Self-consistent \textit{ab initio} DΓA approach

Josef Kaufmann,\textsuperscript{1} Christian Eckhardt,\textsuperscript{2,1} Matthias Pickem,\textsuperscript{1} Motoharu Kitatani,\textsuperscript{3} Anna Kauch,\textsuperscript{1} and Karsten Held\textsuperscript{1}

\textsuperscript{1}Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria
\textsuperscript{2}Institute for Theoretical Solid State Physics, RWTH Aachen University, 52074 Aachen, Germany
\textsuperscript{3}RIKEN Center for Emergent Matter Sciences (CEMS), Wako, Saitama, 351-0198, Japan

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We present and implement a self-consistent DΓA approach for multi-orbital models and \textit{ab initio} materials calculations. It is applied to the one-band Hubbard model at various interaction strengths with and without doping, to the two-band Hubbard model with two largely different bandwidths, and to SrVO\textsubscript{3}. The self-energy feedback reduces critical temperatures compared to dynamical mean-field theory, even to zero temperature in two-dimensions. Compared to a one-shot, non-self-consistent calculation the non-local correlations are significantly reduced when they are strong. In case non-local correlations are weak to moderate as for SrVO\textsubscript{3}, one-shot calculations are sufficient.

I. INTRODUCTION

Strongly correlated materials are becoming more and more relevant for technological applications. They are also utterly fascinating, not least because their theoretical study is intrinsically difficult. The actual calculation of correlated materials and their properties usually requires a combination of \textit{ab initio} methods and simplified model approaches. A very successful \textit{ab initio} method for studying strongly correlated materials is the combination of density functional theory \cite{1, 2} with the dynamical mean-field theory \cite{3-7} (DFT + DMFT) \cite{6-12}, which is capable of describing local electronic correlations very accurately. In systems where nonlocal correlations play an important role, e.g., in two-dimensional or layered systems, DMFT cannot predict the correct low temperature behavior. Cluster and diagrammatic extensions of DMFT \cite{13, 14} have been developed to cure this problem.

One such method is the \textit{ab initio} DΓA \cite{15-17} which extends the concept of the dynamical vertex approximation (DΓA) \cite{18, 19} to realistic materials calculations. It inherits from DMFT the non-perturbative treatment of strong local correlations, but on top of this also includes non-local correlations. To this end, a two-particle ladder is built with the local DMFT irreducible vertex and the non-local Green’s function as building blocks. These ladder diagrams then yield a non-local contribution to the self-energy.

Hitherto such \textit{ab initio} DΓA calculations have been restricted to so-called “one-shot” calculations without an update of the DMFT vertex and non-local Green’s function. Obviously, such a one-shot calculation is only expected to be reasonable as long as the non-local corrections to DMFT remain small. It also does not suppress the DMFT critical temperatures nor modifies the DMFT critical exponents. In the case of DΓA calculations for one-band models, so-far a Moriyasque λ-correction \cite{19, 20} was devised as a cure. It imposes a sum rule on the spin (or alternatively spin and charge) susceptibility, reduces the critical temperature and yields reasonable critical exponents\cite{21-23}. Superconductivity in cuprates \cite{24} and nickelates \cite{25} is described surprisingly accurate, even correctly predicted in the latter case. The extension to the multi-orbital case however makes this Moriyasque λ-correction impractical. One would need to introduce and determine various λ parameters for all spin-orbital combinations.

Another route has been taken in the closely related dual fermion approach \cite{26} with ladder diagrams \cite{27}. Here, the Green’s function is updated with the calculated non-local self-energy in a so-called “inner self-consistency”. Hitherto applied to one-band model Hamiltonians such as the Hubbard \cite{28} and Falicov-Kimball model \cite{29} yields very reasonable critical temperatures and exponents. Also a self-consistent update of the dual fermion vertex has been discussed \cite{30-32}.

In case of the DΓA such an update of the Green’s function has also been made, however only for the much more involved parquet DΓA \cite{33-37} \cite{38}. Here, besides the self-consistent update of the Green’s function and self-energy, all three scattering (ladder) channels are mutually fed back into all other channels through the parquet equation \cite{39-42}. The drawback is the extreme numerical effort needed to solve the parquet equations, which limits the method to one-band models so far \cite{33, 34, 36, 43}.

In this paper we present a self-consistent ladder DΓA (sc-DΓA) for multi-orbital models and materials. We update the Green’s function lines, as it is also done in parquet and dual fermion approaches but neither in the original \textit{ab initio} DΓA method nor in previous ladder DΓA calculations. This allows for a self-energy feedback into the ladder diagrams contained in the Bethe-Salpeter equation, and leads to substantial damping of the fluctuations in the respective scattering channel. Since this approach only requires a repeated evaluation of the \textit{ab initio} DΓA equations, its application to multi-orbital models is straightforward. Our results demonstrate that sc-DΓA works well for single- and multi-orbital systems and also when doping away from integer filling.

The paper is organized as follows: In Section II we introduce the Hubbard model (HM), our notation, and the DMFT. Furthermore we give an overview over the different variants of DΓA that were hitherto used. In
Section III we introduce our new way of doing DΓA self-consistently. Then, in Section IV, we present results for
the single-orbital Hubbard model on the square lattice
with nearest-neighbor hopping. This model has already
been extensively studied and our results can be compared
to the literature. Finally, in Section V, we present results
for SrVO$_3$ at room temperature.

II. MODEL AND FORMALISM

A. Multi-orbital Hubbard model

The Hamiltonian of the multi-orbital Hubbard model is

$$H_{\text{HM}} = \frac{1}{V_{\text{BZ}}} \int_{\text{BZ}} \text{d}k \sum_{lm\sigma} h_{lm}(k) \hat{c}_{kl\sigma} \hat{c}_{km\sigma} + \sum_{i} \sum_{il'm'n'm'} U_{il'm'n'} \hat{c}_{il\sigma} \hat{c}_{il'm\sigma} \hat{c}_{il'm'n\sigma} \hat{c}_{il'n\sigma}. \quad (1)$$

Here, the first term is the underlying tight-binding model, which can be obtained 	extit{ab initio} by Wannierization of a
bandstructure from density functional theory. The in-
tegral over the crystal momentum $k$ is taken over the
first Brillouin zone (BZ) with volume $V_{\text{BZ}}$. The operator
$\hat{c}_{km\sigma}^\dagger$ ($\hat{c}_{km\sigma}$) creates (removes) an electron with spin $\sigma$ in the Wannier orbital $m$ at momentum $k$ (the Fourier
transformed operators are labeled with unit cell index $i$
instead of $k$). The second term of Eq. (1) contains the
interaction of the electrons. While in principle 	extit{ab initio}
DΓA can include non-local interactions, we restrict our-
ourselves here to local ones. That is, in each unit cell $i$, the
matrix $U_{il'm'n'}$ parameterizes scattering events in which
local orbitals $l,l',m,m'$ are involved. In cases, where the
unit cell contains multiple atoms, the matrix elements
of $U_{il'm'n'}$ are non-zero only when all indices correspond
to interacting orbitals of the same atom (i.e., are local
interactions). This restriction can be relaxed, in principle,
to include also non-local interactions within the unit
cell, either defining the whole unit cell as “local” or in-
cluding the bare non-local interactions within the (then
non-local) vertex building block for ladder DΓA.

