Electronic correlation at the 2P-level:

An intro to diagrammatic extensions of DMFT with applications of DTA (spin fluctuations, pseudogap, superconductivity)

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- *1. Intro:* DMFT as a starting point
- 2. Basics of its diagrammatic extensions

- 3. How *nonperturbative* information is ``encoded'' in the DMFT vertex functions
- 4. D Γ A algorithms: different flavours
- 5. Pedagogical discussion of relevant results

Conclusions & Outlook

DMFT in a nutshell

$$
\sum_{i} \sum_{j=i} = \delta_{ij} \Leftrightarrow \Sigma(\vec{k}, \omega) = \Sigma(\omega)
$$

the self-energy is **local !!**

high connectivity/dimensions

v W. Metzner & D. Vollahardt, PRL (1989)

v A.Georges & G. Kotliar, PRB (1992)

è **local,** but **all orders** included**!!** è **non perturbative** in **U!!**

DMFT algorithm: Self-consistency at the 1P level

★ starting point :

1P- and 2P-self-consistency of DMFT \star **1P-level :** $G_{ii} = G_{AIM}$ (DMFT self-consistency) \sum \vec{k} $G(\vec{k}, \nu) = G_{AIM}(\nu)$ always verified in DMFT calculations \sum \star **2P-level :** $\boldsymbol{\Gamma}_{ijkl}^{2PI} = \boldsymbol{\Gamma}_{jij}^{2PI} \delta_{ijk} \delta_{jl} = \boldsymbol{\Gamma}_{AlM}^{2PI} \sum \ \sum \ \chi(\vec{q}, \omega) = \chi_{AIM}(\omega)$ **d = ∞** DMFT is exact ✓

 \bar{q} $\sin d = \infty : \chi(\vec{q}, \omega) \equiv \chi_{AIM}(\omega) \ \forall \vec{q} \text{ (except special momenta)}$

v A. Georges et al. RMP (1996)

v A. Georges et al. RMP (1996); A. Katanin et al. PRB (2009); G. Rohringer & AT, PRB (2016); L. Del Re & AT, PRB (2021)

From ∞ dimensions to ... "reality" !

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Diagrammatic extensions of DMFT

★ **Dynamical Vertex Approximation (DA)**

[⌘ *AT, Katanin, Held, PRB (2007)*]

★ **Dual Fermion (DF)** & **Dual Bosons (DB)** [⌘ *Rubtsov, Lichtenstein …, PRB (2008); Ann. Phys (2012)*]

★ **1Particle Irreducible approach**

[⌘ *Rohringer, AT et al., PRB (2013)*]

★ **DMF2RG**

[⌘ *Taranto, …,& AT; PRL (2014); Vilardi , Taranto & Metzner, PRB (2019)*]

★ **TRILEX, QUADRILEX**

[⌘ *Ayral & Parcollet, PRB 2015; PRB (2016)*]

REVIEWS OF MODERN PHYSICS, VOLUME 90, APRIL–JUNE 2018

Diagrammatic routes to nonlocal correlations beyond dynamical mean field theory

Diagrammatic extensions of DMFT

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2P-Feynman diagrams: (local) Green's & vertex functions

2P-Green's function:
$$
G_{\sigma_1, \sigma_2, \sigma_3, \sigma_4}^{(2)}(\tau_1, \tau_2, \tau_3, 0) = \langle \hat{c}_{\sigma_1}(\tau_1) \hat{c}_{\sigma_2}^{\dagger}(\tau_2) \hat{c}_{\sigma_3}(\tau_3) \hat{c}_{\sigma_4}^{\dagger}(0) \rangle
$$

Its Fourier Transform: $G_{\sigma_1 \sigma_2 \sigma_3 \sigma_4}^{(2)}(\omega, \nu, \nu') = \int_0^\beta d\tau_1 d\tau_2 d\tau_3 e^{i\nu\tau_1} e^{-i(\nu + \omega)\tau_2} e^{i(\nu' + \omega)\tau_3} G_{\sigma_1 \sigma_2 \sigma_3 \sigma_4}^{(2)}(\tau_1, \tau_2, \tau_3, 0)$

\rightarrow computable for AIM

single band: **ED** & **NRG** *[Kugler et al. PRX, (2021)]* general multi-band case: **CTQMC** *[TRIQS, w2dynamics, ALPS, ….]*

the lowest order :

1) parquet equation:

Relation to the physics?

