Unifying spin-fluctuations and DMFT: TRILEX and vertex-based approaches

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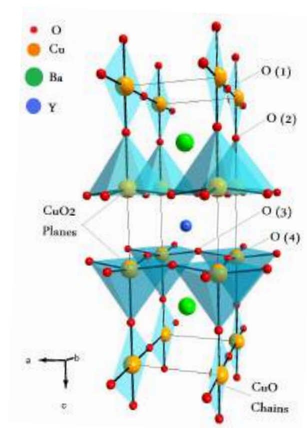
Solve the Quantum Many-Body Problem ?

Quantum Embedding methods (DMFT and beyond)

High-Tc cuprate superconductors



Exact diagonalization (small systems)

Tensor network (DMRG, …)

Quantum Monte Carlo (auxiliary field)

Machine Learning

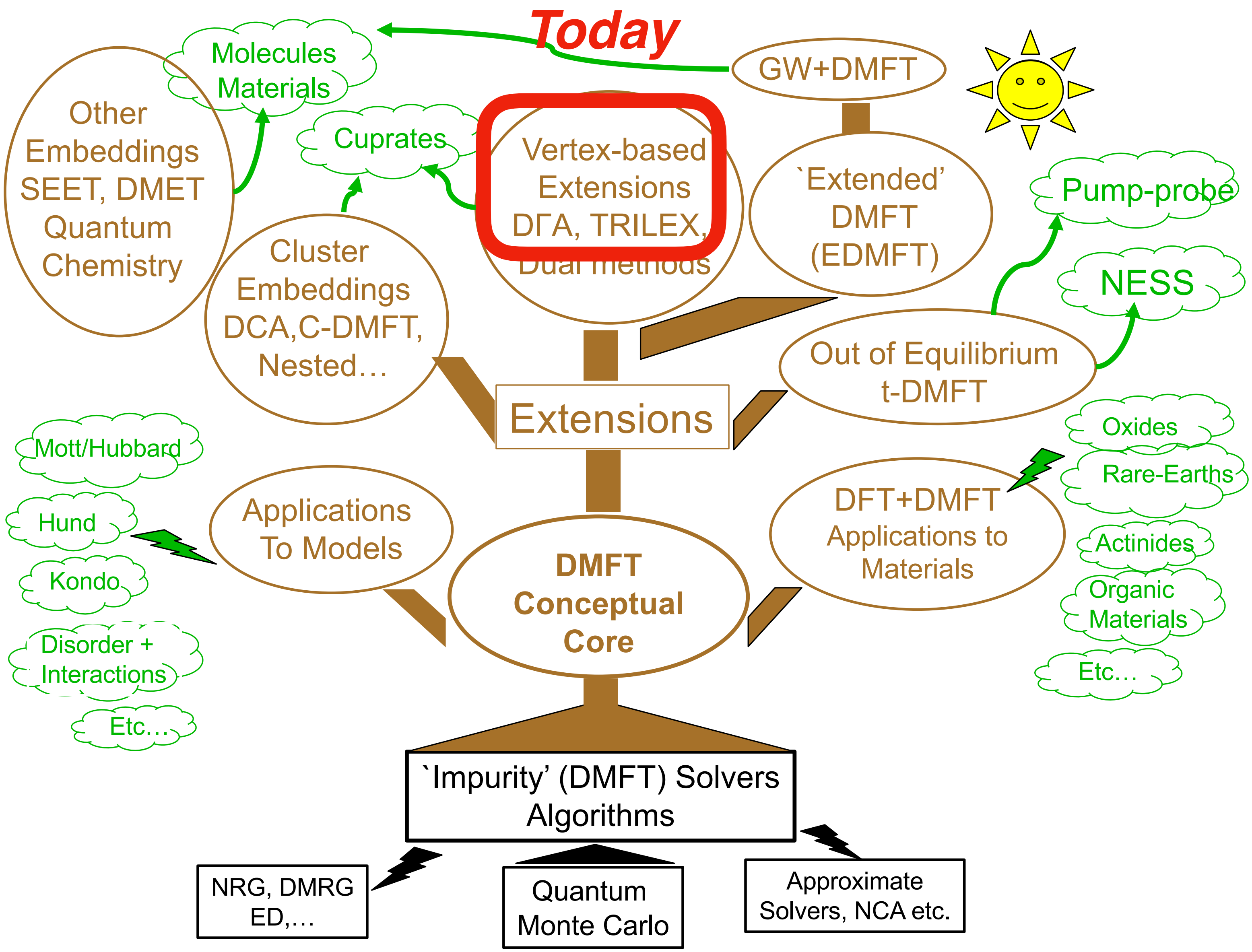
Hubbard model

$$H = -\sum_{\langle ij \rangle, \sigma=\uparrow,\downarrow} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U n_{i\uparrow} n_{i\downarrow}$$

High order perturbation theory "diagrammatic" QMC

…

DMFT family tree [lecture 1]



What is missing in DMFT ?

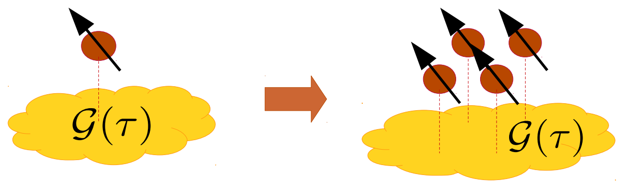
- Short range spatial correlations
- Control : small parameter ?

} Cluster DMFT

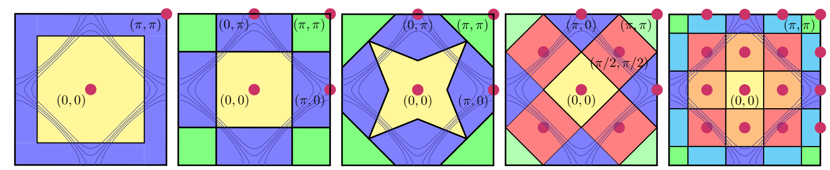
Cluster DMFT

- A few atoms + self-consistent bath

Real space



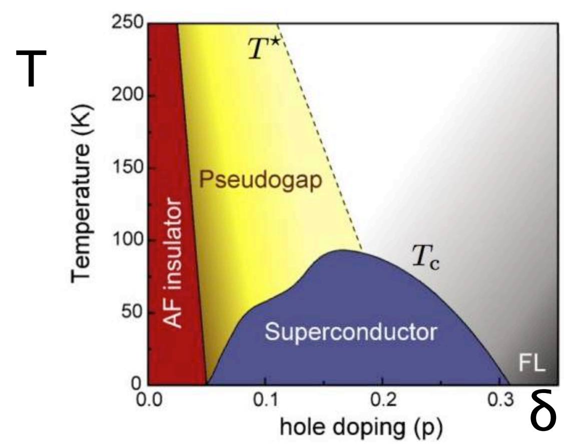
Reciprocal space
Brillouin zone patching



- Short range fluctuations. K-dependence of self-energy.
- Control parameter = size of cluster / momentum resolution

Hubbard model & high Tc superconductors

A lot of authors & works e.g. Capone, Civelli, Ferrero, Georges, Gull, Haule, Imada, Jarrell, Kotliar, Lichtenstein, Katsnelson, Maier, Millis, Tremblay, Werner, OP, ...



- Pseudo-gap (node vs antinode, Fermi Arcs), d-wave SC dome
- But solving large clusters is hard, specially at low T.

What is missing in (cluster) DMFT ?

- Short range spatial correlations
- Control : small parameter ?

} Cluster DMFT

- Long range correlations / interactions
- Feedback of low energy collective modes onto one particle properties.

} Vertex methods (Trilex, DGA, Quadrilex). See also EDMFT, GW + DMFT

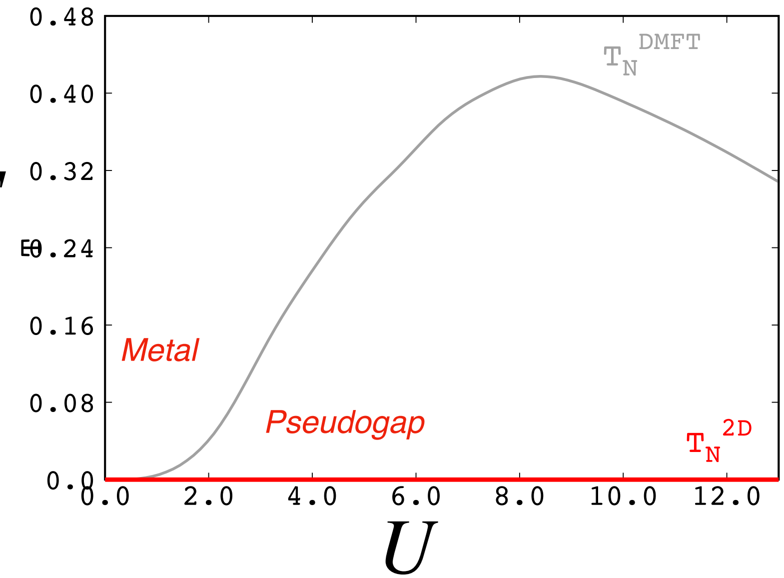
  - e.g. at quantum critical points (beyond Hertz-Millis theory)

Let us look at a simpler problem …

Weak coupling 2d Hubbard model

- Half filled.
- DMFT has AF order (mean field).
- Mermin-Wagner theorem
  long range AF fluctuations.

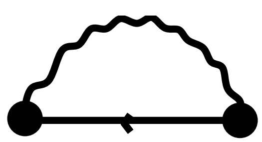
$$Q = (\pi, \pi) \qquad \xi \sim e^{a/T}$$

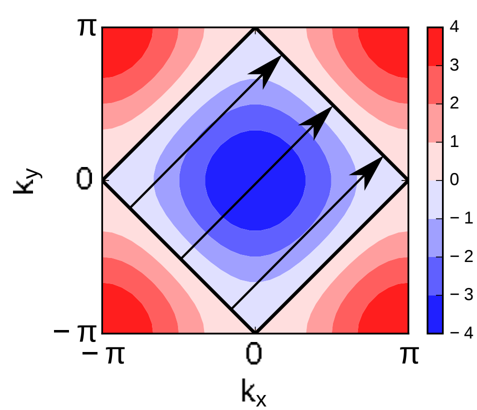


- AF fluctuations destroys the Fermi liquid, opens pseudogap *(Vilk-Tremblay 1997)*

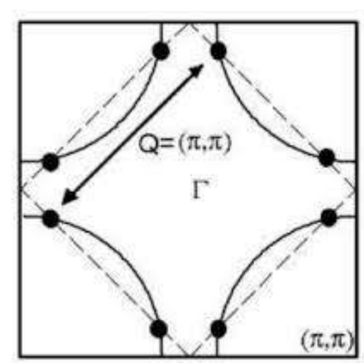
Fermi surface and nesting

$$\Sigma(k, i\omega) \approx$$





$t' = 0$



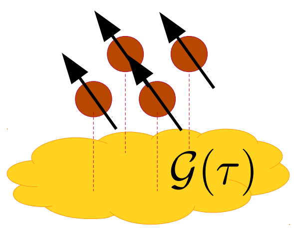
$t' \neq 0$

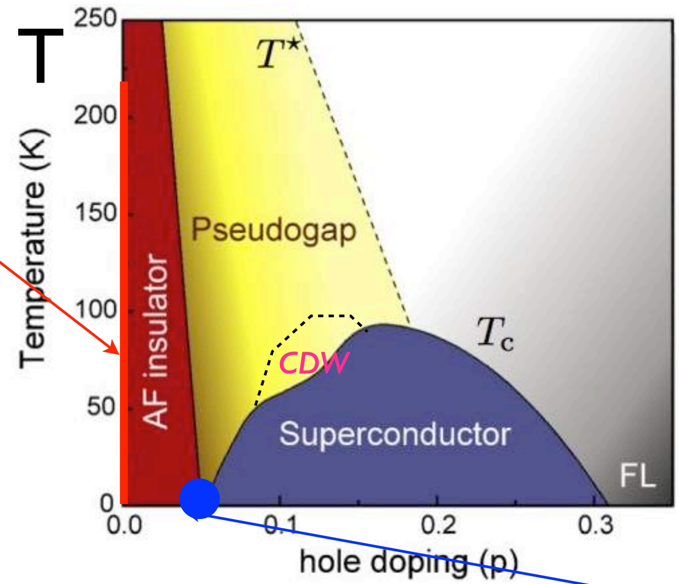
- Benchmark for
  methods beyond DMFT.

Goal : Mott physics & long range fluctuations

Doped Mott insulators

Anderson '87, Kotliar Liu '88, ...

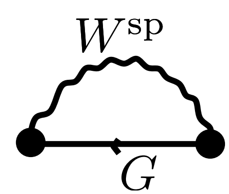




Spin Fluctuation Theory

Pines '90, Chubukov '92, ...

$\Sigma(k, i\omega) \approx$



- Mott physics & short range correlations
- Cluster DMFT.

- Effect of AF fluctuations

Formalism with
Spin Fluctuation theory at weak coupling & (cluster) DMFT at strong coupling ?

Reminder : one particle Green functions

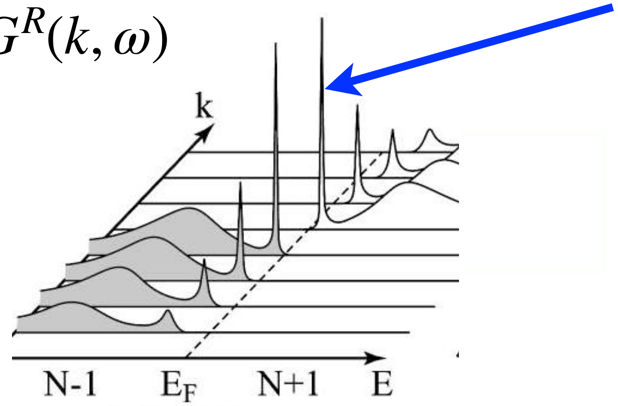
$$G(x,\tau) = -i\langle T_\tau c(x,\tau) c^\dagger(0,0)\rangle$$

Self-energy $$\Sigma = G_0^{-1} - G^{-1}$$

- Experiments : Photoemission (ARPES). STM.
- In Fermi liquid, at low energy, Σ encodes properties of the quasi-particles, e.g. effective mass, quasi-particle weight, lifetime.

$$A(k,\omega) = -\frac{1}{\pi} Im G^R(k,\omega)$$

Quasi-particle peak



Correlated Fermi liquid

Two particle physics in DMFT ?

- DMFT : self-consistent problem on <u>one-particle Green function</u>

$$S_{\text{eff}} = -\iint_0^\beta d\tau d\tau' c_\sigma^\dagger(\tau)\mathcal{G}_\sigma^{-1}(\tau-\tau')c_\sigma(\tau') + \int_0^\beta d\tau\ U n_\uparrow(\tau) n_\downarrow(\tau)$$

$$G_{\sigma \text{imp}}(\tau) \equiv -\left\langle T c_\sigma(\tau) c_\sigma^\dagger(0)\right\rangle_{S_{\text{eff}}} \qquad \Sigma_{\sigma\ latt}(k, i\omega_n) = \Sigma_{\sigma\ imp}(i\omega_n)$$

$$\Delta = t^2 G$$

- Questions :
  - Part I : How to compute susceptibilities in DMFT ? transport ?
  - Part II : Self-consist on two-particle Green function ? U ?

Part I

Susceptibility in DMFT

Static susceptibility

- Static susceptibility at simple q : solve DMFT in ordered phase

$$\chi \propto \frac{\partial m}{\partial h}\Big|_{h=0}$$

- Need a more general method for
  - Frequency dependency
  - Momentum dependency (incommensurate order)
  - General χ tensor (multiple possible instability)

Kubo formula

- Quantum linear response theory
  Response of operator A to a field coupled to B

$$\chi_{AB}(t-t') = -i\theta(t-t')\langle[A(t), B(t')]\rangle$$

- A, B : quadratic in the fundamental operators

$$A = A_{ab}c_a^\dagger c_b \qquad B = B_{cd}c_c^\dagger c_d$$

E.g. : susceptibilities $A = B = \sum_{i\sigma} (-1)^\sigma c_{\sigma i}^\dagger c_{\sigma i}$, conductivity (A = B = J)

- Requires the computation of two-particle Green functions

$$\sim \langle c_a^\dagger(t) c_b(t) c_c^\dagger(0) c_d(0)\rangle$$

Two particle Green functions

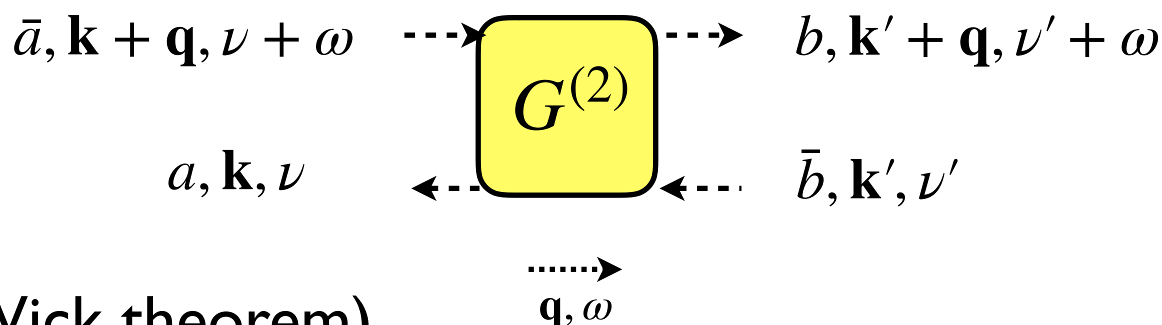
- Definition

$$G^{(2)}_{\bar{a}a\bar{b}b}(x_1, x_2, x_3, x_4, \tau_1, \tau_2, \tau_3, \tau_4) \equiv -i\langle T_\tau c^\dagger_{\bar{a}}(x_1, \tau_1) c_a(x_2, \tau_2) c^\dagger_{\bar{b}}(x_3, \tau_3) c_b(x_4, \tau_4)\rangle$$

a,b : multi-index orbital, spin

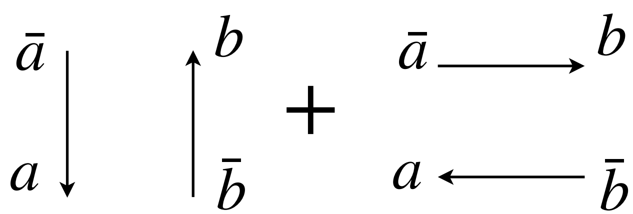
- Rank 4 tensor, with 3 frequencies/momenta

$$G^{(2)}_{\bar{a}a\bar{b}b}(k, k', q, \nu, \nu', \omega) =$$



- Non interacting case (Wick theorem)

$$G^{(2)}_{\bar{a}a\bar{b}b} =$$



$G_{0a\bar{a}}G_{0b\bar{b}}$ $\qquad$ $-G_{0a\bar{b}}G_{0b\bar{a}}$

Two particle Green functions

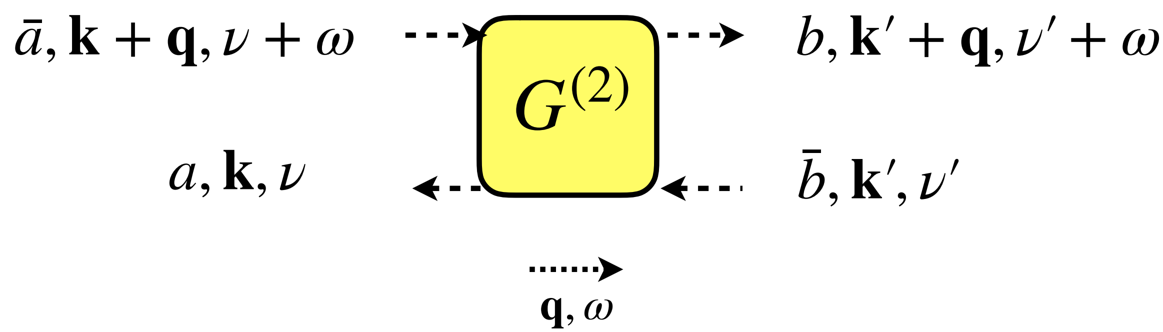
- Definition

$$G^{(2)}_{\bar{a}a\bar{b}b}(x_1, x_2, x_3, x_4, \tau_1, \tau_2, \tau_3, \tau_4) \equiv -i\langle T_\tau c^\dagger_{\bar{a}}(x_1, \tau_1) c_a(x_2, \tau_2) c^\dagger_{\bar{b}}(x_3, \tau_3) c_b(x_4, \tau_4)\rangle$$

a,b : multi-index orbital, spin

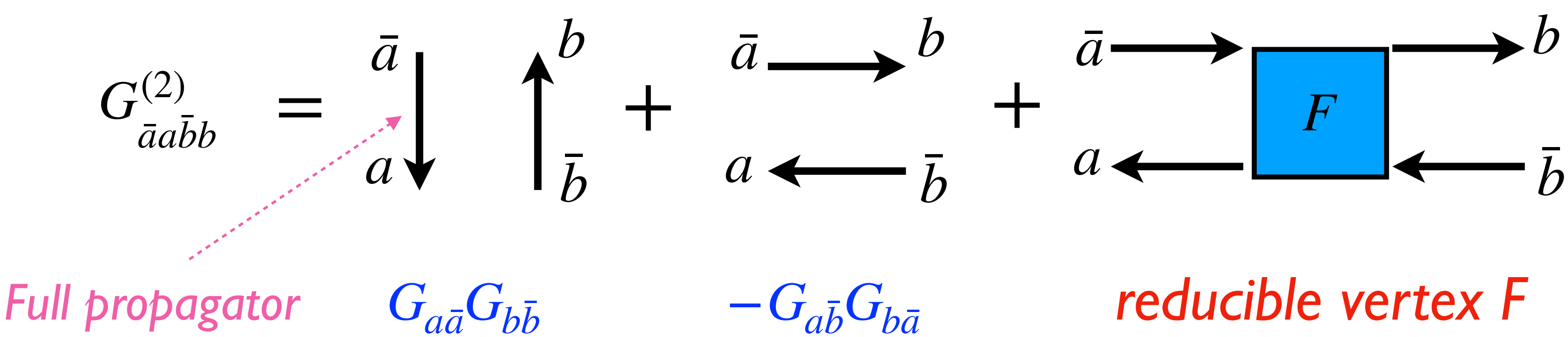
- Rank 4 tensor, with 3 frequencies/momenta

$$G^{(2)}_{\bar{a}a\bar{b}b}(k, k', q, \nu, \nu', \omega) =$$



- Perturbative expansion

$$G^{(2)}_{\bar{a}a\bar{b}b} =$$



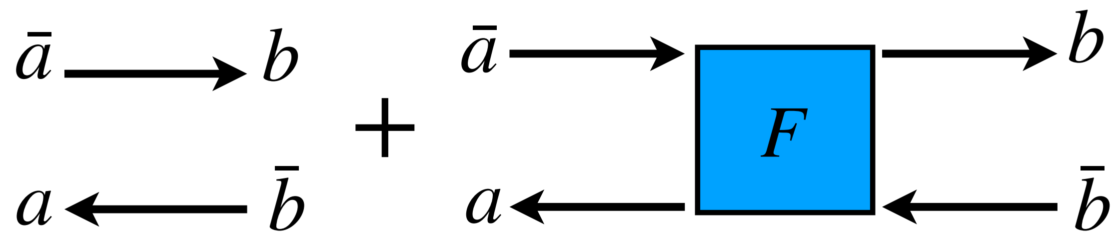
- In Fermi liquid, interactions between quasi-particles.

Generalized susceptibilities

- Generalized susceptibility (remove disconnected part, <A>)

$\tilde{\chi}_{0\;\bar{a}a\bar{b}b}$

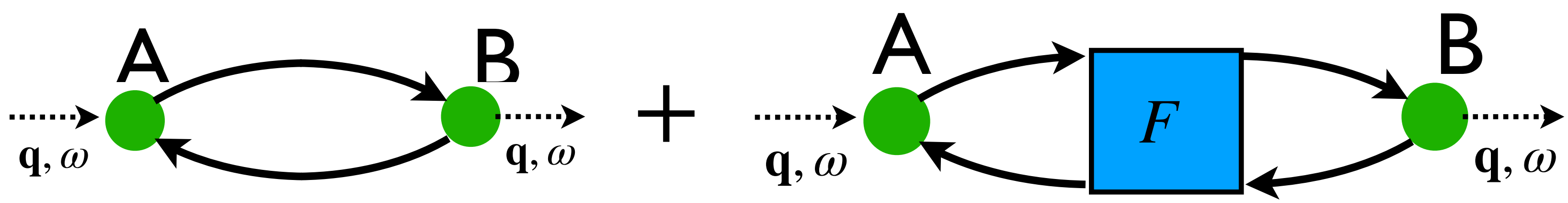
$\tilde{\chi}_{\bar{a}a\bar{b}b} =$



- Susceptibility : contract with A and B, sum over frequencies/momenta

$$\chi(q,\omega) = \sum_{\nu\nu' k k'} \tilde{\chi}_{\bar{a}a\bar{b}b}(q,k,k',\omega,\nu,\nu')A_{\bar{a}a}(k)B_{\bar{b}b}(k')$$

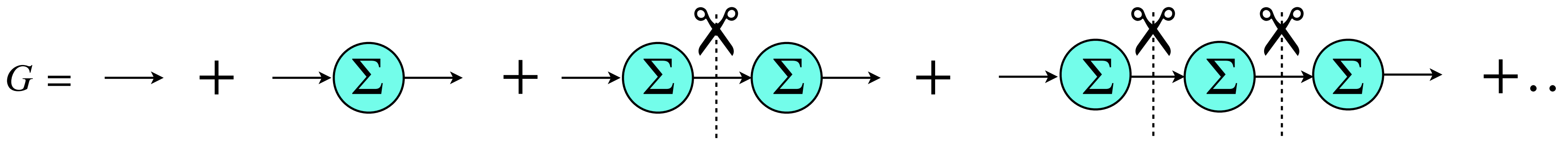
$\chi_{AB}(q,\omega) =$



Lindhard function *Vertex corrections*

Reminder : Dyson Equation

- Dyson equation for the one particle Green function

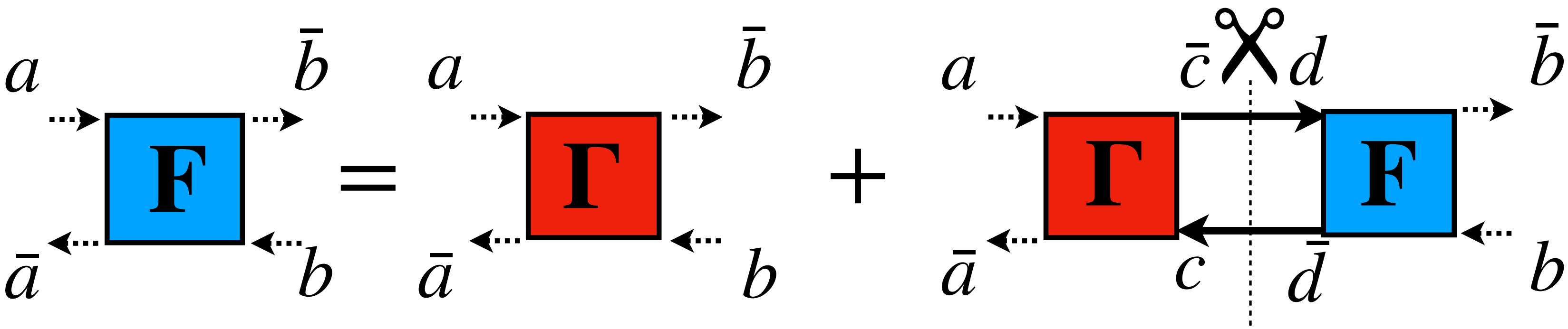


- Self-energy : 1PI (particle irreducible) diagrams

$$G = G_0 + G_0 \Sigma G \qquad\qquad \Sigma = G_0^{-1} - G^{-1}$$

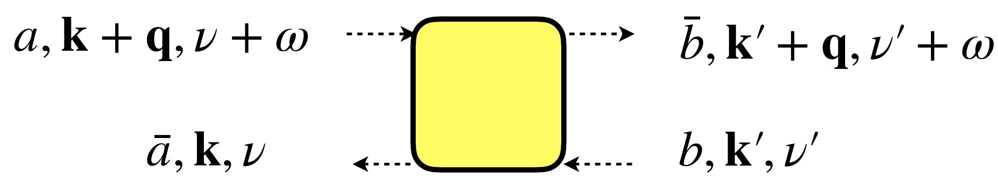
Bethe-Salpeter equation

- Reducibility in particle-hole channel



$$F^{\nu\nu'\omega}_{a\bar{a}b\bar{b};kk'q} = \Gamma^{\nu\nu'\omega}_{a\bar{a}b\bar{b};kk'q} + \sum_{c\bar{c}d\bar{d},k_1,\nu_1} \Gamma^{\nu\nu_1\omega}_{ab\bar{a}\bar{b};kk_1q}\tilde{\chi}^{\nu_1\omega}_{0c\bar{c}d\bar{d},k_1k_1q} F^{\nu_1\nu'\omega}_{d\bar{d}b\bar{b};k_1k'q}$$

- Matrix equation
  grouping indices
  $I = (a, \bar{a}, k, \nu)$ $J = (b, \bar{b}, k', \nu')$
  diagonal in (q,ω)



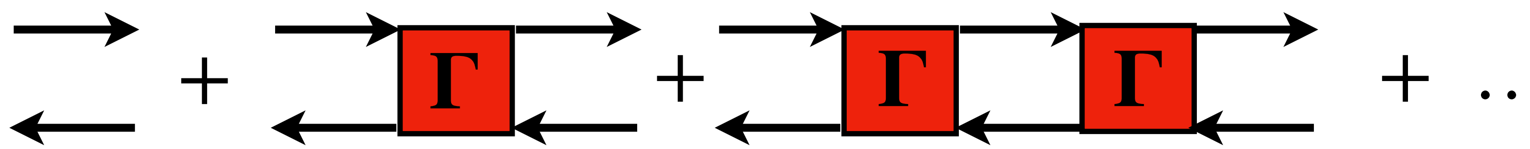
$$F = \Gamma + \Gamma\tilde{\chi}F$$

- $\Gamma_{a\bar{a}b\bar{b}}(k, k', q, \nu, \nu', \omega)$: Irreducible vertex in the particle-hole channel

Bethe-Salpeter equation

- Relation (exact) between the irreducible vertex Γ and χ

$\tilde{\chi} =$



$\tilde{\chi}_0$

$$\tilde{\chi} = \tilde{\chi}_0 + \tilde{\chi}_0 \Gamma \tilde{\chi} \Longleftrightarrow \Gamma = \tilde{\chi}^{-1} - \tilde{\chi}_0^{-1}$$

- Approximations for Γ
  - RPA : $\Gamma \propto U$
  - DMFT ?

DMFT

Cf. A. Georges et al. Rev. Mod. Phys. 1996

- DMFT : atomic approximation of Luttinger-Ward functional

$$\Phi[G] \approx \sum_i \phi_{atomic}[G_{ii}] \qquad \Sigma_{ij}^{latt} = \frac{\delta \Phi}{\delta G_{ji}} = \delta_{ij} \Sigma^{imp}$$

- Impurity model : auxiliary problem to solve the approximation.

- The irreducible vertex Γ

$$\Gamma_{ijkl}^{lattice} = \frac{\delta^2 \Phi}{\delta G_{ji} \delta G_{lk}}$$

- In DMFT susceptibilities

$$\Gamma_{ijkl}^{lattice} \approx \delta_{i=j=k=l} \Gamma_{imp}$$

$$\Gamma_{lattice}(k, k', q, \nu, \nu', \omega) \approx \Gamma_{imp}(\nu, \nu', \omega)$$

Susceptibilities in DMFT

Cf. A. Georges et al. Rev. Mod. Phys. 1996

M. Jarrell et al., '90

- Solve DMFT
- Compute impurity two-particle functions
- Use BSE for impurity and lattice

} *Numerically harder* — *e.g. noise control in BSE inversion.*

$$G_{imp} \longrightarrow \tilde{\chi}_{imp,0} \longrightarrow \Gamma_{imp} \longrightarrow \Gamma_{lattice} \longrightarrow \tilde{\chi}_{lattice} \longrightarrow \chi_{lattice}(q,\omega)$$

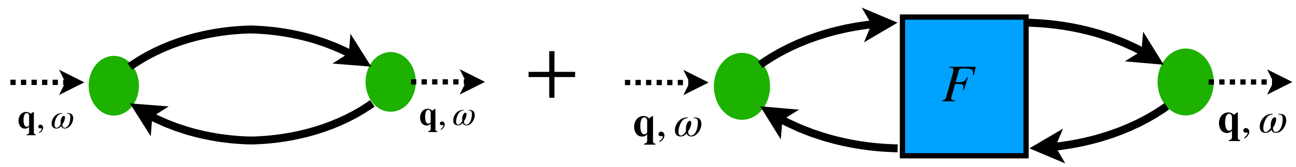
$$G^{(2)}_{imp} \longrightarrow \tilde{\chi}_{imp} \nearrow$$

$$\Gamma_{imp} = \tilde{\chi}^{-1}_{imp} - \tilde{\chi}^{-1}_{imp,0} \qquad \tilde{\chi}^{-1}_{lattice} = \Gamma_{lattice} + \tilde{\chi}^{-1}_{lattice,0}$$

Does not feedback in DMFT self-consistency loop

Are vertex corrections important ?

$\chi_{AB}(q,\omega) =$

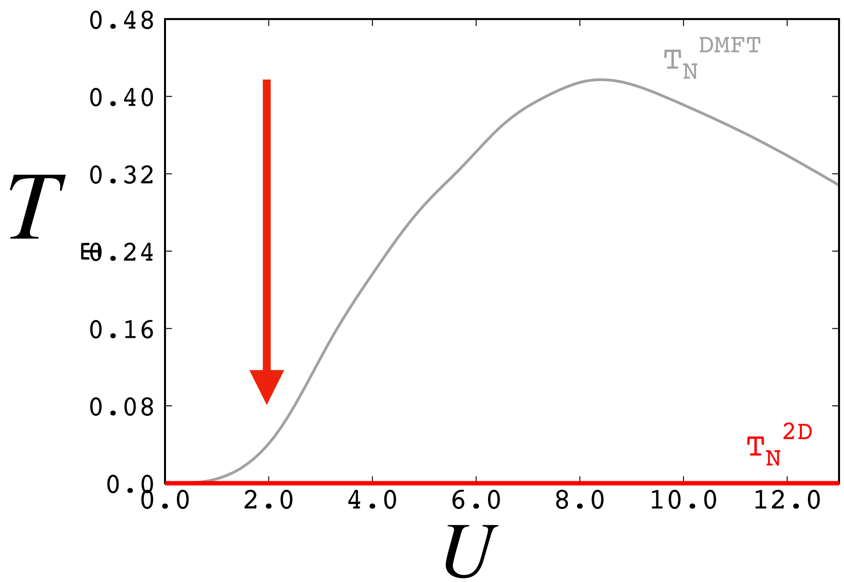


- Magnetic susceptibility
  - Non interacting case. Lindhard function $\chi_{\text{charge}} = \chi_{\text{spin}} \propto G_0 G_0$
  - Mott insulator: charge gap vs low energy spin excitations
- Conductivity
  - Cancellation of vertex corrections by symmetry in DMFT

Simple example

- 1 band Hubbard model, 2d square lattice, DMFT.

M. Jarrell 92
Curves from T. Schaefer

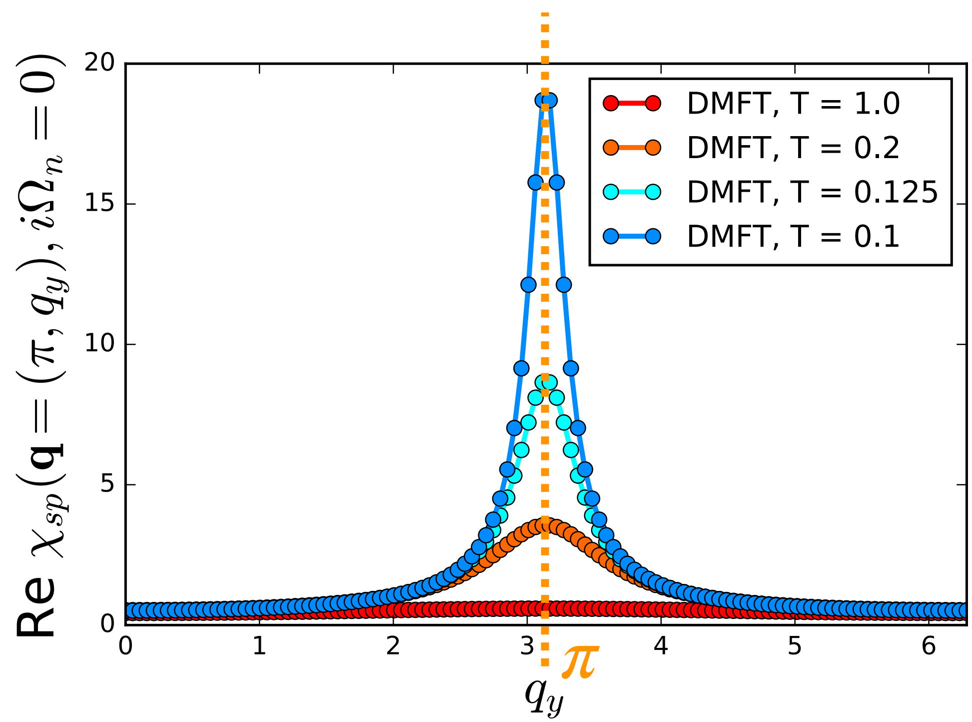


Ornstein-Zernike form

$$\chi(q, i\Omega_0) = \frac{A}{(q - Q_{AF})^2 + \xi^{-2}}$$

$$Q_{AF} = (\pi, \pi)$$

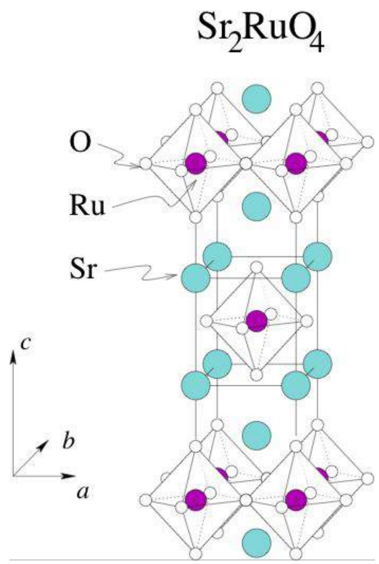
$\chi(q = (\pi, q_y), \omega = 0)$



Sr_2RuO_4

- Ab initio : DFT + DMFT

Cf Talk by Hugo Strand
ArXiv:1904.07324

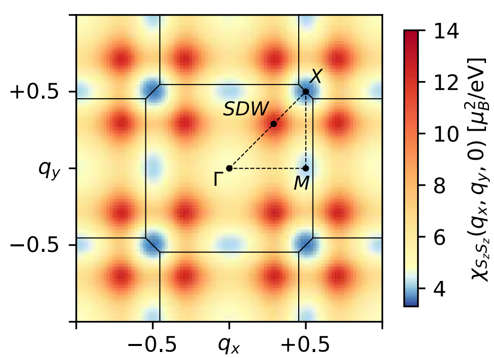


Cf Talk by Manuel Zingl
ArXiv:1902.07324

Magnetic susceptibility

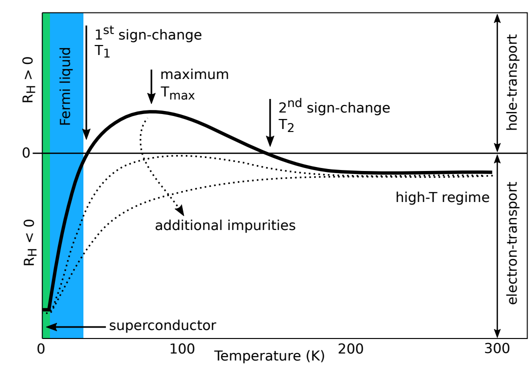
$$\chi_{ab}(q, \omega = 0)$$

- Structure of magnetic excitations ?



Hall effect

- Origin of sign change of Hall coefficient with T ?



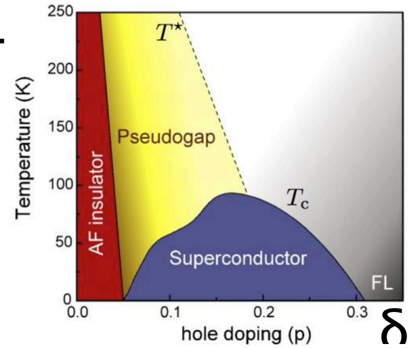
Cluster DMFT susceptibilities: examples on Hubbard model

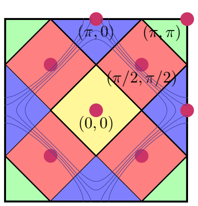
Pseudogap in cuprate

Xi Chen et al. Nat.Comm 2016

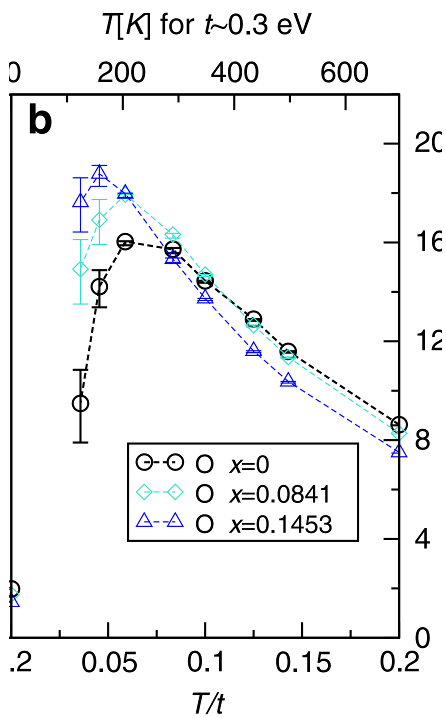
Relaxation rate vs T for different doping

$$\frac{1}{T_1 T} \propto \lim_{\nu \to 0} \sum_q f(q) \frac{\chi''(q,\nu)}{\nu}$$





$$\frac{1}{T_1 T}$$

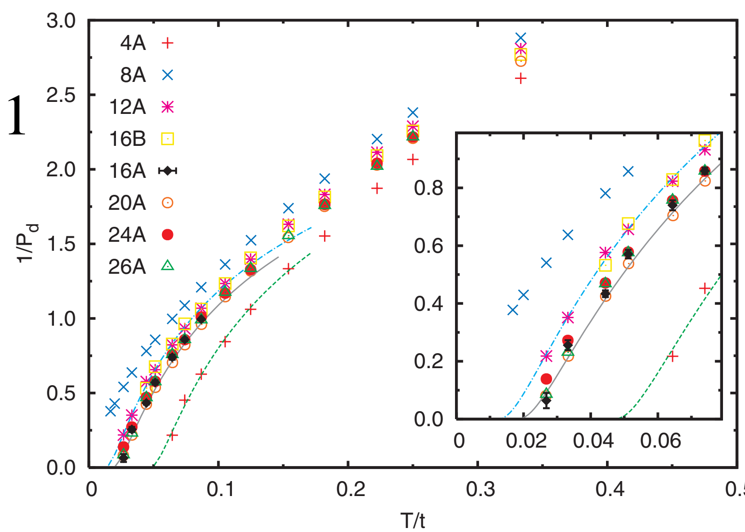


Superconductivity

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

Large clusters χsc
U = 4t
Tc ≈ 0.02t

χ^{-1}



T/t

Part II

Beyond (cluster) DMFT

Trilex, DΓA, Quadrilex

A self consistent approximation at the two-particle level

Toschi et al. (2007)

T. Ayral et al. (2015-2016)

Functionals

- A general method in statistical physics:
  - Find relevant physical quantity X
  - Build a functional $\Gamma(X)$ using Legendre transforms.
  - Approximate the "complicated" part of $\Gamma(X)$
- Examples:
  - magnetic transition X =m
  - Density functional theory $X = \rho(x)$, electronic density
  - DMFT, X = G

Trilex, Quadrilex, DΓA
X = Some two-particle Green function

DMFT

- Hubbard model action. Add a quadratic source h

$$S = \int d\tau d\tau' \sum_{ij} c^\dagger_{i\sigma}(\tau)\left(g^{-1}_{0ij} + h_{ij}\right)(\tau-\tau')c_{\sigma j}(\tau') + \int d\tau U \sum_i n_{i\uparrow}(\tau) n_{i\downarrow}(\tau)$$

- Free energy is a function of h

$$\Omega[h] = -\log \int \mathcal{D}[c^\dagger c] e^{-S[h]}$$

$$G_{ij}(\tau-\tau') = -\left\langle c_i(\tau) c^\dagger_j(\tau')\right\rangle = \frac{\partial \Omega}{\partial h_{ji}(\tau'-\tau)}$$

- Legendre transform to eliminate h for G.

$$\Gamma[G] = \Omega[h] - \mathrm{Tr}(hG)$$

$$\Gamma[G] = \underbrace{\mathrm{Tr}\ln G - \mathrm{Tr}(g_0^{-1}G)}_{U=0 \text{ term}} + \Phi[G]$$

$$\frac{\partial \Gamma[G]}{\partial G} = h = 0$$

$$\Sigma_{ij} = \frac{\delta \Phi}{\delta G_{ji}}$$

Idea

- Functional of one-particle Green function

$$\Gamma[G,\lambda] = \underbrace{\mathrm{Tr}\ln G - \mathrm{Tr}(g_0^{-1}G)}_{U=0 \text{ term}} + \Phi_{LW}[G]$$

- Eliminate λ by Legendre transform
- Higher functionals of vertex, two particle functions
  De Dominicis, Martin, Math. Phys. 1, 1964.
- Idea : these objects are more local than the self-energy. Approximation on these functionals rather than Φ_{LW}.