The physics of the Hubbard model is usually studied
in the framework of the Green’s function formalism. Our
computational methods additionally employ the Matsu-
bara formalism, where the one-particle Green’s function
for a system in thermal equilibrium at temperature
$T = 1/\beta$ is defined by

$$G_{lm}^k = -\int_0^\beta d\tau e^{i\nu \tau} \langle T_\tau \hat{c}_{kl} \hat{c}_{km}(0) \rangle. \quad (2)$$

Here, the 4-index $k = (i\nu, k)$ combines Matsubara fre-
quency $i\nu$ and crystal momentum $k$; $\tau$ is the imaginary
time. Spin indices were omitted here, since we consider
only paramagnetic systems with spin-diagonal Green’s
functions. The interacting Green’s function contains (in-
finitely) many connected Feynman diagrams that are, via
the Dyson equation (DE), captured by the self-energy:

$$\Sigma_{lm} = (i\nu + \mu)\delta_{lm} - h_{lm}(k) - [G_{lm}^k]^{-1}. \quad (3)$$

B. Dynamical mean-field theory

In most cases, it is completely infeasible to compute
$G_{lm}$ or $\Sigma_{lm}$ directly through these infinitely many Feyn-
man diagrams. Instead, one is bound to rely on approxi-
mations. In the DMFT approximation the self-energy is
assumed to be strictly local, or momentum-independent.
This becomes exact in infinite dimensions, while it still
remains an excellent approximation in three dimensions,
and even for many two-dimensional systems. As we illus-
rate in Fig. 1 in a very abstract way, DMFT consists of
two steps: First, one uses the $k$-integrated Dyson equation
(3) to obtain the local Green’s function from the
local (k-independent) DMFT self-energy:

$$G_{lm}^\nu = \frac{1}{V_{\text{BZ}}} \int_{\text{BZ}} \text{d}k [i\nu + \mu] \delta_{lm} - h_{lm}(k) - \Sigma_{lm}^\nu \quad (4)$$

Here, the chemical potential $\mu$ is chosen such that the
system contains the desired number of electrons. In the
second step one obtains a new local self-energy, which is
in principle the sum of all self-energy diagrams built from
the above propagator and the local interaction. These
two steps can be iterated until convergence.

In practice the second step is usually solved by intro-
ducing an auxiliary Anderson impurity model (AIM), since
a direct summation of all diagrams is infeasible. For the
AIM, on the other hand, it is possible to cal-
culate correlation functions like the one-particle Green’s
function $g_{\nu}^\nu$ on the impurity numerically exactly.
C. Local correlations on the two-particle level

Despite the success of DMFT, additional efforts are necessary in order to access also the momentum dependence of the self-energy. There are several diagrammatic extensions of DMFT that result in the momentum dependent self-energy (for a review see Ref. 14). These diagrammatic routes to non-local correlations all rely on two-particle vertices from DMFT. Here locality is assumed on the two-particle level, instead of the one-particle level. Local correlations on the two-particle level [44] are contained in the two-particle Green’s function of the (DMFT) impurity model,

\[ G_{\alpha_1\alpha_2\beta_1\beta_2}^{\nu_1\nu_2\nu_3\nu_4} = \frac{1}{\beta^3} \int_0^\beta d\tau_1 d\tau_2 d\tau_3 e^{i(\nu_1\tau_1 - \nu_2\tau_2 + \nu_3\tau_3 - \nu_4\tau_4)} \langle T_\tau \hat{c}_\alpha(\tau_1) \hat{c}_\beta(\tau_2) \hat{c}_\gamma(\tau_3) \hat{c}_\delta(\tau_4) \rangle, \tag{5} \]

for which we use spin-orbital compound indices \( \alpha, \beta, \gamma, \delta \). In this paper we compute such two-particle Green’s functions by continuous-time quantum Monte Carlo (CTQMC) with worm sampling [45], which is implemented in W2DYNAMICS [46].

The two-particle Green’s function is connected to the fully reducible vertex \( F_{\alpha\beta\gamma\delta}^{\nu_1\nu_2\nu_3\nu_4} \) by

\[ G_{\alpha_1\alpha_2\beta_1\beta_2}^{\nu_1\nu_2\nu_3\nu_4} = g_a^{\nu_1} g_c^{\nu_3} (\delta_{12} - \delta_{14}) - \frac{1}{\beta^3} g_a^{\nu_1} g_b^{\nu_2} g_c^{\nu_3} g_d^{\nu_4} F_{\alpha_1\beta_1\gamma_1\delta_1}^{\nu_1\nu_2\nu_3\nu_4}, \tag{6} \]

where \( \delta_{12} \equiv \delta_{ab} \delta_{cd} \delta_{\nu_1\nu_2} \) and \( \delta_{14} \equiv \delta_{ab} \delta_{cd} \delta_{\nu_1\nu_4} \). Closely related is the generalized susceptibility

\[ \chi_{\alpha_1\alpha_2}^{\nu_1\nu_2\nu_3\nu_4} = \beta \left( G_{\alpha_1\alpha_2}^{\nu_1\nu_2\nu_3\nu_4} - g_a^{\nu_1} g_c^{\nu_3} \delta_{12} \right) \equiv \chi_{0,\alpha_1\alpha_2}^{\nu_1\nu_2\nu_3\nu_4} + \chi_{\text{conn},\alpha_1\alpha_2}^{\nu_1\nu_2\nu_3\nu_4}, \tag{7} \]

with

\[ \chi_{0,\alpha_1\alpha_2}^{\nu_1\nu_2\nu_3\nu_4} = -\beta g_a^{\nu_1} g_c^{\nu_3} \delta_{14}. \tag{9} \]

Since energy conservation constrains \( \nu_1 + \nu_3 = \nu_2 + \nu_4 \), it is sometimes of advantage [47] to make a transition from four fermionic frequencies to a notation with two fermionic and one bosonic Matsubara frequency.

If we choose the bosonic frequency as \( \omega_{\text{ph}} = \nu_1 - \nu_2 \), the Bethe-Salpeter equation (BSE) in the particle-hole channel can be solved separately at each bosonic frequency. In the particle-particle channel, we have to choose \( \omega_{\text{pp}} = \nu_1 + \nu_3 \) instead. Furthermore, the Bethe-Salpeter equations can be diagonalized in spin space by the following linear combinations:

\[ F_{d,\ell,m,n} = F_{\uparrow\uparrow\downarrow\downarrow} + F_{\uparrow\downarrow\uparrow\downarrow}, \tag{10} \]
\[ F_{m,\ell,m,n} = F_{\uparrow\uparrow\downarrow\downarrow} - F_{\uparrow\downarrow\uparrow\downarrow}, \tag{11} \]
\[ F_{s,\ell,m,n} = F_{\uparrow\uparrow\uparrow\downarrow} + F_{\uparrow\downarrow\uparrow\downarrow}, \tag{12} \]
\[ F_{t,\ell,m,n} = F_{\uparrow\uparrow\uparrow\downarrow} - F_{\uparrow\downarrow\uparrow\downarrow}. \tag{13} \]

The Bethe-Salpeter equations for the impurity in the particle-hole (ph) channel are thus

\[ F_{\nu,\nu',\omega}^{\nu,\nu',\omega} = \Gamma_{\nu,\nu',\omega}^{\nu,\nu',\omega} + \sum_{m,n,h,m'} \lambda_{\nu,\nu',\omega,m,n,h,m'}^{\nu,\nu',\omega} F_{\nu,\nu',\omega}^{\nu,\nu',\omega}, \tag{14} \]

where \( r = d,m \) denotes the afore-defined channel and \( \omega \equiv \omega_{\text{ph}} \) is the bosonic frequency. For better readability we will adopt the shorthand notation

\[ F_{r} = \Gamma_{r} + \sum_{\nu,\nu',\omega} \chi_{0,r}^{\nu,\nu',\omega} F_{r}, \tag{15} \]

where all quantities are matrices in an orbital-frequency compound index.