• generalized local charge susceptibility for i Ω =0

v P. Chalupa et al., PRL (2021); S. Adler., …, & AT, SciPost Phys. (2024)

Anderson Impurity Model

• wide-band limit, half-filling

Physical response of the AIM • w2dynamics – CT-HYB

M.Wallerberger, *et.al,* CPC **235,** 388 (2019)

Physical response of AL & AIM • w2dynamics – CT-HYB

M.Wallerberger, *et.al,* CPC **235,** 388 (2019)

1.Step: Non interacting case/bubble term

2.Step: weak vs. strong-coupling

e.g.: intermediate temperature region $(T_K < T < U)$

v *P. Chalupa, T. Schäfer, M. Reitner, D. Springer, S. Andergassen, and A.T., PRL 126 056403 (2021)*

Phase diagram of the Hubbard model <u>idse diugrani of the Habit</u>

Algorithmic challenges

I. Approaches based on 2PI vertices

parquet-based methods

1 dynamical vertex approximation (**DA**)

QUADRILEX

 $\overline{\delta^2 \Phi_{LW}}$

 $\delta^2 G$

 $\neg 2PI$

=

c

[A. Toschi et al., PRB (2007); O. Gunnarsson et al., PRB (2016) T. Ayral et al. , PRB (2016); G. Rohringer et al. , PRB (2018); ….]

II. Multivaluedness of LW functional

iterative/self-consistent (=``bold'') Diagrammatic resummation

Diagrammatic Monte Carlo

Nested Cluster Schemes

[E. Kozik et al., PRL (2015); A.Stan et al., NJP (2015); R. Rossi et al. , PRB (2015); J. Vucicevic, et al. PRB (2018), ….]

The underlying physics of the nonperturbative regime

n′

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the dynamical vertex approximation (DΓA): a 2PI-based approach

AT, A. Katanin, K. Held, PRB (2007)

See also: PRB (2009), PRL (2010), PRL (2011), PRB (2012), PRB (2015), … Review: RMP (2018)

DMFT: all **1-particle** irreducible diagrams (=self-energy) are **LOCAL** !!

An inspiring example : DCA calculations of **k**-dependent vertex functions

... of increasing 2P-irreducibility

DCA, 2d-Hubbard model, $U=4t$, $n=0.85$, $v=v'=π/β$, $ω=0$, s. Th. Maier et al., PRL (2006) T=0.5t $-t$ t_t $\bf{DCA}, \ 2$ d-Hubbard model, **U**=4t, n=0.85, ν=ν'=π/β, ω=0, s.Th. Maier et al., PRI

Flowchart of the (full fledged) DA algorithm

Flowchart of the (full fledged) DA algorithm

Flowchart of the full fledged DA algorithm

➜ *Possible simplification, if the nonlocal fluctuation of one channel dominate:*

Possible simplification: the ladder DA algorithm

And … what about self-consistency?

 \cdot For the theory of the **QUADRILEX** approach, s. T. Ayral & O. Parcollet, PRB (2016)

Self-consistency of the ladder DA algorithm

*An approximation for the self-consistency: Moriya DA or ``*λ-*DA''*

A. Katanin et al, PRB (2009); G. Rohringer & AT, PRB (2016); J. Stobbe & G. Rohringer, PRB (2023)

² [−] *^U* ! ω**q** 2 $\frac{1}{2}$! *G*ν **k***G*^ν+^ω **^k**+**^q** *,* (3) A or Δ DFA $\prime\prime$ \boldsymbol{p} as a measure as \boldsymbol{p} 0*,***q** = −βδνν! **k** \mathbf{F} \overline{a} ⁰*,***^q** [−]! νν1ω Γ_{total} is the series the self-consistency ℓ calculates the full vertex on \mathcal{L} Salpeter equation in the relevant scattering channels. For \mathbf{r} is the formalism via a renormalization \mathbf{r} nressions for the Moriva D**Γ**Α or ``λ-D**Γ**Α' magnetism [49] as follows: **e Moriya D** Γ **A** corresponding to the charge \sim \sim \sim \mathbf{W} in Eq. (1) *Explicit expressions for the Moriya DΓA or ``λ-DΓA''*