Two ways to implement this idea :Trilex, DΓA

I - TRILEX

T. Ayral & O.P. Phys. Rev. B 92, 115109 (2015)
T. Ayral & O.P. Phys. Rev. B 94, 075159 (2016)
T. Ayral, J Vucicević, and O.P. Phys. Rev. Lett. 119, 166401 (2017)

Electron-boson language

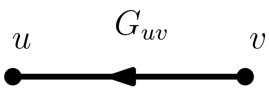
$$S_{\mathrm{eb}} = \bar{c}_u \left[-G_0^{-1}\right]_{uv} c_v + \frac{1}{2}\phi_\alpha \left[-W_0^{-1}\right]_{\alpha\beta} \phi_\beta + \lambda_{uv\alpha}\bar{c}_u c_v \phi_\alpha$$

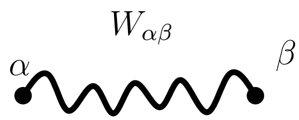
$$\varphi_\alpha \equiv \langle \phi_\alpha \rangle$$
$$W^{\mathrm{nc}}_{\alpha\beta} \equiv -\langle \phi_\alpha \phi_\beta \rangle$$
$$G_{uv} \equiv -\langle c_u \bar{c}_v \rangle$$

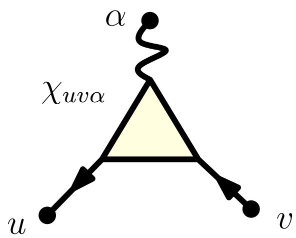
- Hubbard model : decouple in spin/charge channel.
- Coulomb interaction. Beyond GW + DMFT ?
- Electron-phonon.
- Low energy effective spin fermion model.

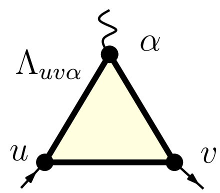
The 3PI functional

De Dominicis Martin, Math. Phys. 1, 1964.









$$G^{(3)}_{uv\alpha} \equiv \langle c_u \bar{c}_v \phi_\alpha \rangle$$

$$\Lambda_{uv\alpha} \equiv G^{-1}_{xu} G^{-1}_{vw} W^{-1}_{\alpha\beta} G^{(3)}_{wx\beta}$$

$$\Gamma_3[G, W, G^{(3)}] \equiv \Gamma_2[G, W, \lambda] + \lambda \cdot G^{(3)}$$

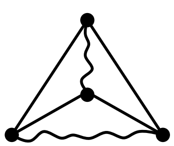
$$\Gamma_3[G, W, G^{(3)}] = -\mathrm{Tr}\log\left[G^{-1}\right] + \mathrm{Tr}\left[\left(G^{-1} - G_0^{-1}\right) G\right]$$

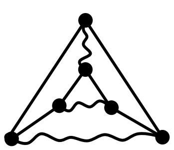
$$+ \frac{1}{2}\mathrm{Tr}\log\left[W^{-1}\right] + \frac{1}{2}\mathrm{Tr}\left[W W_0^{-1}\right]$$

$$+ \frac{1}{2}\Lambda_{ux\alpha} G_{wx} G_{uv} W_{\alpha\beta} \Lambda_{wv\beta} + \mathcal{K}[G, W, G^{(3)}]$$

$\Phi[G, W]$

3PI diagrams

 $\in \mathcal{K}$

 $\notin \mathcal{K}$

$$\Lambda_{uv\alpha} = \lambda_{uv\alpha} - \frac{\partial \mathcal{K}[G, W, G^{(3)}]}{\partial G^{(3)}_{uv\alpha}}$$

3PI diagrams

Vertex corrections

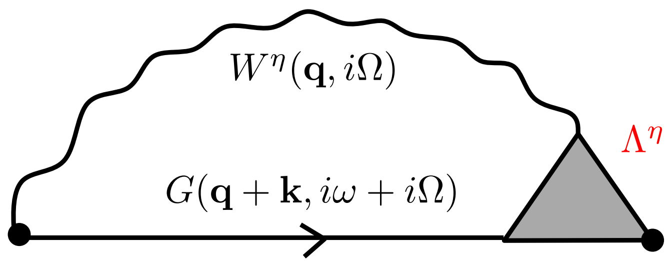
"3PI Dyson equation"

TRILEX (triply-irreducible local expansion).

$$\mathcal{K}^{\rm latt}(G, W, G^{(3)}) \approx \sum_i \mathcal{K}_{atomic}(G_{ii}, W_{ii}, G^{(3)}_{iii})$$ + *Cluster Trilex*

$$\boxed{\Lambda^\eta(\mathbf{q}, \mathbf{k}, i\omega, i\Omega) \approx \Lambda^\eta_{\rm imp}(i\omega, i\Omega)}$$

$$\Sigma(\mathbf{k}, i\omega) = \sum_{\eta=ch,sp}$$



Weak coupling, U ⟶0

- No vertex correction: Λ =λ
- Spin fluctuation diagram

Atomic limit, t⟶0

- Exact in this limit
- Mott physics (DMFT)

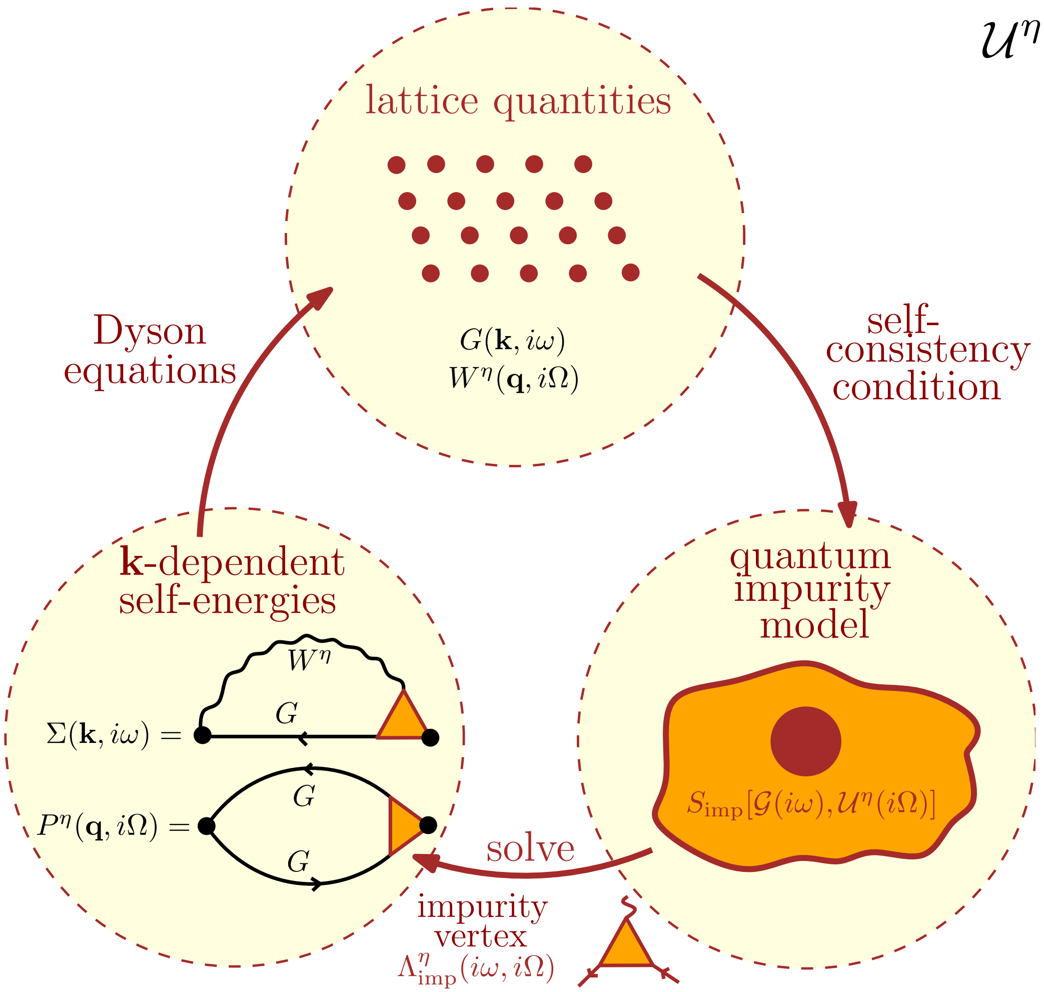
Spin-fluctuation and DMFT are two “asymptotic” regimes of TRILEX.

Summary of equations

T. Ayral & OP Phys. Rev. B 92, 115109 (2015),
Phys. Rev. B 94, 075159 (2016)

$$\mathcal{G}(i\omega) = \left[G_{\text{loc}}^{-1}(i\omega) + \Sigma_{\text{loc}}(i\omega)\right]^{-1}$$

$$\mathcal{U}^{\eta}(i\Omega) = \left[\left[W_{\text{loc}}^{\eta}(i\Omega)\right]^{-1} + P_{\text{loc}}^{\eta}(i\Omega)\right]^{-1}$$

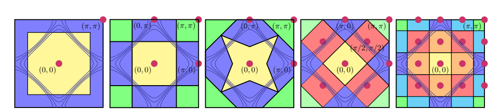


Self-consistent impurity model

$$S_{\text{imp}} = -\iint_0^{\beta} d\tau d\tau' \sum_{\sigma} c^*_{\sigma\tau}\mathcal{G}(\tau-\tau')c_{\sigma\tau'}$$
$$+\frac{1}{2}\iint_0^{\beta} d\tau d\tau' \mathcal{U}^{ch}(\tau-\tau')n(\tau)n(\tau')$$
$$+\frac{1}{2}\iint_0^{\beta} d\tau d\tau' \mathcal{U}^{sp}(\tau-\tau')\vec{S}(\tau)\cdot\vec{S}(\tau')$$

Retarded interaction (charge & spin)

- Cluster TRILEX & benchmark

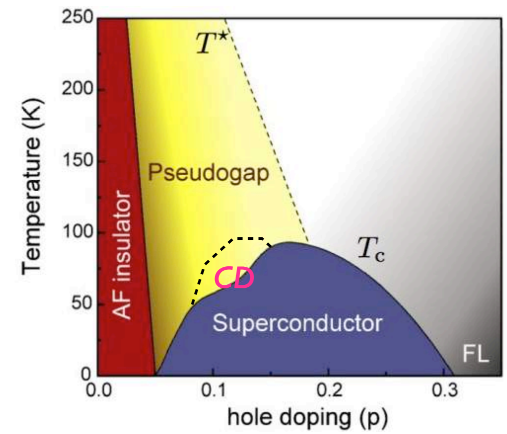


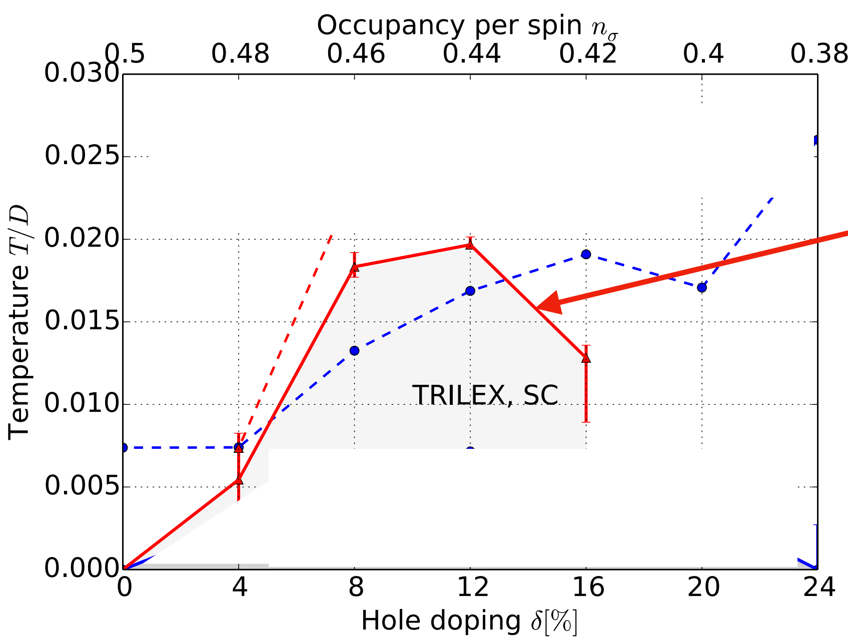
T. Ayral et al. Phys. Rev. Lett. 119, 166401 (2017)

Superconductivity

J. Vucicevic, et al. Phys. Rev. B 96, 104504 (2017)

- Proof of concept, with Hubbard model
- d-SC with one site impurity model (≠ cluster DMFT).
- From high temperature, compute leading instability.





Strong interaction

d-SC & Mott physics

SC disappear close to Mott insulator

- Comparison cluster DMFT ?

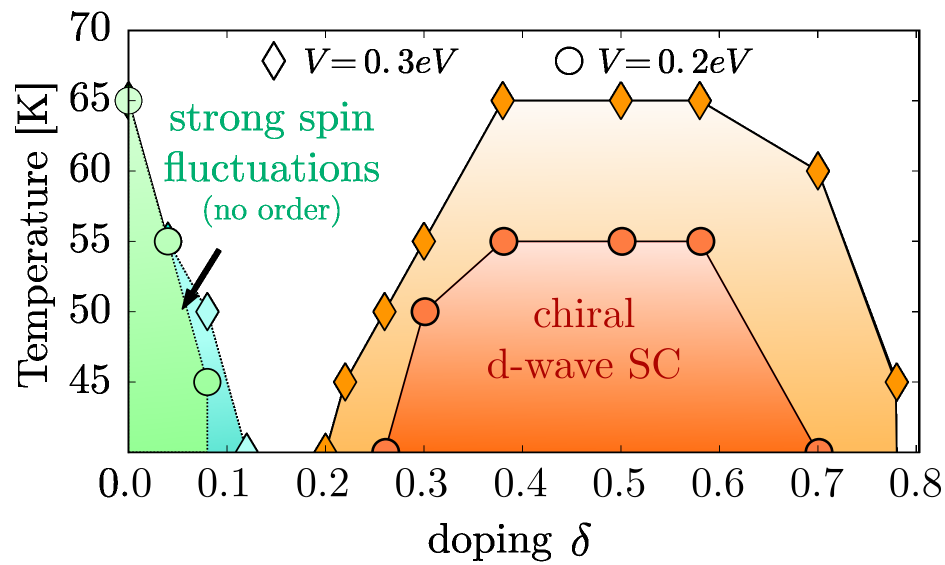
Long range interaction & superconductivity

X. Cao, T. Ayral, Z. Zhong, OP, D. Manske, P. Hansmann Phys. Rev. B 97, 155145 (2018)

- Adatoms on a Si(111) surface.
- Extended Hubbard model with long range Coulomb interaction, triangular lattice

$$H = \sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \frac{1}{2} \sum_{ij} U_{ij} n_i n_j - \mu \sum_i n_i$$

$$U_q = U_0 + V \sum_{i \neq 0} \frac{e^{iqR_i}}{|R_i|}$$



- Prediction : (chiral) d-wave superconductivity (TRILEX and EDMFT)

2- DΓA / Quadrilex

Toschi, A., A. A. Katanin, and K. Held, Phys. Rev. B 75, 045118 (2007)

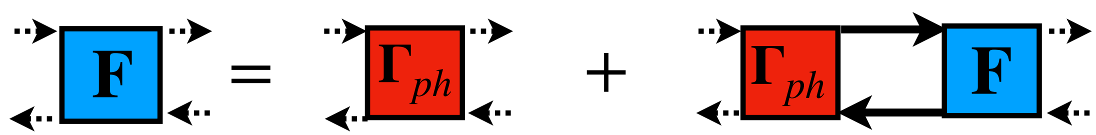
Rohringer et al. Rev. Mod. Phys 90 025003 (2018)

Ayral, O.P. Phys. Rev. B 94, 075159 (2016)

Parquet equations

- 3 Channels for two-particle reducibility $r = ph, \overline{ph}, pp$
- Bethe Salpeter equation in each channel
  Φ_r, Γ_r: reducible/irreducible vertex in channel r

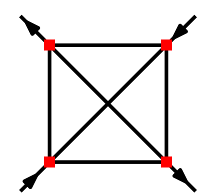
$$F = \Gamma_r + \Phi_r$$

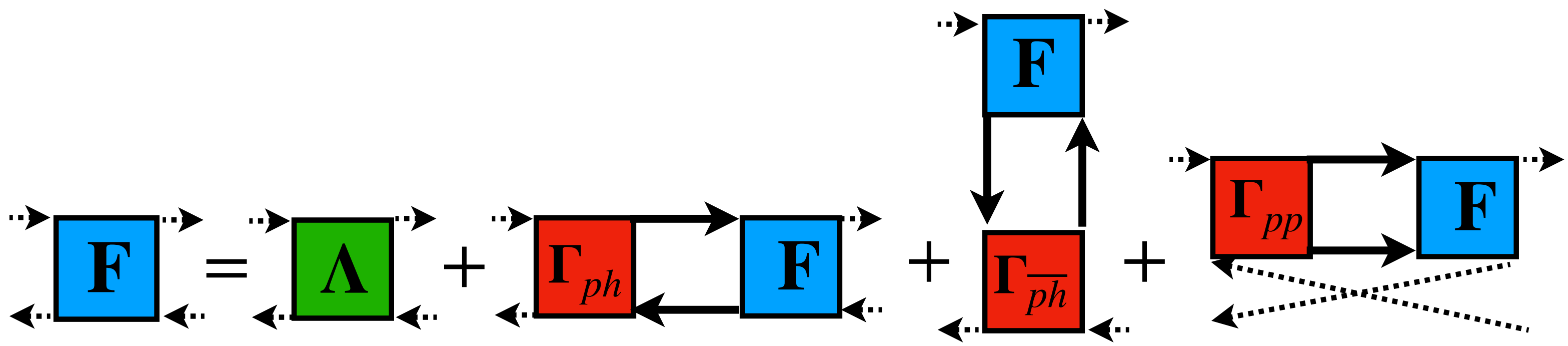


$$\Phi_r = \Gamma_r \tilde{\chi}_{0r} F$$

- $\Lambda^{(4)}$: Fully irreducible vertex (in all channels)

First order of Λ





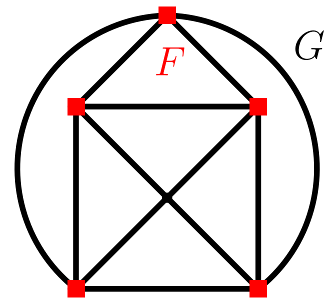
$$F = \Lambda^{(4)} + \Phi_{ph} + \Phi_{\overline{ph}} + \Phi_{pp}$$

Quadrilex/DΓA

- Second Legendre transform *De Dominicis, Martin, Math. Phys. 1, 1964.*

4PI diagrams

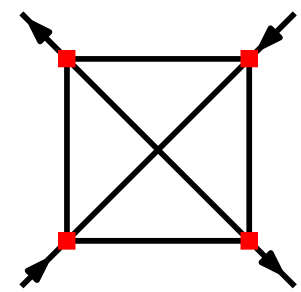
$$\Gamma_4[G, G^{(2)}] \equiv \Gamma[G, U] - \frac{1}{2} U \cdot G^{(2)}$$



$$\Gamma_4[G, G^{(2)}] = \Gamma_{4,0}[G, G^{(2)}] + \mathcal{K}_4[G, G^{(2)}]$$

$$\Lambda^{(4)}_{u\bar{u}v\bar{v}} = \lambda^{(4)\mathrm{bare}}_{u\bar{u}v\bar{v}} - 2\frac{\partial \mathcal{K}_4[G, G_2]}{\partial G_{2\bar{u}u\bar{v}v}}$$

$$T\Omega = \langle H \rangle + T\Gamma_4$$



- Quadrilex approximation *T.Ayral & OP (2016)*

$$\mathcal{K}_4^{\mathrm{QUADRILEX}}[G_{\mathbf{R}_1\mathbf{R}_2}, G_{2,\mathbf{R}_1\mathbf{R}_2\mathbf{R}_3\mathbf{R}_4}] \equiv \sum_{\mathbf{R}} \mathcal{K}_4[G_{\mathbf{RR}}, G_{2,\mathbf{RRRR}}].$$

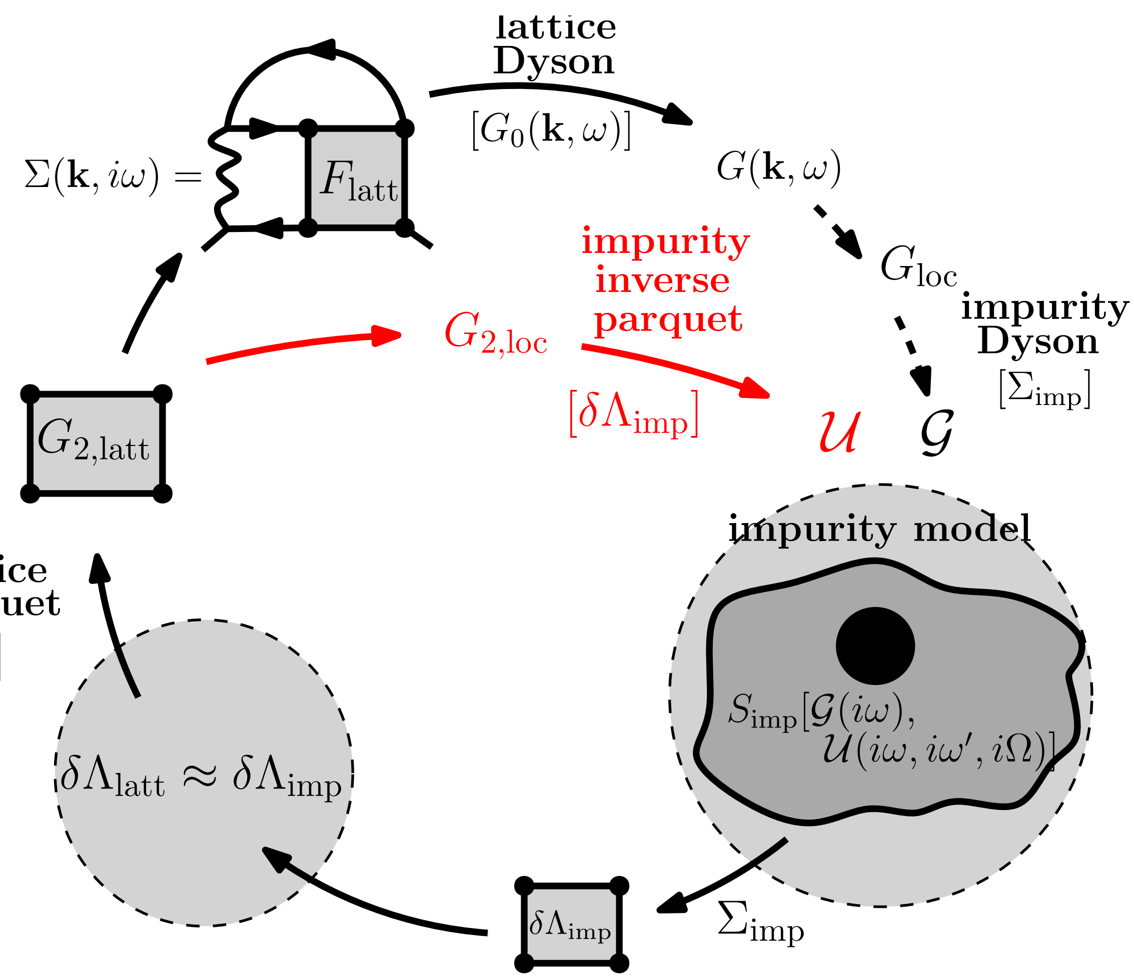
- Solvable with impurity model

$$S^{\mathrm{Quadrilex}}_{imp} = -\int d\tau d\tau' c^\dagger_\sigma(\tau) \mathcal{G}^{-1}(\tau - \tau') c_\sigma(\tau') +$$
$$\frac{1}{2}\int d\tau_1 d\tau_2 d\tau_3 d\tau_4 \mathcal{U}_{\sigma_1\sigma_2\sigma_3\sigma_4}(\tau_1, \tau_2, \tau_3, \tau_4) c^\dagger_{\sigma_1}(\tau_1) c_{\sigma_2}(\tau_2) c^\dagger_{\sigma_3}(\tau_3) c_{\sigma_4}(\tau_4)$$

DΓA vs Quadrilex

- DΓA Toschi et al. 2007
  No renormalisation of the interaction in the impurity model

- Both Quadrilex/DΓA are (in theory) cluster-controlled.



Ladder DΓA

A. Toschi et al (2007)
Rohringer et al. Rev. Mod. Phys 90 025003 (2018)

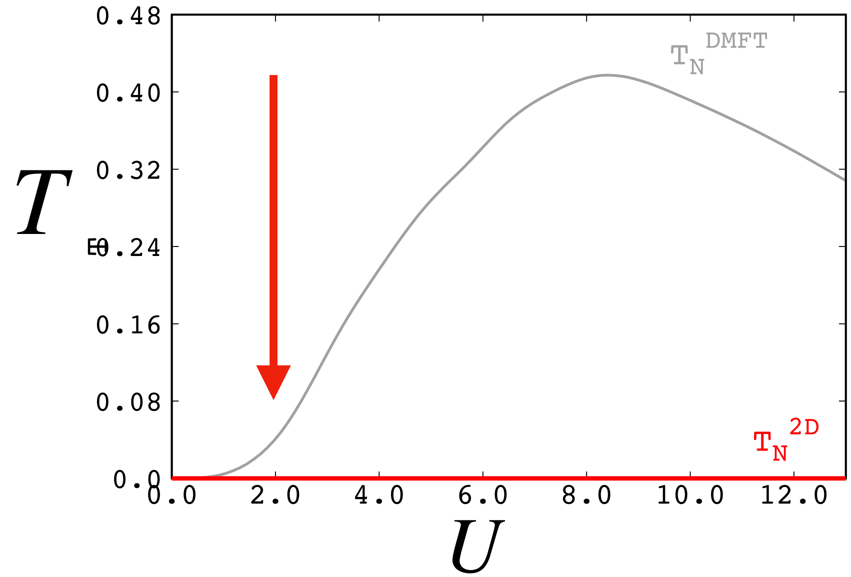
- Solving Parquet equations is hard ! (not a matrix equation).
- In most cases, further approximation are made.
  - Ladder DGA
    - Approximation on the irreducible vertex in PH channel only Γ
    - Solve Bethe-Salpeter in this channel, recompute self-energy

$$\Gamma_{latt} = \Gamma_{imp}$$

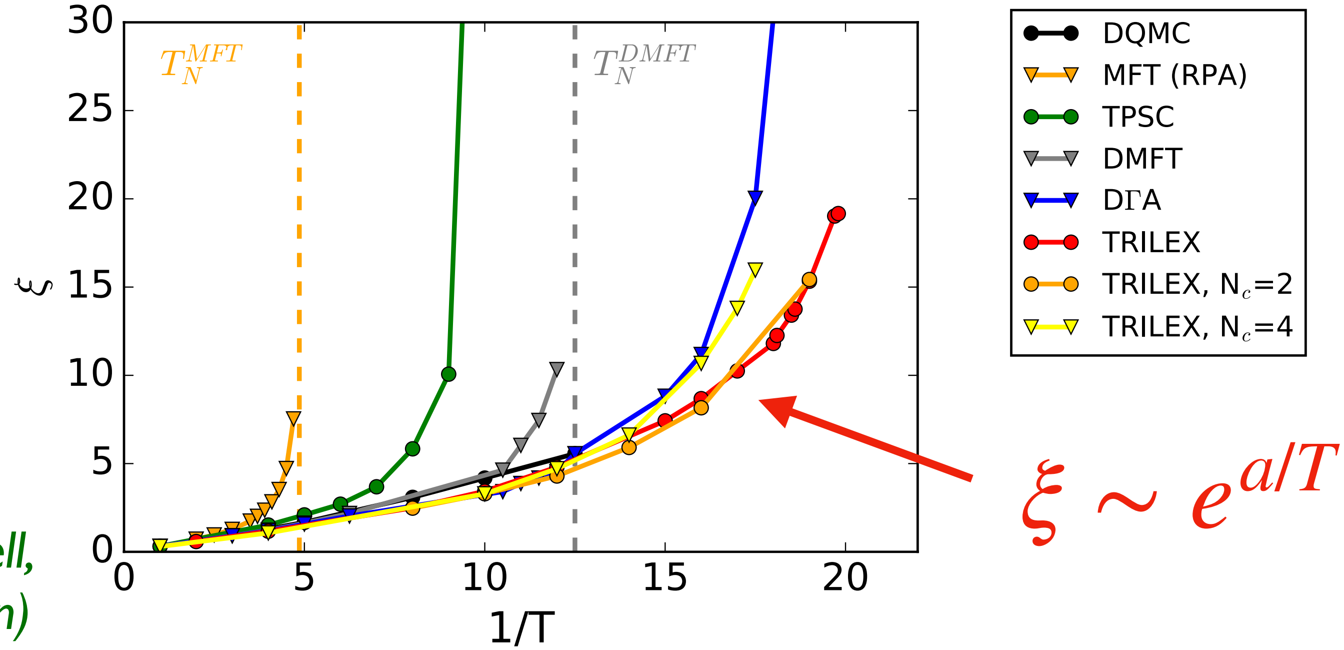
  - One shot computation (no self-consistency).
  - "Moriya" correction (ad-hoc constant to adjust some sum rules)

Weak coupling 2d Hubbard model

- Half filled.
- DMFT has AF order (mean field).



- Correlation length ξ (T) (from a fit of χ(q,0)), U= 2t

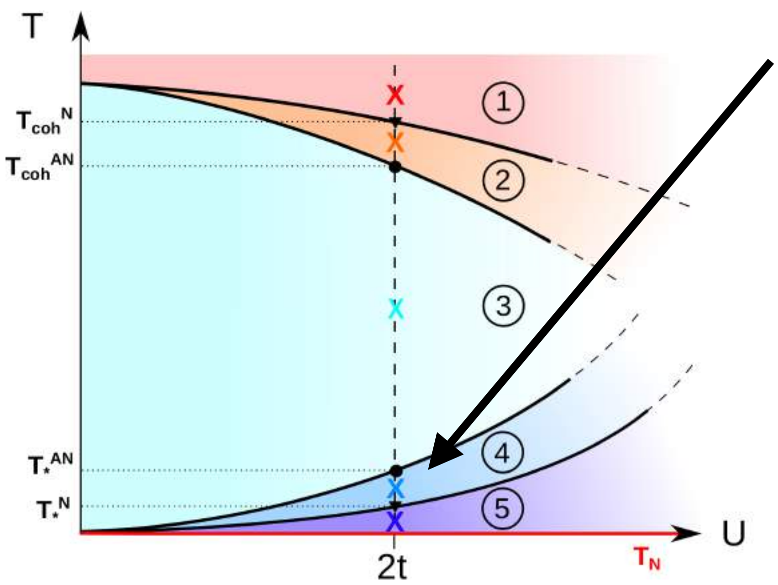


From T. Schaefer, N. Wentzell, Y.Y. He et al. (in preparation)

Weak coupling Hubbard model

- Schematic phase diagram

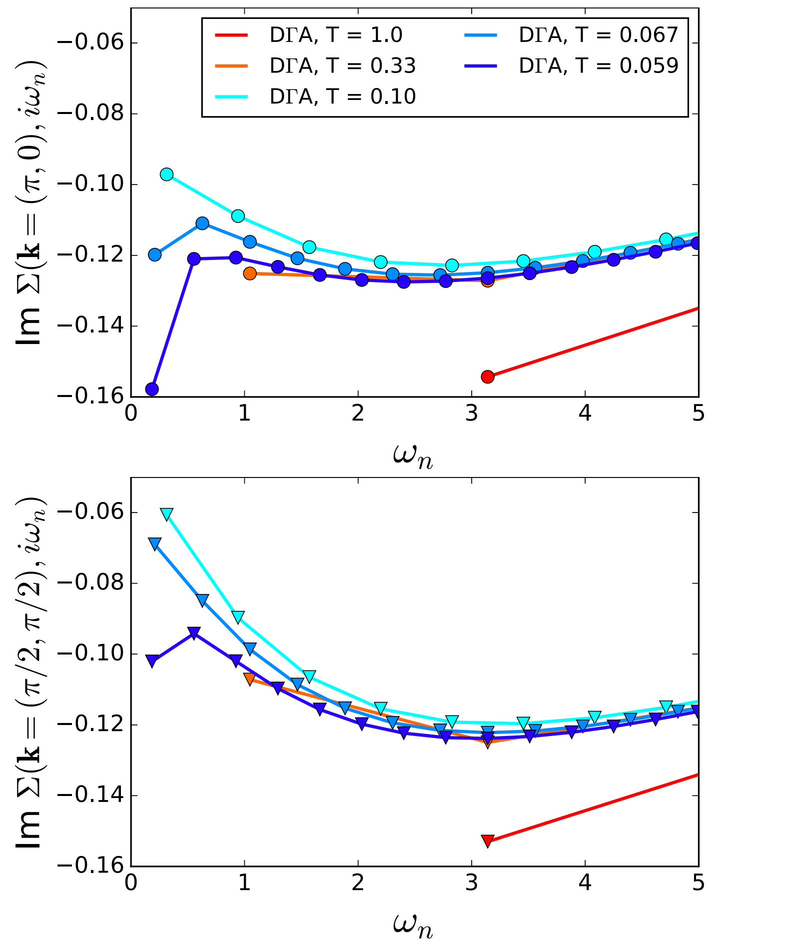
$T_{Néel}$ *in DMFT*



$Im\Sigma(k, \omega)$ in DΓA

Antinode

Node

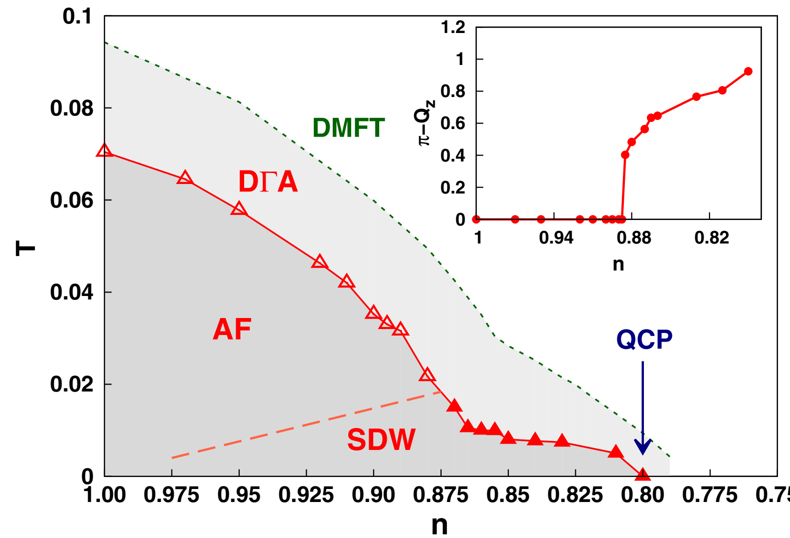


- See also diagrammatic QMC
  F. Simkovic et al.(arXiv:1812.11503)

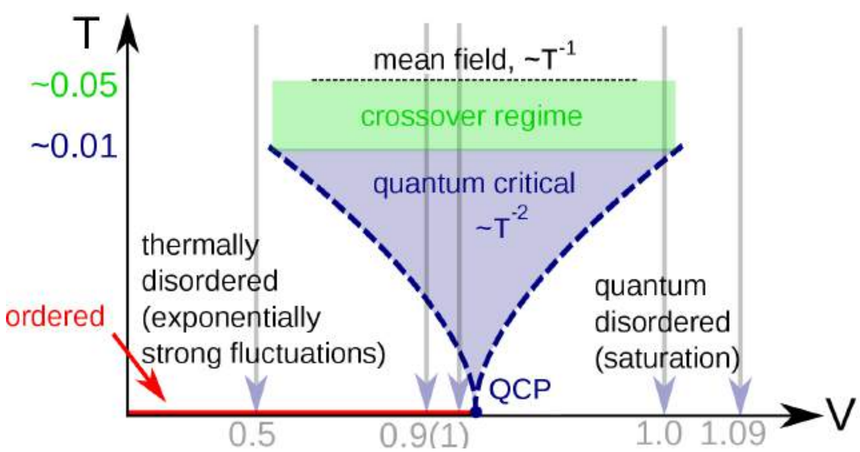
T. Schaefer et al. PRB 125109 (2015),
J. Magn. Magn. Mat. 400, 107(2016)
(and in preparation)

Quantum critical points

- 3d Hubbard model.
  QCP destruction of AF by doping
  - Computation of critical exponents
  - Control ? Clusters ?



T. Schaefer et al.
Phys. Rev. Lett. 119, 046402 (2017)

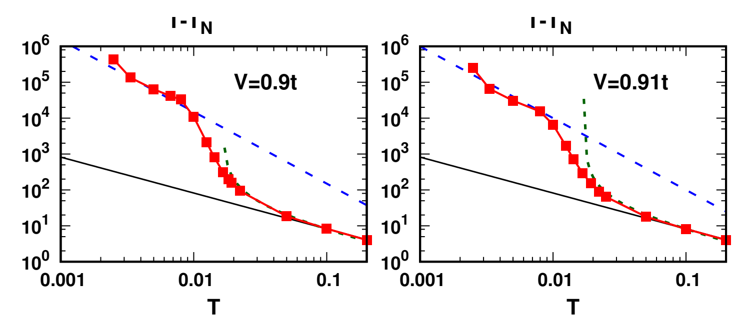


T. Schaefer et al.
Phys. Rev. Lett. 122, 227201 (2019)

- Periodic Anderson model

$$\mathcal{H} = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} d^\dagger_{\mathbf{k}\sigma} d_{\mathbf{k}\sigma} + \varepsilon_f \sum_{i\sigma} f^\dagger_{i\sigma} f_{i\sigma}$$
$$+ U \sum_i n_{f,i\uparrow} n_{f,i\downarrow} + V \sum_{i,\sigma} \left[d^\dagger_{i\sigma} f_{i\sigma} + f^\dagger_{i\sigma} d_{i\sigma} \right]$$

$$\chi \sim T^{-2}$$

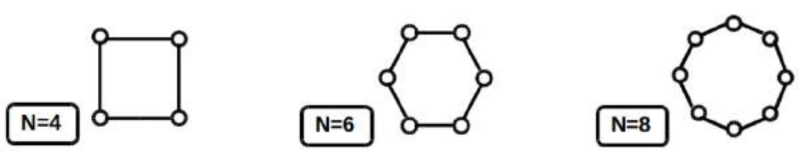


DΓA with full parquet equations

- Parquet equations are hard to solve.
  Not a matrix equation.
  Limited to small resolution (or small a systems,).

Yang et al. Phys. Rev. E 80, 046706 (2009),
Tam et al Phys. Rev. E 87, 013311 (2013)
Li et al. Phys. Rev. B 93, 165103 (2016)

- Examples
  - Polariton in strongly correlated systems *A. Kauch et al. arXiv:1902.09342*
  - "Nanorings" benchmarks



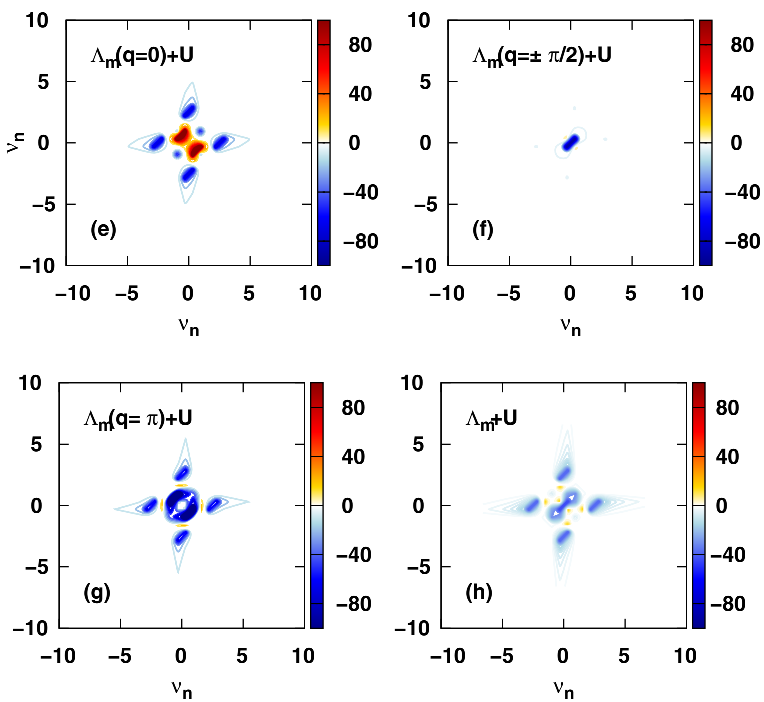
A.Valli et al.
PRB 91, 115115 (2015))

- How local is the irreducible vertex ? Or Trilex vertex ?

How local is the vertex ?

Λ(4)

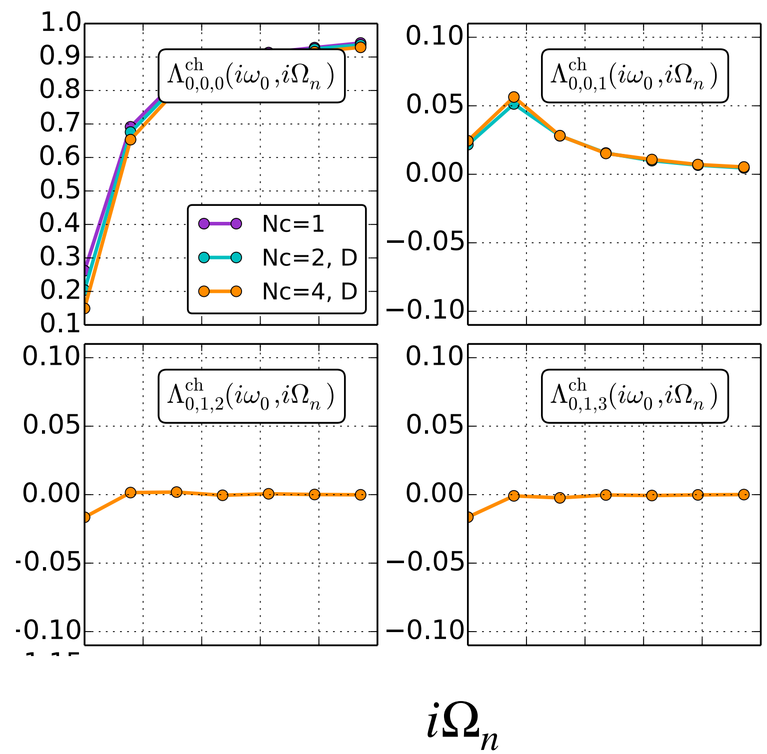
- Some results with cluster DMFT
  T. Maier et al. PRL. 96, 047005. (2006)
- Nanoring benchmarks :
  in some cases, strong q dependence.
  A. Valli et al. PRB 91, 115115 (2015))



- Cluster DΓA corrections ?

Cluster Trilex Λ

- Non local only
  at low frequencies

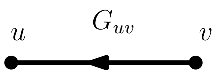


Summary

A family of methods

DMFT (2PI)

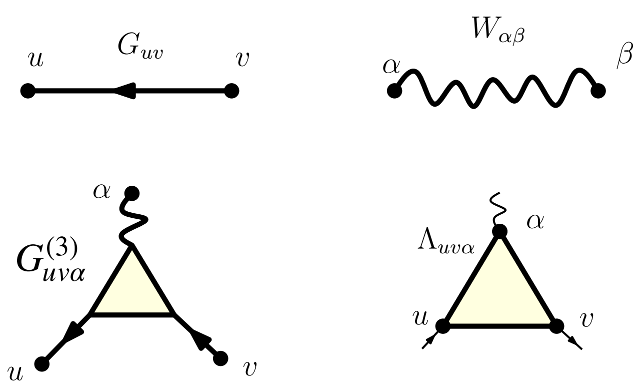
$$\Sigma = \frac{\delta \Phi_{\mathrm{LW}}}{\delta G}$$



Trilex (3PI)

T.Ayral & OP (2015)

$$\Lambda_{uv\alpha} = \lambda_{uv\alpha} - \frac{\partial \mathcal{K}[G, W, G^{(3)}]}{\partial G^{(3)}_{uv\alpha}}$$

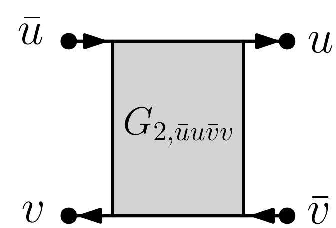


Quadrilex (4PI)/ DΓA

Toschi et al. 2007

T.Ayral & OP (2016)

$$\Lambda^{(4)}_{u\bar{u}v\bar{v}} = \lambda^{(4)\mathrm{bare}}_{u\bar{u}v\bar{v}} - 2\frac{\partial \mathcal{K}_4[G, G_2]}{\partial G_{2\bar{u}u\bar{v}v}}$$



- Beyond DMFT, a family of approaches with two-particle self-consistency
- Solved with an auxiliary quantum impurity model
- Local approximations for vertex instead of self-energy.
- Controlled by cluster extensions

Perspectives

- Work in progress :
  - More applications
  - Can we control DΓA with clusters ?
  - Quadrilex : is it better to have a self-consistent interaction ?

Collaborators

Thomas Ayral

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Nils Wentzell

Thomas Schäfer

Thank you for your attention