D. Dynamical vertex approximation

The DFA is a diagrammatic extension of DMFT that assumes locality of the irreducible vertex, which is taken as input from an auxiliary impurity problem (usually from a converged DMFT solution to the original problem).

Since its original formulation in Ref. 48, the DFA was developed in three main directions (often called different DFA flavors):

(i) the original parquet formulation (p-DFA), where the locality is assumed on the level of the fully irreducible vertex \( \Gamma \) – this flavor treats the smallest set of diagrams as local, and correspondingly it is computationally most demanding [35, 37];

(ii) ladder-DFA (in combination with DFT input also called \textit{ab initio} DFA [15–17]), where it is the irreducible vertex in the particle-hole channel (\( \Gamma_{\text{ph}} \)) that is assumed local;

(iii) \( \lambda \)-corrected DFA (usually also called ladder-DFA), where as in (ii) the irreducible vertex \( \Gamma_{\text{ph}} \) is taken as local. However, after the solution of the Bethe-Salpeter equations (a non-local version of Eq. (15)), a sum rule is imposed on the susceptibility by introducing the so-called Moriyasque \( \lambda \)-correction [19, 20, 49] to the susceptibility and self-energy.

Below we first briefly review these three existing flavors, as this allows placing the new flavor (sc-DFA; introduced in the next Section) into its proper methodological context.

1. Parquet-DFA

The parquet-scheme is a method to self-consistently calculate 1-particle and 2-particle quantities [39–42] (it is closely related to the multiloop generalization [50, 51] of the functional renormalization group (fRG) method [52]). Given a one-particle Green’s function \( G \) and the
fully 2-particle irreducible [53] 2-particle vertex $\Lambda$, one can iterate the parquet equation

$$F_r = \Lambda_r + \sum_{r'} c_{r'} \Gamma_{rr'} \chi_0 F_{r'},$$

and the lattice BSE

$$F^q_r = \Gamma^q_r + \Gamma_r^q \chi^q_0 F^q_r$$

(16)

(17)
to obtain the (in general non-local) vertices $F_r$ and $\Gamma_r$. Here the index $r = d, m, s, t$ is as defined earlier the channel index, $c_r$ denotes a real prefactor, and Eq. (16) is diagonal in the bosonic variable (4-index $q$). In our short notation $F^q_r$ and $\Gamma^q_r$ are matrices in two fermionic multi-indices as before. The parquet equation Eq. (16) is not diagonal in the bosonic 4-index and its evaluation requires evaluation of the per definition reducible vertices $\Phi_r$ at different frequency and momentum combinations (for explicit formulation see e.g. Ref. 35).

The Green’s function entering the above Eqs. (16)-(17) via $\chi_0$ can also be updated, since the full vertex $F$ is related to self-energy through the Schwinger-Dyson equation (SDE, see e.g. Ref. 35).

The SDE together with the Dyson equation and Eqs. (16)-(17) constitute a closed set with only one input quantity: $\Lambda$. For an exact $\Lambda$, the parquet scheme produces the exact one- and two-particle quantities. In practice, for example $\Lambda = U$ is taken, which is the lowest order in perturbation expansion widely known as the parquet approximation [40,41]. In the parquet DGA method $\Lambda$ is assumed local and taken from a converged DMFT calculation [54].

Truncated unity approximation. The parquet scheme is numerically extremely costly [35]. We thus employ an additional approximation. Specifically, we transform the fermionic momentum dependence of the 2-particle reducible vertices $\Phi_r$ into a real space basis, leaving only the bosonic momentum $q$:

$$\tilde{\Phi}_{r}^{\ell \ell'} q = \frac{1}{N} \sum_{k,k'} (f^{k\ell})^{*} \Phi_{r}^{kk'} q f^{k'\ell'}$$

(18)

where $f^{k\ell}$ are basis functions (typically known as form factors) of a suitable transformation-matrix which we choose to obey certain symmetries. Exploiting the relative locality [37,55] of the reducible vertices $\Phi$ in their two fermionic momenta we limit the number of basis functions $f^{k\ell}$ used for the transformation (hence the name truncated unity). This amounts to setting to the more nonlocal parts (in the fermionic arguments) of the 2-particle reducible vertices to zero.

$$\tilde{\Phi}_{r}^{\ell \ell'} q = 0 \text{ for } \ell, \ell' > l_{\text{max}}.$$

(19)

The calculations to transform the entire parquet-scheme including convergence studies in the number of basis functions can be found in Refs. 37 and 56. The truncated unity implementation (TUPS) [37] with 1 or 9 form factors was used to generate the comparison data in Sec. IV.

2. Ladder-DGA

Even with the truncated unity approximation the parquet-DGA is numerically very costly. It also suffers from the presence of divergencies [57–61] in the fully irreducible vertex $\Lambda$ that is directly taken as input. Therefore it is often preferable to use ladder-DGA, where the locality level is risen to the irreducible vertex in the particle-hole channel $\Gamma_{d/m}$.

Then, DGA becomes significantly simpler and essentially consists of two steps: First one has to compute the Bethe-Salpeter equations

$$F^q_r = [1 - \Gamma^q_r \chi^q_0]^{-1} \Gamma^q_r$$

(20)
in the particle-hole channels $r = d, m$. Since the irreducible vertex can also exhibit divergences, it is better to reformulate the above equation. This is done by expressing $\Gamma$ by Eq. (15) and rearranging the terms, as shown in Ref. 15. Then one arrives at

$$F^q_r = [1 - \chi_0^{nl,q}]^{-1} \Gamma^q_r$$

(21)

containing only the full reducible vertex $F$, and the non-local part of the bubble $\chi_0^{nl,q} = \chi_0 - \chi_0^\omega$.

The momentum-dependent reducible vertices $F_{r}^q$ from the longitudinal and transversal particle-hole channels are then combined. We do not need to calculate the latter explicitly, because it can be obtained from the former through the crossing-symmetry [14]. The combined vertex $F$ is then

$$F_{d,nlh}^{k \ell} = F_{d,nlh}^{r \nu r} + F_{d,nlh}^{nl,v\nu} - \frac{1}{2} F_{d,h}^{nl,\nu r} - \frac{3}{2} F_{d,h}^{m,\nu r}$$

(22)

(see also Eq. (54) in Ref. 15). Vertices labeled “$nl$” are non-local, i.e. $F_{r,nlh}^{nl,v\nu} = F_{r,nlh}^{r \nu r} - F_{r,nlh}^{r \nu r}$.