(I) :
$$
\langle \chi_{\text{rel}}(\mathbf{q}, \omega) \rangle = \langle \chi_{\text{rel}}(\mathbf{q}, \omega) = ([\chi_r(\mathbf{q}, \omega)]^{-1} \cdot \langle \chi_{\text{rel}}) \rangle + \langle \chi_{\text{llm}} \rangle + \langle \chi_{\text{llm}} \rangle + \langle \chi_{\text{llm}} \rangle
$$

\nin channel $r(\text{eg. } m, d)$ to the term.

\n(II) :
$$
\chi_{r=m,d,\dots}^{\lambda}(\mathbf{q}, \omega) = ([\chi_r(\mathbf{q}, \omega)]^{-1} \cdot \langle \chi_{\text{rel}} \rangle)^{\frac{1}{\text{mass}}} \cdot \langle \chi_{\text{rel}} \rangle
$$

\nconvection of theorem

\n(III) :
$$
\sum_{k}^{\lambda,\nu} = \frac{Un}{2} - U \sum_{\omega q} \left[1 + \frac{1}{2} \gamma_{d,q}^{\nu\omega} (1 - U \chi_{d,q}^{\lambda,\omega}) - \frac{3}{2} \gamma_{m,q}^{\nu\omega} (1 + U \chi_{m,q}^{\lambda_m,\omega}) - \sum_{\nu'} \chi_{0,q}^{\nu'} \epsilon_{\text{rel}}^{\nu\nu'\omega} \right] G_{k+q}^{\nu+\omega}.
$$

\n(III) :
$$
\sum_{k}^{\lambda,\nu} = \frac{Un}{2} - U \sum_{\omega q} \left[1 + \frac{1}{2} \gamma_{d,q}^{\nu\omega} (1 - U \chi_{d,q}^{\lambda,\omega}) - \frac{3}{2} \gamma_{m,q}^{\nu\omega} (1 + U \chi_{m,q}^{\lambda_m,\omega}) - \sum_{\nu'} \chi_{0,q}^{\nu'} \epsilon_{\text{rel}}^{\nu\nu'\omega} \right] G_{k+q}^{\nu+\omega}.
$$

 $(1 \pm l$ $J \chi_{r,\mathbf{q}}^{\omega}$ $\int u \int_{r,\mathbf{q}}^{\nu\nu'\omega}$ and $\chi_{0,\mathbf{q}}^{\nu\nu'\omega} =$ $-\beta \delta_{\nu\nu'}$ \sum **c** $\left\langle \right\rangle$ $G^\nu_{\bf k} G^{\nu+\omega}_{\bf k+q}$, for further details, s. J. Stobbe & G. Rohringer, PRB (2023). function to a finite bath, it does not suffer from any statistical \mathcal{L} $- \beta \delta$, $\sum G^{\nu} G^{\nu + \omega}$ for further details s. I. Stobbe & G. Robringer, PRR $-\rho o_{\nu\nu'} \sum_{\mathbf{k}} \mathbf{G}_{\mathbf{k}} \mathbf{G}_{\mathbf{k}+\mathbf{q}}$, for further details, s. J. Stoppe & G. Kommiger, FKB. \mathbf{z} α \mathcal{V}^* $\gamma_{r,\mathbf{q}}^{\nu\omega} = \sum$ ν' $(\chi_{0,\mathbf{q}}^{\nu\nu'\omega})$ $\frac{\partial \nu^{V' \omega}}{\partial \mathbf{q}} \bigl(1 \pm U \, \chi_{r,\mathbf{q}}^{\omega} \bigr) \bigr)^{-1} \chi_{r,\mathbf{q}}^{\nu \nu' \omega} \quad \text{and} \ \ \chi_{0,\mathbf{q}}^{\nu \nu' \omega}$ [34,41,43,46], where only the spin channel has been renor- $-\beta\delta_{\nu\nu'}$ $\sum G_{\bf k}^{\nu}G_{{\bf k}+\alpha}^{\nu+\omega}$, for further details, s. J. Stobbe & G. Roh $\overline{\mathbf{k}}$ $\chi_{0,\mathbf{q}}^{\nu\nu'\omega} = -\beta \delta_{\nu\nu'} \sum$ **k** $G_{\mathbf{k}}^{\nu}G_{\mathbf{k}+\mathbf{q}}^{\nu+\omega}$, for further detai J. Stobbe & G. Rohringer, PRB (2023). with $\gamma_{r,\mathbf{q}}^{\nu\omega}=\sum(\chi_{0,\mathbf{q}}^{\nu\nu}\alpha(1\pm U\chi_{r,\mathbf{q}}^{\omega}))\left[\chi_{r,\mathbf{q}}^{\nu\nu}\right]\alpha^{2}\omega^{2}$ and $\chi_{0,\mathbf{q}}^{\nu\nu'\omega}=-\beta\delta_{\nu\nu'}\sum G_{\mathbf{k}+\mathbf{q}}^{\nu}$, for further details, s. J. Stobbe & G. Rohringer, PRB (2023).

