DoFun 3.0: Functional equations in Mathematica

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Abstract
We present version 3.0 of the Mathematica package DoFun for the derivation of functional equations. In this version, the derivation of equations for correlation functions of composite operators was added. In the update, the general workflow was slightly modified taking into account experience with the previous version. In addition, various tools were included to improve the usage experience and the code was partially restructured for easier maintenance.

Keywords: Dyson-Schwinger equations, functional renormalization group equations, correlation functions, quantum field theory, composite operators

1. Introduction
Computer algebra systems are an integral part of particle physics and physics in general. Many specialized tools exist and supplement generic programs like Mathematica [1]. Especially in perturbative calculations in high-energy physics they are indispensable, see, e.g., [2-4]. In recent years, non-perturbative functional methods, see [5-17] for reviews, have also reached a point where the help of computer algebra systems is helpful or even mandatory. To assist in these cases, a range of dedicated tools was developed [18-23].

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Here, we present a continuation of that work with a new and extended version 3 of the program DoFun (Derivation Of FUNctional equations) \cite{18,20}. Its purpose is the derivation of Dyson-Schwinger equations (DSEs), functional renormalization group equations (RGEs) and - added in this version - correlation functions of composite operators. The output can be arranged in such a way that it is compatible with other programs to perform traces, like FormTracer \cite{23}, FORM \cite{24,28}, HEPMath \cite{29} or FeynCalc \cite{30,32}, and can be exported to numeric code for numeric calculations \cite{22}.

In the past, DoFun was helpful in several projects using large systems of equations which are extremely tedious or even impossible to derive manually. But even for manually manageable cases a computer-assisted derivation is very useful. Examples for the usage of DoFun include Yang-Mills theory and QCD in various gauges in vacuum, e.g., \cite{33,53} and beyond, e.g., \cite{54,60}, effective models for QCD, e.g., \cite{57,61,67}, asymptotic gravity \cite{68} and other models \cite{69}. DoFun is often used in combination with other programs like Form \cite{25,28}, FormTracer \cite{23}, CrasyDSE \cite{22} or xPert \cite{70}.

Since publication of version 2 it became apparent that some aspects of DoFun should be improved to optimize the workflow and in particular to fully incorporate some cases which were not included in the original version. A main consequence of this is a change in the handling of fields. Originally the natures of fields were guessed from the input. While this makes many use cases simple, it leads to problems for other cases, e.g., complex scalar fields. Thus, fields have to be defined now explicitly which avoids ambiguous situations.

A totally new feature is the derivation of correlation functions for composite operators. It relies on a simple identity, but the calculations can be quite cumbersome as typically many fields are involved which lead to many loops. We also added a few new useful tools, for example, the identification of 1PI diagrams or the extraction of diagrams of a certain type by name. The graphical representation was also modified using now Graph[] instead of GraphPlot[] which is slightly more versatile.

Finally, we moved the code to a public git repository (https://github.com/markusqh/DoFun) to make use of a modern development infrastructure and provide a platform for bug reporting.

In the following we first explain how to install DoFun and get access to the documentation. Sec. 2 also contains a quick start guide. In Sec. 3 we give a short overview of the derivation of functional equations. Sec. 4 contains some additional details. We summarize in Sec. 5. The appendices contain various summaries of new functions and usage changes from version 2 to 3. For the readers familiar with DoFun 2, changes they have to consider are listed there as well. Readers who want to get started right away should read the installation instructions and can then continue with the provided documentation that includes examples.

2. Installation and quick start guide

DoFun was developed in Mathematica 11.3 and tested in Mathematica 12. Using it in earlier versions down to 10.0 was not fully tested. It will not work with versions older than version 10.0, since functionality introduced in that version is used. In versions 10.0 to 10.2 functionality is limited due to modifications introduced in 10.3.

DoFun can be installed with the installation script from the git repository by evaluating

\begin{verbatim}
In[1]:= Import["https://raw.githubusercontent.com/markusqh/DoFun/master/DoFun/DoFunInstaller.m"]
\end{verbatim}

This will put DoFun in Mathematica’s application folder.\footnote{On a typical Linux system this would be ".Mathematica/Applications."} Alternatively, one can download it from https://github.com/markusqh/DoFun/releases and copy it manually to the applications folder.

The documentation of DoFun is available in Mathematica’s Documentation Center: Add-ons and Packages \rightarrow DoFun. Direct access to the documentation of a function is also possible via ??function or pressing F1 when the cursor is inside the function name.

DoFun is loaded by evaluating

\begin{verbatim}
In[2]:= Needs[DoFun`]
\end{verbatim}
The first step is typically to define the fields which will be used with the newly introduced function `setFields[]`. For example, a real bosonic field $A$, a pair of fermionic fields $\eta$ and $\bar{\eta}$, and a pair of complex bosonic fields $\phi$ and $\bar{\phi}$ are defined by

```
In[3]:= setFields[{A}, {{eta, etabar}}, {{phi, phibar}}];
```

As basic ingredient one needs an action. It can be given in symbolic form as a list of propagators and vertices which themselves are given as lists of fields, e.g.,

```
In[4]:= action = {{A, A}, {eta, etabar}, {{phi, phibar},
{A, phibar, phi}, {A, etabar, eta}};
```

This is all one needs to start with the derivation of DSEs, flow equations and correlation functions of composite operators using the commands `doDSE[]`, `doRGE[]` and `doCO[]`. Detailed descriptions for options of these functions can be found in the Documentation Center. For the first two we also refer to the article on DoFun 2.0 [20]. Below in Sec. 3.3 we discuss some aspects specific to `doCO` and present an example.

The resulting equations can be plotted with the functions `DSEPlot[]`, `RGEPlot[]` and `COPlot[]`. If desired, one can provide as second argument plot specifications for the fields as illustrated in the example in Sec. 3.4.

### 3. Derivation of functional equations

In this section, the derivation of Dyson-Schwinger and flow equations is described. More details can be found in the articles on DoDSE [11] and DoFun 2 [20], but we reproduce the main steps as a quick reference. We also discuss differences in the implementation in DoFun 3. In Section 3.4 the equations for composite operator correlation functions are discussed and exemplified using the energy-momentum tensor.

#### 3.1. Basic definitions

A basic quantity for all derivations is the effective action $\Gamma[\Phi]$ which depends on the collective field $\Phi$. An index encodes the field type, the position or momentum argument and all indices associated with an internal symmetry group. Repeated indices are summed and integrated over if not noted otherwise. The effective action is defined via a Legendre transformation:

$$
\Gamma[\Phi] := \sup_J (-W[J] + J_i \Phi_i).
$$

(1)

The $J_i$’s are the sources for the fields $\Phi_i$. The generating functional $W[J]$ is related to the bare action $S[\phi]$ as follows:

$$
Z[J] = \int D[\phi] e^{-S[\phi] + \phi^i J_i} =: e^{W[J]}.
$$

(2)

The fields $\phi$ that appear here are the quantum fields which are related to the average fields $\Phi$ by

$$
\Phi_i \equiv \langle \phi_i \rangle_J = \frac{\delta W}{\delta J_i} = Z[J]^{-1} \int D[\phi] \phi_i e^{-S[\phi] + \phi^i J_i}.
$$

(3)

Setting the sources $J$ to zero leads to the physical expectation values of the fields $\phi$: $\Phi_{\text{phys}} := \langle \phi_i \rangle_{J=0}$.

For the effective action a vertex expansion around the physical ground state is employed:

$$
\Gamma[\Phi] = \sum_{n=0}^{\infty} \frac{1}{\sqrt{n!}} \sum_{i_1...i_n} \Gamma_{i_1...i_n} (\Phi_{i_1} - \Phi_{i_1,\text{phys}}) \ldots (\Phi_{i_n} - \Phi_{i_n,\text{phys}}).
$$

(4)
The $N_{i_1...i_n}$ are symmetry factors. The physical $n$-points functions $\Gamma^{i_1...i_n}$ are obtained by derivatives of the effective action and setting the sources to zero:

$$\Gamma^{ij} := \Gamma^{ij}_{J=0} \bigg|_{\Phi = \Phi_{\text{phys}}} = \frac{\partial^2 \Gamma[\Phi]}{\partial \Phi_i \partial \Phi_j} \bigg|_{\Phi = \Phi_{\text{phys}}},$$  \hspace{1cm} (5a)

$$\Gamma^{i_1...i_n} := \Gamma^{i_1...i_n}_{J=0} \bigg|_{\Phi = \Phi_{\text{phys}}} = \frac{\partial^n \Gamma[\Phi]}{\partial \Phi_{i_1} \partial \Phi_{i_2} ... \partial \Phi_{i_n}} \bigg|_{\Phi = \Phi_{\text{phys}}},$$  \hspace{1cm} (5b)

The (field-dependent) propagators are the inverse of the two-point functions:

$$D^{ij} := \frac{\delta W[J]}{\delta J_i \delta J_j} = \left( \frac{\partial^2 \Gamma[\Phi]}{\partial \Phi^2} \right)^{-1}^{ij}.$$  \hspace{1cm} (6)

Again, the physical propagators are obtained for $J = 0$:

$$D^{ij} = D^{ij}_{J=0}.$$  \hspace{1cm} (7)

In the following we will need the derivatives of propagators, fields and vertices with respect to fields. With the relations

$$\frac{\delta}{\delta \Phi_i} \Gamma_{j_1...j_n} = \frac{\delta \Gamma}{\delta \Phi_j} \Gamma_{j_1...j_n},$$  \hspace{1cm} (8)

and

$$\frac{\delta}{\delta \Phi_i} D^{jk} = -\epsilon^{jm}_{i} \left( \frac{\partial^3 \Gamma}{\partial \Phi^3} \right)^{-1}^{jk} \left( \frac{\partial \Gamma}{\partial \Phi} \right)^{mn} \left( \frac{\partial \Gamma}{\partial \Phi} \right)^{-1}^{nk},$$  \hspace{1cm} (9)

we arrive at the simple and complete set of derivative rules

$$\frac{\delta}{\delta \Phi_i} \Phi_j = \delta^{ij},$$  \hspace{1cm} (10a)

$$\frac{\delta}{\delta \Phi_i} \Gamma_{j_1...j_n} = \Gamma^{i_1...i_n},$$  \hspace{1cm} (10b)

$$\frac{\delta}{\delta \Phi_i} D^{jk} = -\epsilon^{jm}_{i} D^{jn} \Gamma_{jn} D^{nk}.$$  \hspace{1cm} (10c)

Note that lowering and raising indices is trivial within the convention introduced here. If Grassmann fields are involved, the function $\epsilon^{jm}_{i}$ takes care of corresponding signs due to their anti-commutative nature. It is defined as

$$\epsilon^{jk...}_{i} = \begin{cases} 1 & \text{i bosonic field} \\ (-1)^{\# \text{ Grassmann fields in } jk...} & \text{i fermionic field} \end{cases}$$  \hspace{1cm} (11)

Note that we use only left-derivatives.\(^2\)

In DoFun the effective action $\Gamma[\Phi]$ is generically defined as a list of interactions. For example, a theory with two fields $\phi_1$ and $\phi_2$ with a quartic interaction is represented by

```
In[5]:= {{phi1, phi1}, {phi2, phi2}, {phi1, phi1, phi2, phi2}}
```

At this point no information about the fields is available. It can be provided by the function `setFields`. For the action above we could declare all fields to be bosons by

```
In[6]:= setFields[{phi1, phi2}]
```

\(^2\)In contradistinction to DoFun 2 we do not include a minus sign in the definition of the vertices by default. See Appendix A.3 for details on signs and how to enable the previous behavior for compatibility.

\(^3\)In DoFun 2 left- and right-derivatives were used.
More information is provided in Sec. Appendix A.2 and the Documentation Center.

3.2. Derivation of Dyson-Schwinger equations

The master equation is derived from the integral of a total derivative,

$$0 = \int D[\phi] \left( \frac{\delta S}{\delta \phi_i} + J_i \right) e^{-S + \phi_i J_i} = \int D[\phi] \left. \left( -\frac{\delta S}{\delta \phi_i} \right) \right|_{\phi'_i = \delta / \delta J_i} + J_i \right) Z[J]. (12)$$

Plugging in Eq. (2), we can switch to the generating functional of connected correlation functions, $W[J]$,

$$-\delta S \bigg|_{\phi_i = \frac{\delta W[J]}{\delta J_i} + \frac{\delta}{\delta J_i}} + J_i = 0, (13)$$

where

$$e^{-W[J]} \left( \frac{\delta}{\delta J_i} \right) e^{W[J]} = \frac{\delta W[J]}{\delta J_i} + \frac{\delta}{\delta J_i}, (14)$$

was used. Performing a Legendre transformation we obtain the master equation for 1PI functions:

$$\frac{\delta \Gamma}{\delta \Phi_i} = \left. \frac{\delta S}{\delta \phi_i} \right|_{\phi_i = \Phi_i + D \frac{\delta}{\delta \Phi_j}}. (15)$$

By applying further derivatives and setting the sources to zero at the end, DSEs for any $n$-point function can be obtained. For more details we refer to Refs. [17, 20, 71] and for a short description of a graphical derivation to Ref. [18].

The implementation of the derivation in DoFun is as follows:

- Perform the first derivative.
- Replace the fields according to Eq. (15).
- Perform additional derivatives.
- Set the sources to zero and get the physical propagators and vertices.
- Get signs from ordering the fermions in a canonical way and the $\epsilon$-functions.
- Identify equal diagrams.

Note that equal diagrams could be identified earlier leading to fewer intermediate expressions. However, we use the algorithm described above, because it is simpler. In case the number of diagrams gets so large that Mathematica cannot handle them anymore, an experienced user could try as a first simplification to modify this aspect of the algorithm in the package code.

The algorithm described above is performed by the function doDSE. It takes as input an action and the derivatives to perform. The result is a symbolic expression which can be plotted with DSEPlot or transformed to an algebraic expression with getAE. For explicit examples we refer to the Documentation Center and the article on DoFun 2 [20]. In Sec. 3.4 a short example for getAE can be found.

3.3. Derivation of functional renormalization group equations

We will follow here the standard derivation of the flow equation for the so-called effective average action given in Ref. [72]. For flow equations we introduce a momentum scale $k$ in the bare action $S[\phi]$ via a regulator term. It serves to integrate out quantum fluctuations in a controlled way:

$$\Delta S_k[\phi] = \frac{1}{2} \phi_i R_{ij}^k \phi_j. (16)$$
All functionals depend now on $k$. In the limit $k \to 0$, the full effective action is recovered. The effective average action, defined by a modified Legendre transformation,

$$\Gamma_k[\Phi] = -W_k[J] + J_i \Phi_i - \frac{1}{2} \Phi_i R_k^{ij} \Phi_j,$$

is used instead of the standard effective action $\Gamma[\Phi]$. This leads to $k$-dependent correlation functions $\Gamma_k^{ij}$. The master equation, which describes the dependence of the effective average action on the scale $k$, is the Wetterich equation,\footnote{72},

$$\partial_k \Gamma_k[\Phi] = \frac{1}{2} \text{Tr} \frac{1}{\Gamma_k^{(2)}[\Phi] + R_k} \partial_k R_k$$

where $\Gamma_k^{(2)}[\Phi]$ is the second derivative of the effective average action. The trace $\text{Tr}$ includes a minus sign for Grassmann fields. $D_{k,J}$ is the field-dependent propagator including the regulator term. Equations for $n$-point functions are obtained by applying $n$ derivatives to Eq. (18) using the differentiation rules from Eq. (10).

The implementation of the derivation in DoFun is as follows:

- Instead of Eq. (18), the following expression is used to minimize the number of diagrams during the derivation (the index $J$ is suppressed here):

$$\partial_t \Gamma_k[\Phi] = \frac{1}{2} \text{Tr} \partial_t \ln \left( \Gamma_k^{(2)}[\Phi] + R_k \right),$$

where $t = \ln(k/\Lambda)$ with $\Lambda$ being a UV cutoff scale. The derivative $\partial_t$ only acts on the regulator $R_k$.

- The starting expression is

$$\frac{1}{2} \epsilon^{ij} \partial_i D^{ij} \Gamma^{ai}.$$

The indices $i$ and $j$ are not closed. This will be done at the end when also the derivative $\partial_t$ is applied.

- Further derivatives are applied with the rules of Eq. (10).

- The sources are set to 0 to obtain physical propagators and vertices.

- The trace is closed by setting $i = j$. If the corresponding propagator belongs to Grassmann fields, a minus sign is added.

- The expressions are reorganized in the canonical way, viz., bosons left of anti-Grassmann fields left of Grassmann fields. Within these three groups external indices are left of internal ones and the latter are organized by the vertex they connect to. This leads to signs from anti-commuting fields and is also required to be able to recognize equal diagrams which are then summed up.

- The derivative $\partial_t$ is applied.

This algorithm is used by the function doRGE which has the same syntax as doDSE, viz., as input an action and the derivatives are required. The output is a symbolic expression. Again we refer to the Documentation Center and the article on DoFun 2\footnote{20} for specific examples.
3.4. Correlation functions of composite operators

Any full correlation function can be expressed in terms of dressed propagators and vertices as

\[ \langle F(\phi) \rangle = F \left( \Phi_1 + D_{ij}^{ij} \frac{\delta}{\delta \Phi_j} \right). \]  

(21)

For correlation functions of composite operators \( O(\phi) \), this leads to

\[ \langle O(\phi(x))O(\phi(y)) \rangle = \left( \Phi_1(x) + D_{ij}^{ij} \frac{\delta}{\delta \Phi_j} \right) O \left( \Phi_1(y) + D_{ij}^{ij} \frac{\delta}{\delta \Phi_j} \right), \]  

(22)

where the \( x- \) and \( y- \)dependence is indicated partially. The derivatives to be performed here are similar to the case of DSEs and we can use the corresponding functions. For \( n \) fields in the expectation value, up to \( n - 2 \) loops can appear.

For the calculation of Eq. 22 in DoFun, it is convenient to write the composite operator as a general \( n \)-point function contracted by an auxiliary function we denote as \( C \). This behaves like a vertex and allows using many functions of DoFun in a straightforward way. To illustrate this, consider the operator \( O_{ij}(x) = \phi_i(x)\phi_j(x) \). The corresponding two-point function can be written as (integration and summation over repeated indices are implied)

\[ \langle O_{ij}(x)O_{kl}(y) \rangle = C_{i,j}^{a,b} C \phi_i(x_1) \phi_j(x_2) \phi_k(x_3) \phi_l(x_4) \]  

(23)

with

\[ C_{i,j}^{a,b} = \delta^{i,j} \delta^{a,b} \delta(x_1 - x) \delta(x_2 - x). \]  

(24)

In the following we go step by step through the derivation of the correlation functions of composite operators using a specific example from QCD. Since in this specific case the result can be simplified further, we show how to realize this with DoFun. The composite operator we will use is the spatial, traceless part of the energy-momentum tensor of Yang-Mills theory:

\[ \pi_{ij}(x) = F_{\mu\nu}^a(x)F_{\nu\mu}^a(x) - \frac{1}{3} \delta_{ij} F_{\mu\nu}^a(x)F_{\nu\mu}^a(x). \]  

(25)

The correlation function we want to calculate is

\[ G_{\pi\pi}(x, y) = \langle \pi_{ij}(x)\pi_{ij}(y) \rangle, \]  

(26)

which, for example, gives access to the shear viscosity via the Kubo relation [73]. We symbolically write the energy-momentum tensor as

\[ \pi_{ij} = \pi_{ij}^{(2)} + \pi_{ij}^{(3)} + \pi_{ij}^{(4)}, \]  

(27)

where the numbers in parentheses indicate the number of gluon fields. \( G_{\pi\pi}(x, y) \) can then be split into parts \( G_{\pi\pi}^{(k,l)}(x, y) \) corresponding to pairs of \( \pi_{ij}^{(k)} \):

\[ G_{\pi\pi}(x, y) = \sum_{k,l=1}^4 \langle \pi_{ij}^{(k)} \pi_{ij}^{(l)} \rangle, \]  

(28)

The minimal number of loops appearing in \( G_{\pi\pi}^{(k,l)}(x, y) \) is \( \lfloor (k + l - 1)/2 \rfloor \), and the maximal number is \( k + l - 2 \), viz., \( G_{\pi\pi}(x, y) \) has up to six loops. We restrict ourselves to two loops here, as expressions become too long otherwise, but the procedure is the same for the dropped expressions. Thus, we only take into account

\[ \tilde{G}_{\pi\pi}(x, y) = \pi_{ij}^{(2,2)} + \pi_{ij}^{(2,3)} + \pi_{ij}^{(3,2)} + \pi_{ij}^{(3,3)} + \pi_{ij}^{(2,4)} + \pi_{ij}^{(4,2)}. \]  

(29)

\footnote{\( \lfloor \cdot \rfloor \) is the floor function.}
The definitions required in DoFun are the following. The composite operator is represented by a field, so we must define it together with the gluon field:

\[
\text{In[7]} := \text{setFields[\{A, FF\}]}
\]

We need to define an action which is given as a list of propagators and vertices, each of which is given by a list of fields. Here we use the Yang-Mills action without ghosts which do not contribute in this case:

\[
\text{In[8]} := \text{action=}\{\{A, A\}, \{A, A, A\}, \{A, A, A, A\}\};
\]

For \(\tilde{G}(x, y)\) we define two auxiliary functions:

\[
\text{In[9]} := \text{F[j_] := Module[\{j1, j2, j3, j4, j5, j6, j7, j8, j9\},}
\]
\[
\text{op[\{FF, j\}, \{A, j1\}, \{A, j2\}]}/2!,
\]
\[
\text{op[\{FF, j\}, \{A, j3\}, \{A, j4\}, \{A, j5\}], \{A, j3\}, \{A, j4\}, \{A, j5\}]/3!,}
\]
\[
\text{op[\{FF, j\}, \{A, j6\}, \{A, j7\}, \{A, j8\}, \{A, j9\}], \{A, j6\}, \{A, j7\}, \{A, j8\}, \{A, j9\}]/4!]]}
\]
\[pi[i_, j_, k_, l_] := \text{op[F[i][[k - 1]], F[j][[l - 1]]}]
\]

The second quantity is the combination of the parts with \(k\) and \(l\) gluon legs. \(\tilde{G}(x, y)\) can then be written as

\[
\text{In[10]} := \text{G1 = pi[i, j, 2, 2] + pi[i, j, 2, 3] + pi[i, j, 3, 2] +}
\]
\[
\text{pi[i, j, 3, 3] + pi[i, j, 2, 4] + pi[i, j, 4, 2];}
\]

The next steps are the replacements of the fields according to Eq. (21) and setting the sources to zero:

\[
\text{In[11]} := \text{G2 = replaceFields[G1];}
\]
\[
\text{G3 = setSourcesZero[G2, action, {}];}
\]

As mentioned above, we only take diagrams up to two loops:

\[
\text{In[12]} := \text{G4 = Select[G3, getLoopNumber[#] <= 2 &];}
\]

The steps from \(G1\) to \(G4\) can be obtained directly with the function doCD:

\[
\text{In[13]} := \text{G4 = doCD[action, G1, getLoopNumber[#] <= 2 &];}
\]

The last argument used is optional and selects here the terms with one and two loops. \(G4\) contains connected and disconnected diagrams. Since the relevant quantity is actually the expectation value of the commutator of the composite operator, the latter will finally vanish, and we drop them here. Of the originally 72 diagrams, many of which are identical, though, now 63 remain:

\[
\text{In[14]} := \text{GConn = getConnected[G4];}
\]

We sum up those graphs:

\[
\text{In[15]} := \text{GConnId =}
\]
\[
\text{identifyGraphs[GConn, \{\{FF, i\}, \{FF, j\}\}]};
\]

Using the plot styles

\[
\text{In[16]} := \text{fieldRules = \{\{A, Red\}, \{FF, Thick, Orange\}\}};
\]

we can plot the result:

\[
\text{In[17]} := \text{COPlot[GConnId, fieldRules]}
\]
It is depicted in Fig. 1. We see three types of diagrams which are not 1PI. They all vanish, because either the combination of a three-gluon vertex and a two-gluon-leg part of $\pi_{ij}$ yields zero due to the color structure or because the combination of a gluon propagator and the three-gluon-leg part of $\pi_{ij}$ yields zero.

We thus continue only with the 1PI part:

```math
In[18]:= G = get1PI[GConnId];
```

This is the final result in symbolic form. A graphical representation is depicted in Fig. 2.