Inserting this into the Schwinger-Dyson equation of motion [15]

$$\chi_{n,m}^{\text{con.k}} = \frac{1}{\beta} \sum_{n,m,n^{'},m^{'}} U_{n,m,n^{'},m^{'}} \sum_{k} F_{d,n^{'},m^{'},k}^{k \ell} F_{d,n^{'},m^{'},k}^{k \ell} G_{h}^{k \ell}$$

(23)
yields the connected part of the momentum-dependent self-energy. In practice this equation is evaluated separately for the summands of $F$ in Eq. (22) [17], such that one can identify the non-local corrections to the DMFT self-energy.

Eqs. (21)-(23) can be evaluated efficiently even for multi-orbital models with $h(k)$ from DFT as input. This is known as the ab initio DGA [15–17]. Hitherto they are evaluated only once, and this flavor is therefore referred to as one-shot DGA (1-DGA) in the following.

3. $\lambda$-corrected DGA

The self-energy obtained in the one-shot ladder-DGA calculation does not always exhibit the correct asym-
totic behavior, especially if the susceptibility is large. In addition, the susceptibilities related to Eq. (21) diverge at the DMFT Néel temperature, violating the Mermin-Wagner theorem [62] for 2-dimensional models. This problem was partially solved by so-called $\lambda$-corrections [19, 20], where one enforces the sum rule for the spin (or spin and charge) susceptibility(ies) by adapting a parameter $\lambda$ (hence the name).

While very successful for one-band models [22–25, 49, 63], this solution is not straightforwardly extensible to multi-orbital systems. The reasons are twofold. Firstly, $\lambda$ would be a matrix with as many independent entries as there are different spin-orbital combinations, resulting in a multi-dimensional optimization problem. Secondly, the solution to this problem is quite likely nonunique and there are at the moment no criteria how the physical matrix $\lambda$ should be chosen. While we do not exclude that a reasonable scheme can be devised for the multi-orbital case in the future (see e.g. [64, 65] for application of sum rules in the multi-orbital two-particle self-consistent approach [66]), we focus here on an alternative scheme, that does not rely on enforcing sum rules.

### III. SELF-CONSISTENT LADDER DΓA

While the $\lambda$-correction is impractical or perhaps not even possible for multi-orbital systems, a one-shot ladder-DΓA calculation as hitherto employed for realistic materials calculations also has severe limits. Where the non-local corrections become strong, its application is not justified. When the DMFT susceptibility diverges at a phase transition, the non-local corrections of a one-shot DΓA calculation are not meaningful any more.

There are two main physical reasons why this is wrong: Firstly, the ladder diagrams of say the particle-hole channel lack insertions from the particle-particle channel, which dampen the particle-hole fluctuations. These diagrams are taken into account only on the level of the impurity. In order to correctly incorporate the non-local contributions to such insertions, we need to evaluate the full parquet scheme that is at the moment numerically too costly for multi-orbital calculations.

Secondly and arguably even more important, the self-energy that enters the propagators in the BSE is still the local DMFT self-energy in a one-shot DΓA. This DMFT self-energy fulfills the local SDE with local $F^{\omega}$, where the non-local contributions do not enter. By using the updated non-local self-energy in the BSE, we can introduce feedback from two-particle non-local correlations to the one-particle quantities. For example, spin fluctuations lead to a reduced life-time which, when included in the ladder Green’s function or self-energy, reduces the spin fluctuations in turn. This mechanism hence suppresses the magnetic transition temperature below the DMFT mean-field value.

#### A. sc-DΓA

The approach we propose here consists in finding a momentum-dependent self-energy for a lattice defined by the tight-binding Hamiltonian $h(k)$, that is consistent with the local irreducible vertex $\Gamma_{ph}$. In practice we use an iterative scheme illustrated in the lower panel of Fig. 1. This procedure bears some formal similarity to DMFT: The first step is again the construction of propagators by the DE [Eq. (3)], with a chemical potential that constrains the electron number. But in contrast to DMFT the self-energy is now momentum-dependent. In the second step we sum up all self-energy diagrams that are generated from the local vertex $\Gamma$. More explicitly, this step consists of the subsequent evaluation of the BSE [Eq. (21)] and SDE [Eq. (23)]. Just as in DMFT, also here the second step is numerically much more expensive than the first (DE) step.

The self-energy resulting from the first iteration of ladder-DΓA is taken to be the input (or “trial”) for the second iteration. Starting from the third iteration, linear combinations of trial and result self-energies from several previous iterations are used as new trials. The linear combination is constructed by the Anderson acceleration algorithm [67, 68]; see also Appendix A. If the result is equal to the trial, the iteration is stopped.

To our knowledge there is no proof of uniqueness or existence of such a fixed point. However, we find the procedure to be convergent over a large range of parameters (cf. Fig. 2 which is discussed in Sec. IV). For convergence it can be crucial to use a DMFT self-energy with very little noise, therefore we use symmetric improved estimators [69] to compute it in CT-QMC. Noise in the vertex however does not have a large influence on the self-energy in DΓA, as recently shown [70].

In case of convergence, the asymptotic behavior of the self-energy is largely repaired with respect to one-shot DΓA calculations. Furthermore, the magnetic susceptibility in two-dimensional models stays finite at all temperatures in agreement with the Mermin-Wagner theorem.

#### B. Ab initio implementation

The sc-DΓA is applicable to ab initio calculations using the ab initio DΓA code [17], with the slight modification of allowing for momentum-dependent self-energies in the input. In the repeated evaluation of Eqs. (21)-(23), we have to generate updated input quantities after every iteration. In Appendix A we provide the details of how this is done in practice in operation with ab initio DΓA.

In the ab initio DΓA implementation the local irreducible vertex is never used explicitly, and the equations are evaluated in terms of the local full vertex $F^{\omega}$ (Eq. (21)) instead of Eq. (20)). As already mentioned, this avoids the computational difficulties coming from using a very large irreducible vertex near or on a divergence line. In-
Indeed, the sc-DΓA scheme can be converged also quite close to the divergence lines (cf. Fig. 2). Let us however note that the local part of self-energy in the converged sc-DΓA calculation is in general not related to $F^\omega$ via the local SDE (as it was the case in a one-shot ladder-DFA). The sc-DΓA corrections to the self-energy modify thus also its local part that is not any more equal to the DMFT solution. One can envisage [14, 15, 71] an update of the local multi-orbital vertex $\Gamma$ which we keep fixed, so that the local Green’s function of the impurity is equal to the local sc-DΓA Green’s function. Such an update is at the moment numerically prohibitively expensive and hence beyond our scope.

C. Relation to p-DΓA

The self-consistency imposed on the self-energy that is obtained by iterative application of BSE (21), crossing symmetry (22) and SDE (23) is reminiscent of the parquet scheme. The main difference is the lack of the full parquet equation (16), which would include also non-local particle-particle insertions in the full vertex $F$. In the full p-DΓA the level of local approximation is also different, since $\Lambda$ contains fewer diagrams than $\Gamma$. In the truncated unity approximation however, $\Gamma$ is also effectively local if we do calculations with only one form factor (1FF p-DΓA). It can be explicitly seen e.g. in Eq. (21) in Ref. [37]. The difference between the irreducible vertices $\Gamma$ in the two approaches is that in sc-DΓA it is taken from DMFT and never updated during the self-consistency cycle, whereas in 1FF p-DΓA it is updated through the parquet equation in every iteration. This update allows for mixing of scattering channels in 1FF p-DΓA, notwithstanding the fact that the non-local contributions from other channels into $\Gamma$ are averaged over momenta.

IV. SQUARE LATTICE HUBBARD MODEL

We begin the application of the sc-DΓA method by considering a relatively simple system, which already has been studied well in some parameter regimes: the one-orbital Hubbard model on a square lattice with nearest-neighbor hopping. The dispersion $h(k)$ in Eq. (1) is then simply

$$ h(k) = -2(\cos(k_x) + \cos(k_y)), $$

(24)

where the nearest-neighbor hopping amplitude is set to $t = 1$ to define our unit of energy for this section (with $h = 1$ setting the frequency unit). Furthermore, the lattice constant $a = 1$ sets the unit of length and $k_B = 1$ the unit of temperature; and the orbital indices $l, m, l', m'$ are restricted to a single orbital at each site.

In Fig. 2 we show the DMFT phase diagram of the Hubbard model on a square lattice at half-filling ($n = 1$ electron per site). With blue crosses we denote points in the phase diagram for which we were able to obtain a converged sc-DΓA solution. Please note, that the sc-DΓA method can be used both below the DMFT Néel temperature (indicated by the gray curve in Fig. 2) as well as between the divergence lines (red and orange curves in Fig. 2). It is only on or directly next to divergence lines that we were not able to obtain convergence.

The phase diagram in Fig. 2 serves as a proof of principle and it is not our intention to discuss the sc-DΓA results in the different parameter regimes in the current paper. Instead, we show selected results for weak ($U = 2$) and intermediate ($U = 4$) coupling, where comparison to other methods is possible, as well as for strong coupling ($U = 8$) and out of half-filling ($n = 0.85$) to show the

Figure 2. Phase diagram of the square-lattice Hubbard model at half-filling. Blue crosses denotes points at which the sc-DΓA could be converged. The DMFT-Néel temperature is shown in gray (from [72]). The brown line indicates the DMFT metal-insulator transition. We also show the first two vertex divergence lines (from [57]).

Figure 3. Static magnetic susceptibility of the square-lattice Hubbard model with $U = 2$ and $n = 1$ at momentum $q = (\pi, \pi)$ as a function of inverse temperature. Different colors and symbols denote different methods. The gray vertical line marks the DMFT Néel temperature.
applicability of the method in this interesting (e.g. with regard to superconductivity) regime.

A. Weak coupling

In order to benchmark the method against known results, we first study a half-filled weak coupling case, with the interaction $U = 2$ (in our units the bandwidth is $W = 8$). This case was intensively studied by various methods in Ref. 63; and in the spirit of Ref. 63 we focus on spin fluctuations and the formation of the pseudogap at low temperature.

In Fig. 3 the static magnetic susceptibility at $q = (\pi, \pi)$ is shown. For $U = 2$ DMFT predicts a phase transition at $T_N \approx 0.08$. The sc-DΓA leads to a seemingly non-diverging antiferromagnetic (AFM) susceptibility; the updated self-energy in the BSE damps the magnetic fluctuations and removes the divergence. In the temperature range accessible, the sc-DΓA susceptibility shows first a $1/(T - T_N)$ behavior, as in DMFT which has a finite Néel temperature $T_N$, and then deviates to a linear behavior on the log-scale of Fig. 3, corresponding to $\chi_{m}(T) \sim \exp(\alpha/T)$ with some constant $\alpha$. Such an exponential scaling with a divergence only at $T = 0$ is to be expected for a two-dimensional system, fulfilling the Mermin-Wagner theorem [62] (cf. also Fig. 13 in Ref. 63).

The sc-DΓA AFM susceptibility is somewhat smaller than the one from $\lambda$-corrected DΓA presented in Ref. 63 (not shown here) as well as slightly smaller than the parquet-DΓA results (shown in Fig. 3 for 1 and 9 form factors). The overall behavior is however well reproduced.

In order to correctly resolve the growing correlation length when lowering the temperature, the size of the momentum grid has to be increased. For the lowest two temperatures shown in Fig. 3 we performed extrapolation to infinite grid size (for details see Appendix B).

With lowering the temperature the growing spin-fluctuations lead to enhanced scattering and suppression of the one-particle spectral weight at the Fermi energy and to opening of a pseudogap [19, 63, 73–76]. Due to the van Hove singularity [77–80] at the antinodal point $k_{AN} = (\pi, 0)$, the suppression happens earlier (upon lowering $T$) at this point than at the nodal point $k_N = (\pi/2, \pi/2)$. The pseudogap behavior of the spectral function is also visible in the imaginary part of self-energy on the Matsubara frequency axis, which we show for different temperatures in Fig. 4. Upon lowering the temperature we first see metallic behaviour at both nodal and antinodal points, followed by increased $|\text{Im}\Sigma(\omega_n = \pi T)|$ first only at the antinodal point (pseudogap) and finally at both nodal and antinodal points.

In Fig. 5 we show the behavior of the imaginary part of the self-energy at the first three Matsubara frequencies for the nodal and antinodal points as a function of inverse temperature. Here we compare the sc-DΓA to parquet-DΓA and $\lambda$-corrected ladder-DΓA [63], and the diagrammatic Quantum Monte Carlo (DiagMC) [63, 81]. For the first Matsubara frequency all the methods lie almost on top of each other down to approx. $1/T = 10$ (at the nodal point differences already become noticeable at $1/T = 10$). For lower temperatures the methods still qualitatively agree, but $|\text{Im}\Sigma(\omega_n = \pi T)|$ grows faster in the $\lambda$-DΓA and quantitatively agrees better with the DiagMC benchmark. In the sc-DΓA, as well as in the p-DΓA, this growth happens at lower temperatures. This is in correspondence to the behavior of AFM susceptibility, which also grows slower in these methods upon lowering the temperature compared to $\lambda$-DΓA and DiagMC, while correctly reproducing the overall behavior.

If we however look at the two larger frequencies (middle and right panel of Fig. 5), the situation is opposite. Here both the p-DΓA as well as sc-DΓA follow the DiagMC benchmark closely up to $1/T = 15$ and do not show any enhancement in $|\text{Im}\Sigma|$ with lowering $T$, while in the $\lambda$-DΓA the $2^{nd}$ and $3^{rd}$ Matsubara frequency follow the behavior of the first one. This is probably a consequence of the $\lambda$-correction that is applied a posteriori to the self-energy. While it works very well for the AFM susceptibility and it gives the correct behavior for the low energy part in the self-energy, that is closely influenced (enhanced) by the strong spin fluctuations, it overestimates this influence for larger energies.

![Figure 4. The imaginary part of sc-DΓA self-energy at $U = 2$ and half-filling for two momenta on the Fermi surface: nodal point, $k_N = (\pi/2, \pi/2)$ and antinodal point, $k_{AN} = (\pi, 0)$. Different colors and symbols denote different temperatures.](image-url)
Figure 5. Inverse temperature dependence of the imaginary part of self-energy at $U=2$ and half-filling for the first three Matsubara frequencies $\omega_n = \{\pi T, 3\pi T, 5\pi T\}$ for two momenta on the Fermi surface: $k_N = (\pi/2, \pi/2)$ and $k_{AN} = (\pi, 0)$. Different colors and symbols denote different methods. The $\lambda$-DG\(A\) and DiagMC data in this figure were kindly provided by the authors of [63].

B. Intermediate coupling

Next, we increase the interaction to $U=4$ but stay at half-filling. Since we already enter a regime, where the numerically exact methods are limited to high temperatures, we do not show comparisons to benchmarks. We focus here on the comparison to parquet-D\(\Gamma\)A and the $\lambda$-corrected DG\(A\).

In Fig. 6 we show the static magnetic susceptibility as a function of momentum $q$ for two temperatures. We choose $T=0.25$ for also comparing with the DMFT result that diverges for slightly lower temperature. Already for $T=0.25$ we see a large difference to the DMFT result. As for the different DG\(A\) methods, the results fall almost on top of each other with the exception of 1FF p-D\(\Gamma\)A, where the susceptibility is somewhat larger close to the $M$-point. For the lower temperature of $T=0.1$ the situation is quite different. Although all methods agree for momenta far from $q=(\pi,\pi)$, close to it the results differ significantly, as it was the case for $U=2$. The sc-D\(\Gamma\)A susceptibility is again the smallest, followed by the p-D\(\Gamma\)A results.

In Fig. 7 we show the imaginary part of self-energy as a function of Matsubara frequency for the same two temperatures as in Fig. 6. For $T=0.25$ the DG\(A\) methods agree well, although not any more quantitatively as it was in the weak-coupling case for this temperature. Here the 1FF p-D\(\Gamma\)A result is noticeably different: at $U=4$ the 1FF approximation is not sufficient any longer at this temperature (cf. Ref. [37]). For $T=0.1$ at the antinodal point we already start to see the pseudogap behavior of self-energy in the sc-D\(\Gamma\)A and p-D\(\Gamma\)A methods, whereas in $\lambda$-DG\(A\) the pseudogap sets in at a higher temperature of $T \approx 0.17$ [49]. Except for the first Matsubara frequency, the three DG\(A\) methods are in excellent, almost quantitative agreement. As in the $U=2$ case, the difference in the first Matsubara frequency is likely to be caused by much smaller AFM susceptibility in sc-D\(\Gamma\)A as compared to $\lambda$-DG\(A\).

An open question remains why the sc-D\(\Gamma\)A produces sizably smaller AFM susceptibility than the $\lambda$-DG\(A\) upon going to low temperatures. For the case of $U=2$ it is also significantly smaller than the DiagMC result [63]. An intuitive partial understanding can be gained by looking at the p-D\(\Gamma\)A results for one and nine form factors (1FF and 9FF). As already mentioned in Sec.IIIC and explained in Ref. 37, for the 1FF approximation to p-D\(\Gamma\)A the irreducible vertex $\Gamma$ is also local. But contrary to sc-
DMFT, it is updated after each update of the self-energy. Therefore when the damping effect of self-energy at low temperature becomes big, it can be counterbalanced by a larger $\Gamma$ which results in a larger susceptibility (cf. Figs. 3 and 6). In sc-D$\Gamma$A this vertex stays the same throughout the calculation; the two-particle feedback onto the self-energy is reduced [82]. There is also no feedback from the particle-particle channel that is present in p-D$\Gamma$A.

In the truncated unity p-D$\Gamma$A we can make $\Gamma$ systematically less local by using more form factors. It has also a strong effect on the susceptibility, as the 9FF p-D$\Gamma$A results show. In the case of $U = 2$ the susceptibility is larger for 9FF, it is however smaller than the 1FF result for $U = 4$ (cf. Fig. 6). Similar (opposite) tendencies of the AFM susceptibility were seen for the two values of $U$ in Ref 37. Although the convergence study in Ref 37 shows that at $T = 0.25$ the 9FF p-D$\Gamma$A result is converged with respect to the number of form factors, it is quite likely not the case for much lower temperatures.

In the $\lambda$-corrected D$\Gamma$A the vertex is also local and not updated. The imposed sum rule however imitates the mutual feedback of the one- and two-particle quantities.
in Ref. [87]. We observe that the frequency \( \omega_{\text{max}} \), at which the splitting occurs, moves to lower values as the temperature is lowered. It could be interpreted as sharpening of the dispersion relation upon lowering the temperature.

In the right panels of Fig. 10 the corresponding self-energy for the lowest temperature in Fig. 8, \( T = 0.05 \), is shown. The imaginary part becomes slightly smaller at the lowest Matsubara frequencies in D\( \Gamma \)A. In stark contrast to the particle-hole symmetric systems studied above, the momentum dependence is rather small and visible mainly in the real part. This results in a slight deformation of the Fermi surface, which we can see in the left panels of Fig. 10. While purely local correlations cannot change the shape of the Fermi surface with respect to the tight-binding model, non-local correlations of D\( \Gamma \)A in this case make the Fermi surface slightly more “quadratic”, since in the nodal direction the real part of the self-energy at low frequencies is larger than DMFT. Furthermore, we observe that spectral weight is redistributed and more concentrated at the corners.

Our results demonstrate that sc-D\( \Gamma \)A works very well also in the doped case. This has been a weak spot for 1-D\( \Gamma \)A since in contrast to the symmetric half-filled model, non-local correlations change the filling. If the Coulomb interaction is rather large and we are close to half-filling, this effect is rather weak. Indeed previous 1-D\( \Gamma \)A calculations have hence focused on this parameter regime. However, in other cases the filling of the DMFT serving as an input to the one-shot calculation can and will be quite different from the filling of the 1-D\( \Gamma \)A. This renders a self-consistent treatment with an adjustment of the chemical potential obvious, so that the filling remains as that for which the vertex \( \Gamma \) was calculated.

V. MULTI-ORBITAL CALCULATIONS

A. Two-orbital model

In order to demonstrate that self-consistent D\( \Gamma \)A also works for more than one orbital, we consider next a simple two-orbital model on a square lattice. Here, electrons...
can hop only to neighboring atoms with hopping amplitudes $t_1 = 1$ and $t_2 = 0.25$ for the two orbitals. This gives rise to a wide and a narrow cosine band with bandwidth 8 and 2, respectively. Along a high-symmetry path, the bandstructure is shown in Fig. 11 (left) and the Fermi surface of the non-interacting tight-binding model in Fig. 11 (right). This tight-binding model is supplemented by a Coulomb repulsion parametrized in the Kanamori form with intra-orbital interaction $U = 4$, Hund’s coupling $J = 1$, and inter-orbital interaction $V = U − 2J$. The spin flip and pair hopping processes are of the same magnitude $J$. Considering the different band widths, the wide band will be weakly correlated, since $U$ is only one half of the band width. The narrow band, however, is strongly correlated since $U$ is twice as large as its band width.

In the context of an orbital-selective Mott transition [91–106], such simple half-filled two-band models with different bandwidths and intra-orbital hopping have been studied very intensively in DMFT. Early calculations however did not include the spin flip and pair hopping processes, but only the density-density interactions for technical reasons. In this situation, the tendency toward an orbital selective Mott transition is largely exaggerated: a spin $S_z = \pm 1$ formed by the Hund’s exchange cannot undergo a joint SU(4) Kondo effect, while the spin-1 of the SU(2)-symmetric interaction can. As we are primarily interested in testing the sc-DΓA method, we consider here the case where the model is doped away from half-filling or $n = 2$ electrons per site. Specifically, we consider the doping $n = 1.7$. This gives rise also to a non-zero real part of the self-energy and (slightly) different fillings of the two orbitals; and hence tests various aspects at the same time.