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DΓA (=beyond DMFT) results in 3 dimensions

✔ **phase diagram** computed by **λ-DΓA:**

single band ${\bm H}$ ubbard ${\bm m}$ odel with nearest neibouring hopping in ${\bm d}$ =3 (@ half-filling), in unit of $\,t=$ 2 $\overline{\sqrt{6}}$

-DΓA results in 3 dimensions

✔ **phase diagram**: one-band Hubbard model in **d=3** (half-filling)

G. Rohringer, AT, et al., PRL (2011)

G. Rohringer, AT, et al., PRL (2011)

DΓA results in 3 dimensions: a quantitative comparison The transition curves *T*N(*U*) for DMFT (orange circles), the A results in **5** amierisions. a quantitutive companson in lD\$Adm giving rise to a higher transition temperature *T*^N

✔ **phase diagram** computed by **λ-DΓA:** picted in Fig. 6 where also results obtained with other methods

single band **Hubbard model** with nearest neibouring hopping in **d=3** (@ half-filling)

-DΓA results: the critical region

-DΓA results in 3 dimensions: the spectral properties

A. Katanin et al, PRB (2009); G. Rohringer & AT, PRB (2016)

-DΓA results in 3 dimensions: the spectral properties

From ∞ dimensions to ... "reality" !

3 *"There is life" … out of half-filling: -DΓA study of the* pseudogap in 2D

A (diverging) elephant in the room (of DΓA) ? $\mathbf{r} = \infty$ The DMFT calculations of the generalized local charge time \mathbf{I} to \mathbf{C} sample the one and two-particle Green's functions in the one and two-particle G

Should be DΓA called rather …``D∞A'' ?

[credit: G. Sangiovanni, 2013]

the number of crossed ¹ *^c* -lines and can then be used to *DRAME INC. INCKIV THIS* \cdots , i.e. \cdots , \cdots Hubbard model, coming from *U* = 0. Dashed red and orange lenhant is **not** a dr (HA) according to [9] as reference, where *nHA* is the number *No, luckly this elephant… is not a dangerous one:*

Working with 2PI vertices : The (non-problematic) ladder case

By exploiting the following identity the ladder diagrams of DTA can be exactly rewritten ...

... eliminating any explicit appearance of the (possibly dangerous) Γ_{am} !

G. Rohringer, AT , et al., PRB (2013); G. Rohringer et al., RMP (2018)

And, remarkably, this works **even** *at the parquet-DΓA level !!*

ü Important progress achieved by *Jae-Mo Lihm*, *Seung-Sup Lee*, *F. Kugler* & *D. Kiese*

(no spoiler here: preprint in preparation)

Conclusions:

