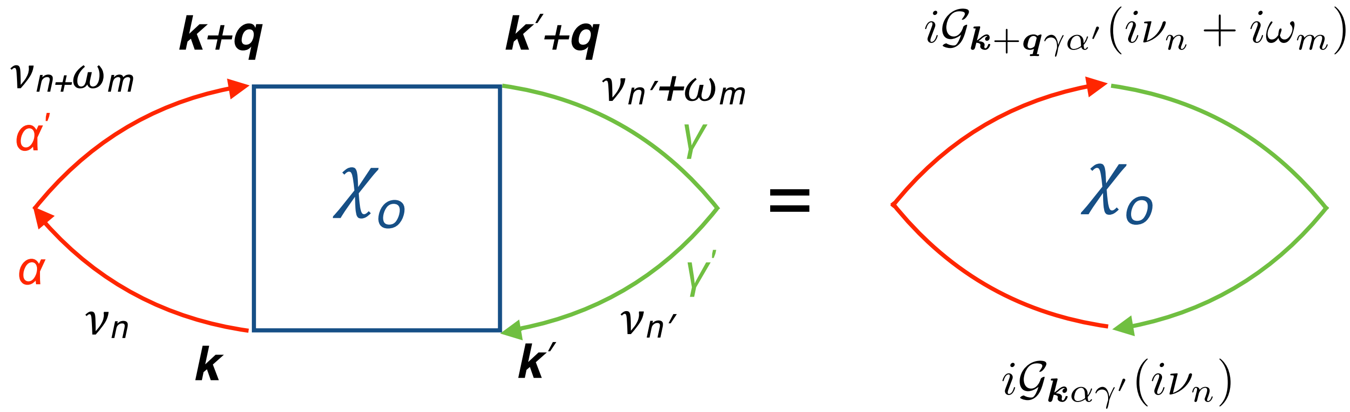
$$\chi_{zz}(\boldsymbol{q};0) = \frac{C_{1/2}(1-\sigma_m^2)}{T - (1-\sigma_m^2)T_{\boldsymbol{q}}}$$

divergence at critical temperature

Curie-Weiss susceptibility

χ_0 term

atomic limit



$$\chi^{\sigma\sigma'}_{n,n'}(0) = -\beta\delta_{nn'}\delta_{\sigma\sigma'}\frac{1}{4}\left[\frac{1}{i\nu_n + U/2} + \frac{1}{i\nu_n - U/2}\right]\left[\frac{1}{i\nu_n + U/2} + \frac{1}{i\nu_n - U/2}\right]$$

$$\chi^0_{zz}(0) = \frac{1}{4}(g\mu_B)^2\sum_\sigma \frac{1}{\beta^2}\sum_n \chi^{\sigma\sigma}_{n,n}(0) = \frac{1}{4}(g\mu_B)^2\frac{\beta e^{\beta U/2}}{1+e^{\beta U/2}}\left[\frac{1}{1+e^{\beta U/2}} + \frac{1}{U\beta}\left(\frac{1-e^{-\beta U}}{1+e^{-\beta U/2}}\right)\right]$$

X_0 term

atomic limit

$$\chi^0_{zz}(0) = \frac{1}{4}(g\mu_B)^2 \sum_\sigma \frac{1}{\beta^2} \sum_n \chi^{\sigma\sigma}_{n,n}(0) = \frac{1}{4}(g\mu_B)^2 \frac{\beta e^{\beta U/2}}{1+e^{\beta U/2}} \left[\frac{1}{1+e^{\beta U/2}} + \frac{1}{U\beta}\left(\frac{1-e^{-\beta U}}{1+e^{-\beta U/2}}\right)\right]$$

large U: weakly temperature dependent

$$\chi^0_{zz}(0) \sim (g\mu_B)^2/4U$$

small *t/U* limit?

X_0 term

in the $t=0$ limit

$$G(i\nu_n) = \frac{1}{i\nu_n + \mu - \Sigma(i\nu_n)}$$

$$\Sigma(i\nu_n) = \mu + \frac{U^2}{4}\frac{1}{i\nu_n}$$

what about the small t/U limit?

let us consider an approximate form for the self-energy

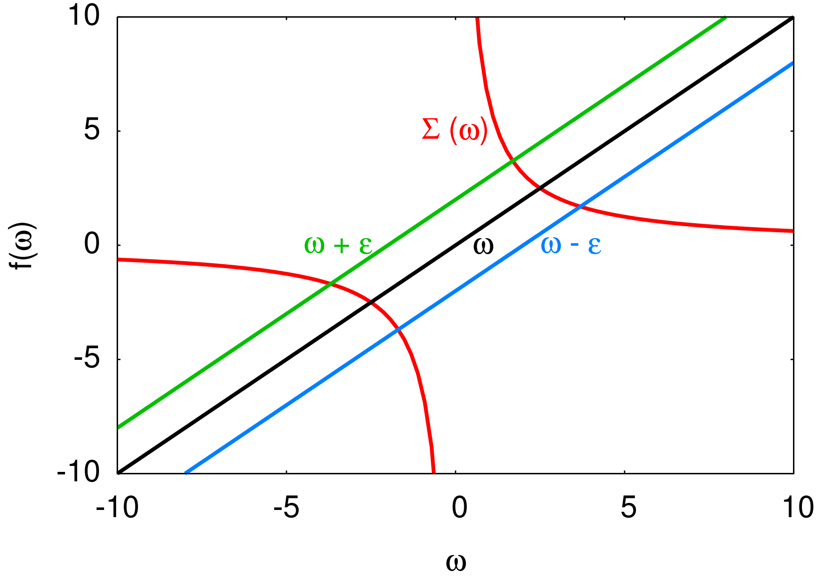
$$\Sigma(i\nu_n) = \mu + \frac{r_U U^2}{4}\frac{1}{i\nu_n}$$

X_0 term

what about the small t/U limit?

$$\Sigma(i\nu_n) = \mu + \frac{r_U U^2}{4}\frac{1}{i\nu_n}$$

$$G_{\boldsymbol{k}}(i\nu_n) = \frac{1}{i\nu_n - \Sigma(i\nu_n) - \varepsilon_{\boldsymbol{k}}} = \frac{1}{E^+_{\boldsymbol{k}} - E^-_{\boldsymbol{k}}}\left[\frac{E^+_{\boldsymbol{k}}}{i\nu_n - E^+_{\boldsymbol{k}}} - \frac{E^-_{\boldsymbol{k}}}{i\nu_n - E^-_{\boldsymbol{k}}}\right]$$



X_0 term

perform Matsubara sums

$$\chi^0_{zz}(\boldsymbol{q};0) = (g\mu_B)^2 \frac{1}{4} \sum_\sigma \frac{1}{\beta^2} \sum_n \chi^{\sigma\sigma}_{n,n}(0)$$

$$= (g\mu_B)^2 \frac{1}{2} \frac{1}{N_{\boldsymbol{k}}} \sum_{\boldsymbol{k}} \left[\underbrace{-I^{++}_{\boldsymbol{k},\boldsymbol{q}} - I^{--}_{\boldsymbol{k},\boldsymbol{q}}}_{A_{\boldsymbol{k},\boldsymbol{q}}} + \underbrace{I^{+-}_{\boldsymbol{k},\boldsymbol{q}} + I^{-+}_{\boldsymbol{k},\boldsymbol{q}}}_{B_{\boldsymbol{k},\boldsymbol{q}}}, \right]$$

"metallic" "insulating"

$$I^{\alpha\gamma}_{\boldsymbol{k},\boldsymbol{q}} = \frac{E^\alpha_{\boldsymbol{k}}\; E^\gamma_{\boldsymbol{k}+\boldsymbol{q}}}{(E^+_{\boldsymbol{k}} - E^-_{\boldsymbol{k}})(E^+_{\boldsymbol{k}+\boldsymbol{q}} - E^-_{\boldsymbol{k}+\boldsymbol{q}})} \frac{n(E^\alpha_{\boldsymbol{k}}) - n(E^\gamma_{\boldsymbol{k}+\boldsymbol{q}})}{E^\alpha_{\boldsymbol{k}} - E^\gamma_{\boldsymbol{k}+\boldsymbol{q}}}$$

X_0 term

at the Γ point

$$\chi^0_{zz}(\mathbf{0};0) \sim (g\mu_B)^2 \frac{1}{4}\frac{1}{N_{\boldsymbol{k}}}\sum_{\boldsymbol{k}} \frac{r_U\, U^2}{[\varepsilon^2_{\boldsymbol{k}} + r_U\, U^2]^{3/2}} \sim (g\mu_B)^2 \frac{1}{4\sqrt{r_U}\, U}\left[1 - \frac{3}{2}\frac{1}{N_{\boldsymbol{k}}}\sum_{\boldsymbol{k}} \frac{\varepsilon^2_{\boldsymbol{k}}}{r_U\, U^2} + \ldots\right]$$

at the M point

$$\chi_0(\boldsymbol{q}_C;0) \sim (g\mu_B)^2 \frac{1}{4\sqrt{r_U}U}\left[1 - \frac{1}{2}\frac{1}{N_{\boldsymbol{k}}}\sum_{\boldsymbol{k}} \frac{\varepsilon^2_{\boldsymbol{k}}}{r_U U^2}\right]$$

in general

$$\chi_0(\boldsymbol{q};0) \sim (g\mu_B)^2 \frac{1}{4\sqrt{r_U}U}\left[1 - \frac{1}{2}\frac{J_{\mathbf{0}}}{\sqrt{r_U}U} - \frac{1}{4}\frac{J_{\boldsymbol{q}}}{\sqrt{r_U}U}\right]$$

$$J_{\boldsymbol{q}} = 2J[\cos q_x + \cos q_y], \qquad J \propto t^2/U$$

χ_0 term & the local vertex Γ

use atomic susceptibility as local susceptibility to determine the vertex via the local Bethe-Salpeter equation

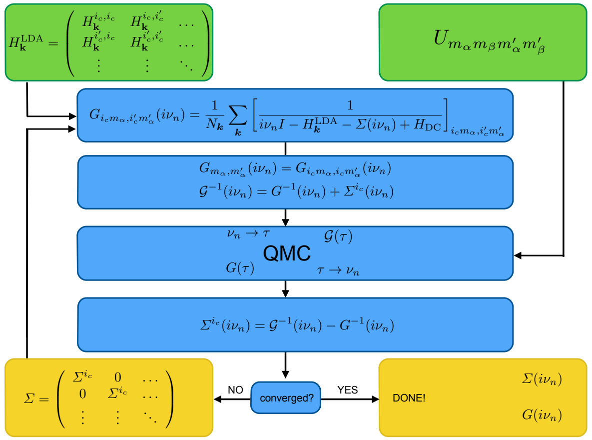
$$\Gamma \sim \left[\frac{1}{\chi^0_{zz}(0)} - \frac{1}{\chi_{zz}(0)}\right] \sim \frac{1}{(g\mu_B)^2}\left[4\sqrt{r_U}U\left(1+\frac{1}{2}\frac{J_{\mathbf{0}}}{\sqrt{r_U}U}\right) - 4k_BT\right]$$

the expected Curie-Weiss behavior

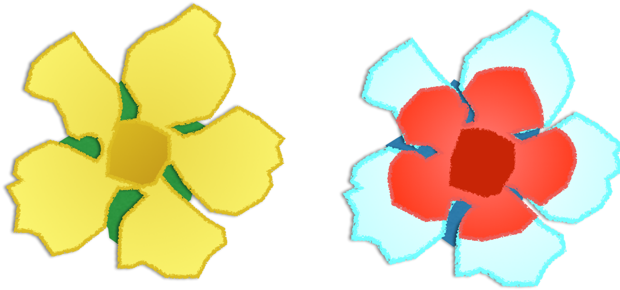
$$\chi_{zz}(\boldsymbol{q};0) = \frac{1}{[\chi^0_{zz}(\boldsymbol{q};0)]^{-1} - \Gamma} \sim (g\mu_B)^2\frac{1}{4}\frac{1}{k_BT + J_{\boldsymbol{q}}/4} = \boxed{\frac{(g\mu_B)^2}{k_B}\frac{1}{4}\frac{1}{T-T_{\boldsymbol{q}}}}$$

conclusion

strongly-correlated systems:
LDA+DMFT method



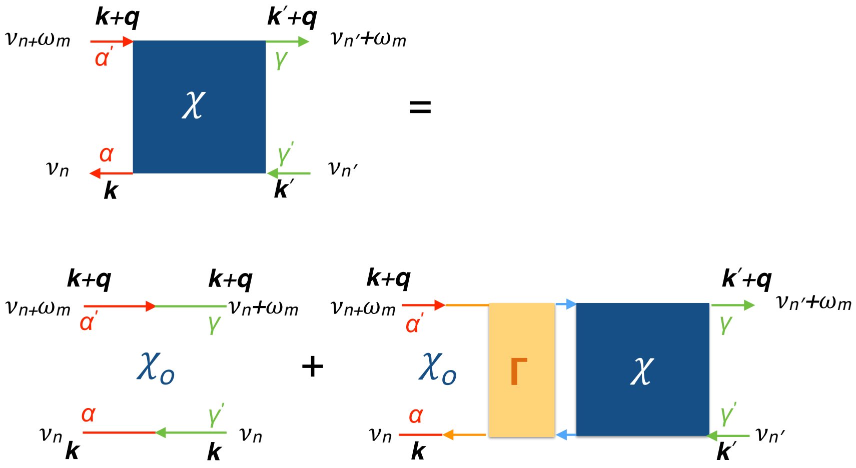
compare to data:
need a response theory



basics of linear-response theory

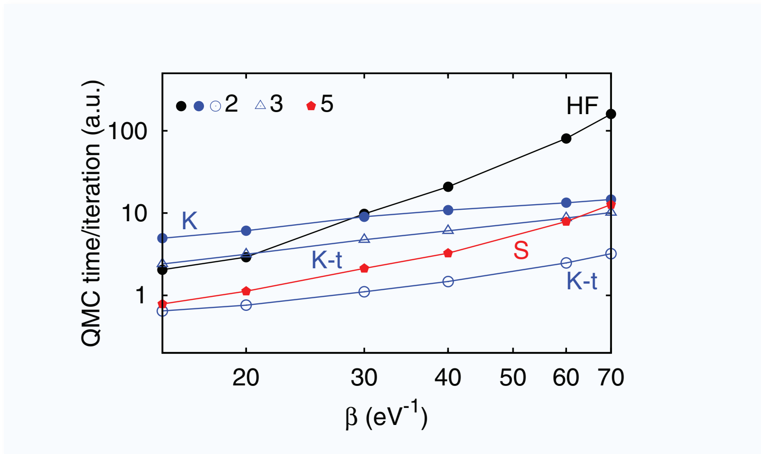
$$\chi_{\hat{P}_\nu \hat{O}_{\nu'}}(\boldsymbol{r},\boldsymbol{r}';t,t') \;=\; i\left\langle\left[\Delta\hat{P}_\nu(\boldsymbol{r};t),\Delta\hat{O}_{\nu'}(\boldsymbol{r}';t')\right]\right\rangle_0 \Theta(t-t')$$

Bethe-Salpeter equation



local-vertex approximation

local susceptibility: QMC methods



CT-HYB vs HF

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thank you!