Ab initio calculations with the dynamical vertex approximation

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We propose an approach for the ab initio calculation of materials with strong electronic correlations which is based on all local (fully irreducible) vertex corrections beyond the bare Coulomb interaction. It includes the so-called GW and dynamical mean field theory and important non-local correlations beyond, with a computational effort estimated to be still manageable.

1 Introduction

Twenty-two years ago Metzner and Vollhardt [1] initiated dynamical mean field theory (DMFT) by investigating fermionic lattice models in the limit of infinite dimensions (\(d=\infty\)). In this limit, the (irreducible) Feynman diagrams for the self energy greatly simplify to their local contribution [1], and non-local interactions reduce to their Hartree contribution [2]. Subsequently, Georges and Kotliar [3] showed that fermionic lattice models are, for \(d=\infty\), mapped onto the self-consistent solution of an auxiliary Anderson impurity model, a most crucial step since this allowed for using well-known impurity solvers. As a direct consequence, the Mott transition [3] and antiferromagnetism [4] were studied by DMFT.

In the last years, DMFT [5,6] along with its cluster [7,8,9,10] and diagrammatic [11,12,13,14,15] extensions became one of the standard approaches for calculating strongly correlated electron systems. It is employed not only for model Hamiltonians but combined with density functional theory in the local density approximation (LDA) [16] also for the realistic calculation of material properties [17,18,19,20,21]. Despite its success, merging LDA with DMFT has severe drawbacks as density functional theory and many body Feynman diagrams are rather orthogonal approaches which do not match nicely. Most noticeable is the so-called double counting problem, arising from the fact that it is unclear how to express, in the DMFT language of Feynman diagrams, the correlations already included in the exchange correlation potential of LDA. But also the calculation of the local Coulomb interaction needed for the DMFT calculation is problematic since DMFT does not include non-local screening effects. These must be taken into account already through a reduced \(U\) value, e.g., calculated by constrained LDA [22,23,24] or by the constrained random phase approximation (cRPA) [25,26].

A way to overcome these two obstacles is to substitute LDA by Hedin’s so-called GW approach [27], which generally gives similar results as LDA but with an improved description of the exchange. Hence semiconductor band gaps are much better described, see, e.g., [29] and for more recent results [30]. This GW+DMFT approach [28] is conceptionally clear and well-defined in terms of Feynman diagrams, see Figures 1, 2. It accounts for the screening of the Coulomb interaction and being determined entirely in terms of Feynman diagrams the subtraction of double counted diagrams becomes a well defined problem. Despite these advantages, the application and further development of the GW+DMFT approach has been stalled since its formulation by Biermann et al. [28]. A first reason for this is that the GW approach is computationally fairly demanding and complex. Hence, mature GW programs were missing in the past, albeit this changed more recently, see e.g. [31,32,33,34]. Second, the GW+DMFT scheme is considerably more involved than LDA+DMFT, in particular, if calculations are done self-consistently and

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Fig. 1  Top: In addition to the Hartree term, the GW approach takes into account the (screened) exchange diagram (single wiggled line: bare Coulomb interaction; double wiggled line: screened Coulomb interaction; double line: interacting Green function; here and in the following $i, j$ indicate the lattice sites and also subsume the spin indices). Bottom: Screening of the Coulomb interaction within the random phase approximation (RPA).

Fig. 2  Feynman diagrams for the DMFT self energy $\Sigma$ in terms of the interacting Green function $G$ (double line). (Here and in the following, we omit the single wiggled line, i.e., use only a dot, if only the bare local interaction is taken. Single wiggled lines are kept if also non-local interactions are included.)

with a frequency dependent (screened) Coulomb interaction. In this situation a full implementation of GW+DMFT appears to be feasible, albeit with quite a considerable effort.

On the other hand, from a mere theoretical perspective, GW+DMFT is a rather ad-hoc merger of two (in their respective field successful) approaches without an underlying principle. In this paper, we point out that \textit{ab initio} calculations with dynamical vertex approximation (DΓA) is a common basis which includes the GW and DMFT diagrammatic contributions as well as non-local correlations beyond in a natural way. \textit{Ab initio} DΓA also realizes Hedin’s original ideas [27] to include vertex corrections beyond GW. Not all vertex corrections are included, which is of course not possible. Instead, only those corrections are incorporated which can be traced back to a fully irreducible local vertex, see Fig. 3. This way we obtain a purely Feynman diagrammatic approach which, while being obviously more involved than GW+DMFT, is computationally still feasible. It should describe weakly correlated systems similarly good as LDA and even better if exchange is important as in semiconductors. It includes the strong local DMFT correlations which are so important for quasiparticle renormalizations, Mott-Hubbard transitions, magnetic moments etc. Finally, it also allows non-local correlations beyond DMFT which provide for the most fascinating aspects of correlated electrons such as spin fluctuations and their interplay with superconductivity, quantum criticality and weak localization.

In the following, we will discuss how to do \textit{ab initio} calculations with the DΓA for actual materials. In Section 2 we introduce the approach in terms of Feynman diagrams which can be translated one-to-one to equations. Let us emphasize, our paper is not a review on previous DΓA calculation [12][13][14][36][37] but instead points out how to do calculations for actual materials. Moreover, in Section 2.1 and 2.2 we show explicitly that GW and DMFT, respectively, are included, as are non-local correlations beyond. Section 2.3 summarizes the algorithm of the proposed scheme and discusses the effort of the algorithm. Finally, Section 3 gives a summary and outlook.
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Fig. 3 Ab initio dynamical vertex approximation:
Besides the bare Coulomb interaction at the lowest order, all local vertex corrections to the fully irreducible vertex $\Gamma_{ir}$ (filled square box) are included. This fully irreducible vertex is calculated numerically from an Anderson impurity model, and is used as input for the parquet equations (see Fig. 4).

2 Ab initio dynamical vertex approximation ($D\Gamma A$)

The basic idea of $D\Gamma A$ is to put the DMFT concept of taking all local contributions of the Feynman diagrams for the self energy (one particle irreducible vertex) to a higher level. That is, requiring the fully irreducible $n$-particle vertex to be local. This approach has been put forward by some of us [12] and, taking a cluster of sites as a starting point, by Slezak et al. [14]; also note related ideas by Kusonose [13]. While $n \to \infty$ yields the exact solution of a given fermionic Hamiltonian, most promising is the $n = 2$ level as this only requires the calculation of two particle response functions (not $n$ particle ones) for an Anderson impurity model [12, 35], a very feasible task. Nonetheless, on this $n = 2$ level most (if not all) of the known correlation physics is already included. The approach was shown to correctly describe pseudogaps [36], the Mermin-Wagner theorem in two dimensions [36], and critical exponents in three dimensions [37]. Its implementation for nanoscopic systems is intriguing as it includes important vertex and weak localization corrections which are important for the conductance [38]. $D\Gamma A$ is closely related to the dual Fermion approach [15] which considers similar diagrammatic expansions, albeit not for the actual Fermions but for dual Fermions. In this sense, the connection between $D\Gamma A$ and dual Fermions is comparable to that of dynamical cluster approximation [7] and cluster DMFT [8] which consider similar clusters in $k$-space and real space, respectively.

As already mentioned, in ab initio $D\Gamma A$ the fully irreducible vertex is approximated by its local contribution ($k$-independent but fully frequency dependent) except for for the lowest order term, i.e., the bare interaction, which is taken with its full spatial dependence see Figure 3:

$$\Gamma_{ij \ ir} = V_{ij} + \text{all local vertex corrections}$$  \hspace{1cm} (1)

From this fully irreducible vertex $\Gamma_{ir}$ in turn, the reducible vertex $\Gamma$ is calculated via the parquet equations [39, 40, 41], see Figure 4 or, neglecting certain channels (e.g., the particle-particle channel), with the corresponding the Bethe-Salpeter equations. While we have been concentrating in the past more on the latter, i.e., the approximative Bethe-Salpeter calculation of the reducible vertex, including a Moriya-like $\lambda$-correction [36], Jarrell and coworkers made remarkable progress in actually solving the parquet equations on a $k$-grid [42]. Hence, a parquet solution is nowadays possible not only for a frequency independent interaction (parquet approximation) but also for a fully frequency dependent vertex which is needed for $D\Gamma A$, at least on a $k$-grid and with a restriction to the most important correlated orbitals.

The so-calculated reducible vertex $\Gamma$ in turn, is directly related to the self-energy $\Sigma$ through the Heisenberg equation of motion (Schwinger-Dyson eq.) [12] (Figure 5) Hartree and Fock term need to be added:

$$\Sigma_{k\nu} = -T^2 \sum_{k'q} V_q G_{k+q, \nu + \omega} G_{k'q, \nu'} G_{k'q+\omega} \Gamma_{k'q, \nu', \omega}.$$  \hspace{1cm} (2)
Fig. 4 Parquet equations connecting the reducible vertex $\Gamma$ (empty squares), the fully irreducible vertex $\Gamma_{ir}$ (filled squares) and the reducible vertex in the particle-particle ($C$) and two particle-hole channels ($Z, \tilde{Z}$) (see [12] for the corresponding equations).

Fig. 5 Heisenberg equation of motion (Schwinger-Dyson eq.) connecting the reducible vertex (empty square box) and the self energy .

Here, $V_{ij}$ denotes the Fourier-transform of $V_{ij}$ which - due to translational symmetry - only depends on the difference $|i - j|$; $G_{k\nu}$ is the Green function at momentum $k$ and fermionic Matsubara frequency $\nu$; $\omega$ is a bosonic Matsubara frequency; and $T$ denotes the temperature.

2.1 Inclusion of $GW$ diagrams

Hitherto DΓA has been applied only to a simple Hubbard model with entirely local interaction. As already indicated in Figure 3 the most natural way to non-local interactions is to include only the bare Coulomb interaction, and assume the locality for all higher order Feynman diagrams for the fully irreducible vertex as in Eq. (1). This way the RPA screening of $GW$ is easily recovered when neglecting the particle-particle...
channel (C) and one of the particle-hole channels (Z). This can be seen from Figure 4 if we consider the last particle-hole (interaction) channel, i.e., $\tilde{Z}$, only: The first term of the right hand side yields exactly the RPA relation between screened interaction ($\tilde{Z}$) and bare one (filled box, fully irreducible vertex) if we replace the reducible vertex $\Gamma$ (empty square) by $\tilde{Z}$. The latter replacement follows from the first line of Figure 3, neglecting the $Z$ and $C$ terms. Inserting this screened $\tilde{Z}$ as part of the reducible vertex into the Heisenberg equation of motion (Figure 5) yields the screened exchange diagram of $GW$. In other words, if we would only take the bare Coulomb interaction for the fully irreducible vertex and restrict ourselves to the interaction channel, we recover the $GW$ approach.

In realistic calculations with many orbitals it might not be possible to include all local vertex corrections to the fully irreducible vertex or to solve the corresponding parquet equations for all orbitals. In this case, it is most reasonable to include these vertex corrections only for the more strongly interacting $d$- and $f$-electrons, whereas for the other orbitals only the bare interaction and (possibly) only the interaction channel is taken into account. That is for these orbitals, only the $GW$ self energy would be included.

2.2 Inclusion of DMFT diagrams and non-local correlations beyond

The DMFT diagrams, on the other hand, are obtained if we restrict the Green function lines in the parquet equations (Figure 4) and in the Heisenberg equation of motion (Figure 5) to their local part. In this case, the exact set of parquet equations and the exact Heisenberg equation of motion connect the local fully irreducible vertex to the irreducible vertices in certain channels, to the reducible vertex and finally the self energy. This way, we have through exact relations generated all local Feynman diagrams for the self energy which is nothing but the DMFT self energy. These local DMFT diagrams account for the major part of electronic correlations, which is, among others, responsible for quasiparticle renormalizations including kinks [43, 44, 45], Mott-Hubbard transitions [3], and magnetism [4, 46, 47] with related spin-polaron physics [48, 49].

At lower temperatures and finer energy scales, more subtle effects of electronic correlations emerge, such as spin fluctuations, quantum criticality, and unconventional superconductivity. Such non-local correlations can be described if we include the non-local Green functions of ab initio DΓA, i.e., non-local lines in Figures 4 and 5. Often such physics can be described in weak coupling perturbation theory. For example, spin fluctuations are understood as the Bethe-Salpeter ladder in terms of the bare Coulomb interaction [50, 51], similarly quantum criticality for weakly correlated magnetic systems [52, 53, 54]. Weak localization [55] and superconductivity [56] on the other hand can be described by the Bethe-Salpeter ladder diagrams of the particle-particle (Cooperon) channel. All this physics is included in ab initio DΓA but in terms of the strongly renormalized fully irreducible local vertex beyond the bare Coulomb interaction. Hence these phenomena previously only well described diagrammatically or weakly correlated electron system can, with DΓA, now be treated for strongly correlated electron systems.

2.3 Ab initio DΓA algorithm

Let us now, for an overview of the proposed approach, present the flow diagram of the ab initio DΓA algorithm, see Fig. 6. Starting point is an appropriate, material-adjusted basis, e.g., obtained by LDA. This LDA calculation is done with the full ab initio Hamiltonian, consisting of kinetic energy $H_{\text{kin}}$, lattice potential $V_{\text{ion}}$, and Coulomb interaction $V_{\text{Coul}}$, within the approximative exchange correlation potential, see, e.g., [21]. For reducing the basis set as well as to identify the more correlated $d$- or $f$-orbitals on given lattice sites, a Wannier function projection is generally necessary, e.g., using Wien2Wannier [57]. Within this Wannier basis, kinetic and lattice potential are identified as a non-interacting Hamiltonian $H_0$; and the Coulomb interaction matrix elements $V_{ij}$ are calculated, which are treated more sophisticatedly in the following DΓA calculation. Let us emphasize that the LDA here only serves to provide an appropriate basis, the LDA approximation itself is not employed for the actual calculation.

With this ab initio starting point, the DΓA self consistency cycle is started. From $H_0(k)$ the local Green function $G_{\text{loc}}$ is calculated (in the first iteration without self energy). The local interaction $V_{ii}$ and
Green function $G_{\text{loc}}$ in turn determine the fully irreducible vertex $\Gamma_{\text{ir}}$. In practice, $\Gamma_{\text{ir}}$ is not calculated via summing up Feynman diagrams but by solving (numerically) an Anderson impurity model (AIM) which has exactly the same local contribution of Feynman diagrams. The numerical effort for calculating this local vertex grows $\sim n_{\omega}^4$ where $n_{\omega}$ is the number of Matsubara frequencies. (The vertex has to be calculated for three Matsubara frequencies and in a Monte-Carlo simulation one needs to test each corresponding time slice once - to get an independent configuration. There a big prefactor of about $O(10^4 - 10^7)$, depending on the Monte Carlo accuracy needed.)

How to extract the fully irreducible vertex from measured two-particle Green functions has already been discussed in [12]. The fully irreducible vertex for the two dimensional Hubbard model was even calculated for a cluster, see [58]. Remarkably, the fully irreducible DCA vertex [58] is barely $k$-dependent which strongly supports our approximation of a purely local vertex even in two dimensions.

After having calculated $\Gamma_{\text{ir}}$, one has to solve the corresponding parquet equations to get the reducible vertex. The effort of this step grows $\sim n_{k}^4 n_{\omega}^4$ ($n_{k}$: number of $k$-point patches; $n_{\omega}$: number of Matsubara frequencies). Hence, for a fine $k$-grid this step becomes the computationally most demanding one. One might however restrict certain orbitals or larger distances to specific channels, i.e., to the simpler Bethe-Salpeter equation. This reduces the effort $[12] [36]$ to $n_{k}^2 n_{\omega}^4$. This simpler approach is also very much in the spirit of Hedin’s original work [27], emphasizing the interaction-channel, which might be of particular importance for the calculation of actual materials.

From the reducible vertex in turn the self energy is obtained through the Heisenberg equation of motion (2). Subsequently, also the $k$-dependent Green function and the local Green function are calculated via the usual Dyson equation. The local Green function in turn allows us to redefine an AIM to recalculate the fully irreducible vertex and to continue with the iteration until convergence.
3 Summary and outlook

Twenty-two years after the invention of DMFT and fourteen years after its merger with LDA we dare to
look into prospective future developments in the field of realistic calculations of strongly correlated materi-
als. We hold that \textit{ab initio} DΓA, which includes the bare non-local Coulomb interaction and all local (fully
irreducible) vertex corrections beyond, has a huge potential as a purely diagrammatic approach in this re-
spect. It does not only include \textit{GW} and DMFT in a natural, unifying way but also non-local correlations
beyond. Hence, it can describe fascinating phenomena of electronic correlations such as antiferromag-
netic spin fluctuations, their interplay with superconductivity, quantum criticality and weak localization
corrections to the conductivity. Actually, most if not all phenomena of strongly correlated electrons we
know appear to be included, at least in principle, via the corresponding Feynman diagrams: \textit{ab initio}
DΓA includes the same kind of Feynman diagrams used in weak coupling perturbation theories and ladder
summations but with the fully irreducible vertex instead of only the bare Coulomb interaction. This way
strong electronic correlations are accounted for. Most of the aforementioned phenomena still need to be
explored by DΓA, as application hitherto concentrated on spin-fluctuations leading to pseudogaps and the
Mermin-Wagner theorem in two dimensions [36] and proper critical exponents in three dimensions [37].

Despite the advantages, the computational effort nonetheless is still manageable, possibly with some
compromises concerning the number of \textit{k}-points for which the full parquet equations instead of the simpler
Bethe-Salpeter equation is solved, and likely with a restriction of the vertex corrections to the more strongly
interacting \textit{d} - or \textit{f}-orbitals. Of course, it still needs to be seen how good this description is in practice for
real materials. Notwithstanding, we feel that implementing \textit{ab initio} DΓA is worthwhile the considerable
effort to do so.

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