In Fig. 13 we show the self-energy at selective k-points. For the given parameters, the 1-DΓA corrections to the self-energy are extremely strong, even exceeding the value of the DMFT self-energy. The reason for this is that we are quite close to an (incommensurate) antiferromagnetic phase transition in DMFT. Immediately before the phase transition, the 1-DΓA corrections become even larger and turn the system insulating.

Similar as for the one-band model, the self-consistency suppresses the antiferromagnetic fluctuations; the actual phase transition occurs only at zero temperature because we are in two dimensions. Hence the sc-DΓA corrections are much weaker at the fixed temperature close to the DMFT phase transition. They will, as a matter of course, become stronger at lower temperatures which are not reachable by 1-DΓA exactly because of the DMFT phase transition. Indeed, Fig. 13 suggests that sc-DΓA is not too distinct from the DMFT result. That is, the self-consistency dampens away much of the one-shot corrections.

However, there is actually a quite important difference: Depending on the k-point the sc-DΓA imaginary part of the self-energy at low Matsubara frequencies is above or below the DMFT self-energy in Fig. 13. This becomes even more obvious in Fig. 12, where we plot the self-energy at the lowest Matsubara frequency strongly depends on the momentum. A strong momentum differentiation of the imaginary part of the self-energy (i.e. the scattering rate) has also been reported for a SrVO$_3$ monolayer [107].

In contrast to the imaginary part, the real part of the self-energy only shows a weak momentum dependence around the DMFT value in Fig. 12. This is different for 1-DΓA where the strong corrections are also reflected in a sizable momentum-dependence of the real part of the self-energy; the strongly correlated band (band 2; blue) also displays a sizable overall shift compared to the DMFT result in 1-DΓA.
But let us turn back to the momentum dependence of the self-energy in sc-DFA. It has a larger influence on the spectral function (Fig. 14) than what one might expect from the Matsubara-frequecy dependence in Fig. 13. In Fig. 14 we see, for all three methods, that the weakly correlated band 1 is still close to the tight-binding starting point in Fig. 11, whereas the strongly correlated band 2 is split into an upper Hubbard band (around $\omega \sim 4$), a lower Hubbard band (around $\omega = -0.5$), and a central quasiparticle peak around the Fermi level ($\omega = 0$). The last is better visible in the zoom-in provided by Fig. 15. The aforementioned momentum differentiation of the self-energy results in a considerably wider central quasiparticle band in sc-DFA than in DMFT or 1-DFA. In 1-DFA the strong fluctuations around the phase transition also smear out the central band when reducing temperature from $T = 0.2$ to $T = 0.1$; $T = 0.05$ is below the DMFT ordering temperature and a one-shot calculation is hence no-longer possible (the reduction of the Néel temperature and susceptibility requires the self-consistency or a Moriya $\lambda$-correction [19]).

In Fig. 16, we further show the spectral weight at the Fermi level in DMFT and sc-DFA, summed over both orbitals. Clearly a Fermi surface close to the tight binding ones is visible. This stems mostly from the wide, less correlated band. The narrow, strongly correlated band is slightly shifted downwards to lower energy and considerably broadened, cf. Fig. 15. Since the band is so flat, this tiny shift results in a sizeable deformation of the spectral weight distribution on the Fermi level: Considering also that $\Sigma(\omega_n)$ averages over a frequency range $\sim T$, we get diffuse arcs around the $M$-point, i.e., $(\pi, \pi)$, which is visible in Fig. 16. However, due to the strong renormalization that is already present in DMFT, the narrow band gives only a small contribution to the spectral weight on the Fermi level.

**B. Strontium vanadate**

As a second, archetypical multi-orbital application we study bulk strontium vanadate SrVO$_3$ at room temperature ($T = 26.3$meV). This material has served as a testbed for the development of realistic materials calculations with strong correlations, and is hence most intensively studied [108–132]. Also the first realistic materials calculations using diagrammatic extensions of DMFT, i.e., *ab initio* DFA, have been performed for this perovskite [15]. SrVO$_3$ is a strongly correlated metal with a quasiparticle renormalization of about two [108]. Electronic correlations also lead to a kink in the self-energy and energy-momentum dispersion relation [110, 133–135]. Theoretical calculations and experiments do not indicate any long-range order.

For this realistic *ab initio* calculation, we start with a Wien2K calculation [136, 137] using the PBE exchange correlation potential in the generalized gradient approximation (GGA) [138], and a lattice constant of $a = 3.8\AA$. The calculated bandstructure is projected onto maximally localized $t_{2g}$ Wannier orbitals [139–141] using wien2wannier [142]. This three-band Wannier Hamiltonian, available open source [143], is supplemented by a...
Figure 14. Momentum-resolved spectral function of the two-orbital Hubbard model at $T = 0.1$ along a high-symmetry path through the Brillouin zone. The first column shows only the component corresponding to the wide band, the second column only the component corresponding to the narrow band. In the third row the full spectral function is shown.

Figure 15. Low-frequency zoom of momentum-resolved spectral function for the two-orbital Hubbard model at temperatures $T = 0.2, 0.1, 0.05$ on a path through the Brillouin zone. In the 1-DGA-spectrum at $T = 0.1$ it is clearly visible that the analytic continuation does not work well in the vicinity of the $\Gamma$-point. This is a typical issue for 1-DGA calculations where non-local self-energy corrections become large.
Kanamori Coulomb interaction including the same terms as for the two-band model and parametrized by $U = 5\text{eV}$ and $J = 0.75\text{eV}$. The difference to earlier \textit{ab initio} DΓA [15–17] calculations, which have been one-shot non-self-consistent calculations, is that we now perform a self-consistent calculation.

As already mentioned, a Moriya-λ correction is extremely difficult for such realistic multi-orbital calculations. There is not only a magnetic and charge λ for every orbital but additionally also various orbital combinations. Hence, we hold that a self-consistent calculation shall be preferable compared to a high-dimensional fit of the various λ parameters. Also conceptionally it is a clearer approach.

In Fig. 17 we compare the self-energy of the one-shot and self-consistent \textit{ab initio} DΓA calculation. In contrast to the two-band Hubbard model study above, the differences are here only minor. The reason for this is that in case of the two-band Hubbard model we were close to the DMFT phase transition, whereas SrVO$_3$ is rather far away from any phase transition. Hence, the 1-DΓA corrections are much smaller to start with. In such a situation, the self-consistency is not necessary. This justifies \textit{a posteriori} the use of non-self-consistent \textit{ab initio} DΓA in Refs. [15–17].

### VI. CONCLUSION

We have presented a self-consistent solution of the ladder DΓA equations where the calculated DΓA self-energy is fed back into the Bethe-Salpeter ladder. This damps the Green’s function and thus the overall strength of the ladder, largely reducing the critical temperatures of DMFT. Hitherto, a similar effect has been achieved by a Moriyasque λ correction for one band-models; multi-orbital models have only been studied by one-shot, non-self-consistent and non-λ-corrected calculations. Applying such a λ correction to multi-orbital or doped systems is difficult, to say the least. One-shot calculations, on the other hand, are disputable whenever the non-local corrections to DMFT become large. Our paper demonstrates that conceptionally clean self-consistent calculations are indeed feasible and work well, also for multi-orbital and doped systems.

For the one-band Hubbard model we have benchmarked the method against previous (λ-corrected and parquet) DΓA and numerically exact DiagMC results at weak coupling. We find an excellent agreement up to the point where the susceptibilities become huge, where self-consistent DΓA yields a somewhat reduced susceptibility. The self-consistency allows applying DΓA even in the close vicinity of the divergence lines of the vertex, at strong coupling and for doped systems.

For the two-band Hubbard model we study the regime close to the DMFT phase transition. Here, the one-shot DΓA corrections are large but the self-consistency mitigates this to a large extent. While the frequency depen-
ence eventually looks similar to that of DMFT, there is a sizable momentum dependence which leads to a widening of the quasiparticle band. In case of SrVO$_3$ we have performed realistic \textit{ab initio} DGA materials calculations. Here, we are not close to any phase transition and the difference between one-shot and self-consistent \textit{ab initio} DGA is minute.

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Appendix A: Implementation

For the practical evaluation of the DGA equations Eqs. (21) to (23), we use the \textit{ab initio} DGA code [17]. Here we describe the details of the implementation, which are closely connected to \textit{ab initio} DGA. Solving the aforementioned equations self-consistently means that the \textit{ab initio} DGA code is executed several times in a loop in order to do a fixed-point iteration. Before each iteration, we create an updated trial input, until the point where the output does not differ from the input any more. Therefore, in order to describe the details of the updates, we have to recapitulate the input structure of \textit{ab initio} DGA first.

Apart from the system-defining parameters (tight-binding Hamiltonian and U-matrix) the following quantities are required as input:

1. lattice self-energy $\Sigma^k$ (can also be momentum-independent)
2. impurity self-energy $\Sigma^\nu_{\text{imp}}$ (can be identical to the lattice self-energy, as in 1-DGA)
3. impurity Green’s function $g^\nu$
4. impurity two-particle Green’s function $G^{\nu\nu'}_{\omega}$

The update proceeds in the two steps described in the following.

1. Update of the self-energy and one-particle Green’s function

This step defines the update. We take trial and result self-energies from several preceding iterations and compose a new trial self-energy $\Sigma_{\text{trial}}^k$ for the $j$-th iteration. This is prediction is usually made by the Anderson acceleration algorithm [67, 68] (also known as Pulay-mixing [144] or direct inversion in iterative subspace, DIIS [145]). This trial self-energy is then used to compute a new local propagator $G^\nu_{\text{loc}}(j)$ by

$$ G^\nu_{\text{loc}}(j) = \frac{1}{V_{\text{BZ}}} \int dk \left[ (iv + \mu)^{(j)} \mathbb{I} - h(k) - \Sigma_{\text{trial}}^k \right]^{-1}, \quad (A1) $$

where the chemical potential $\mu^{(j)}$ is adapted such that the expectation value of the particle number stays at the desired value. The change of the chemical potential usually stays in the range of a few percent. Once the new local Green’s function is determined, we project (downfold) it to the correlated impurity subspaces. Thus, each impurity $I$ obtains its new Green’s function $g^{\nu}_{I}$.  

2. Update of impurity quantities

This step is inherent to our specific implementation of \textit{ab initio} DGA, and not part of the algorithm per se. But since \textit{ab initio} DGA reads the one- and two-particle Green’s function instead of the irreducible vertex, we need to “wrap” the irreducible vertex (unchanged throughout all iterations) in the new impurity propagator by means of the Bethe-Salpeter equation. In order to avoid direct computation of the irreducible vertex, we compute the updated generalized susceptibility for iteration $(j)$ in channel $r$ by

$$ \chi^{(j)}_{r} = \chi^{\text{DMFT}}_{r} \left[ \chi^{\text{DMFT}}_{r} + \chi^{(j)}_{0} - \chi^{(j)}_{0} \left( \chi^{\text{DMFT}}_{0} \right)^{-1} \chi^{\text{DMFT}}_{r} \right]^{-1} \chi^{(j)}_{0} \quad (A2) $$

Note that all susceptibilities in these equations are compound-index matrices in the orbital space of the impurity and fermionic frequencies. The new impurity one-particle Green’s function enters into this equation only through $\chi^{(j)}_{0}$ of Eq. (9), where updated impurity Green’s functions $g^{(j)}_{I}$ are used. The two-particle Green’s function is obtained by dividing through $\beta$ and adding a disconnected part, according to Eq. (7).

Furthermore, it is necessary to compute an updated (“fake”) impurity self-energy by the equation of motion. The reason for this can be seen in Eq. (75) of Ref. [15]. There, the DMFT self-energy appears as a separate term. However, in its essence it is not the DMFT self-energy, but rather the result of the Schwinger-Dyson equation of motion for the impurity[146]. In Ref. [15], this term is subtracted and substituted by the actual DMFT self-energy, in order to mitigate effects of finite frequency
boxes. Therefore, we compute the impurity self-energy from the equation of motion,

\[ \Sigma^{\nu}_{\text{con},m,I} = \frac{1}{\beta} \sum_{\nu'} \sum_{\text{thn}} U_{I,\text{mhn}} G_{\text{con},I,\text{mhn}}^{\nu'} g_{\text{con},I,\text{mhn}}^{\nu} (j) \]  

(A3)

using both the new \((j)\) and the DMFT one- and two-particle Green’s function. The index \(I\) labels the \(I\)-th impurity of the unit cell. Importantly, the frequency boxes have to be identical. Then the difference of these two self-energies is added to the DMFT self-energy and taken as the new (fake) impurity self-energy. In this way the effects of finite-box summation are cancelled. We emphasize that the “fake” impurity self-energy is merely an auxiliary quantity and never used to extract any physical properties of the result. Only the lattice self-energy is subject to physical interpretation in our computations.

**Appendix B: Extrapolation of the susceptibility**

Since we are quite limited in the number of \(q\)-points that we can use in our calculation, we have to do an extrapolation of the magnetic susceptibility. This is possible due to the observation that the inverse of the antiferromagnetic susceptibility depends linearly on the inverse of the number of \(q\)-points. In particular, the extrapolation was necessary for sc-DFA on the square-lattice Hubbard model with \(U = 2\) at \(T = 0.05\) and \(T = 0.04\). There the DFA calculation was done with \(48 \times 48, 64 \times 64, 68 \times 68, 72 \times 72, 76 \times 76, 80 \times 80\) \(k\)- and \(q\)-points. In Fig. 18 and Fig. 19 it is visible that the extrapolation with above mentioned linear relation is indeed possible. Although a deviation from this behavior is to be expected as \(n_q \to \infty\), it can only lead to a small change in the logarithmic plot in Fig. 3 and thus our conclusions remain unchanged.

On the other hand, for \(k\)- and \(q\)-grids of \(48 \times 48\) or larger, we find that the self-energy is practically independent on the number of \(k\)- and \(q\)-points, such that no extrapolation is necessary there.

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