We can use DoFun to convert this to an algebraic expression. However, we will only explain schematically how to do this, as the resulting expressions are very long and not very instructive. As a first step, we define which indices the fields have:

```math
In[19]:= defineFieldsSpecific[{
A[mom, col, lor],
FF[mom, lors, lors]}
]
```

This assigns the gluon field $A$ a momentum, a color and a Lorentz index and the energy-momentum tensor a momentum and two spatial Lorentz indices. In the next step, we would need to define the Feynman rules for the gluon propagator, the three- and four-gluon vertices and the components of the energy-momentum tensor. Once this is done, one can transform the symbolic to the algebraic expressions with

```math
In[20]:= getAE[G, {{FF, i, p, k, l}, {FF, j, -p, m, n}}]
```

The arguments in the lists assign, for example, the external field $FF$ with the index $i$ the momentum $p$ and the spatial Lorentz indices $k$ and $l$. This is the final expression. To continue from here, one can, for example, perform traces or export the expression to a numeric program.

Finally, we show some three-loop diagrams as an example of higher contributions to Eq. (26) in Fig. 3.

4. Some details

This section collects some more detailed information about certain aspects of DoFun.

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5The names of the indices are arbitrary and do not have any special meaning within DoFun.
4.1. Structure of DoFun

The main part of DoFun is contained in three package files:

- **DoDSERGE.m**: This package contains the functions for deriving DSEs, flow equations and composite operator correlation functions.
- **DoFR.m**: This package provides tools to derive Feynman rules from a given action. Changes in version 3 are minor and it should work with old programs without problems. Only signs for fermions should be checked because all derivatives are left-derivatives now.
- **DoAE.m**: This package contains functions to transform symbolic to algebraic expressions. The functionality is basically identical to version 2 with the exception that composite operators were added. It should work with old programs without problems.

Additional files/directories are the following:

- **Kernel/init.m** is called for loading DoFun and automatically checks for updates.
- **DoFunInstall.m** can be called for installing DoFun on a computer. It copies all required files to the appropriate places.
- **Documentation** contains the documentation which can be accessed in the Documentation Center via Add-ons and Packages → DoFun.

4.2. Fields

All fields are assigned a specific type out of the following list: boson, fermion, antiFermion, complex and antiComplex. The field type is obtained with ***fieldType[][]***. To assign these types, the function **setFields[]** is used. It also takes care of setting various other properties of fields, e.g., if they are commuting or anti-commuting, which can be checked with **cFieldQ[]** and **grassmannQ[]**. Fields know about their anti-fields which can be determined with **antiField[]**.

4.3. Treatment of anti-commuting fields

Signs from the anti-commuting nature of fermions are taken into account by the function defined in Eq. (11). It is called **sf[]** and automatically simplifies in many cases. It is inserted whenever needed and only at the end, when all single fields of the superfield are written out, the signs are determined with the function **getSigns[]**.

The notation for vertices uses the following convention for the places of indices:

\[
\Gamma_{ijkl}^{\bar{\psi}_i\psi_j\bar{\psi}_k\psi_l} = \frac{\delta^4 \Gamma}{\delta \psi_l \delta \psi_j \delta \psi_k \delta \bar{\psi}_i}
\]  
(30)

This entails that fields in the derivation functions are put in inverse order, because they are applied from left to right. For example, the DSE corresponding to Eq. (30) is derived by

\begin{verbatim}
In[21]:= doDSE[action, {{psi, l}, {psi, k}, {psibar, j}, {psibar, i}}]
\end{verbatim}
5. Summary

Calculations in quantum field theory can easily become too tedious to perform them manually. Automatizing them not only alleviates the calculations but is in some cases mandatory. The software DoFun we presented here is a tool for functional calculations which can profit from such an automatization. It can derive various functional equations from a given action and yields results in a form suitable for further manipulations by other programs. The present version 3 simplifies some aspects, introduces new tools and adds composite operators to the tool box.

6. Acknowledgments

We thank Jens Braun, Tobias Denz, Marc Leonhardt, Mario Mitter, Coralie Schneider, Nils Strodthoff and Nicolas Wink for useful discussions and input on how to improve DoFun. Funding by the FWF (Austrian Science Fund) under Contract No. P27380-N27 is gratefully acknowledged. The work is also supported by EMMI, the BMBF grant 05P12VHCTG, and is part of and supported by the DFG Collaborative Research Centre SFB 1225 (ISOQUANT) as well as by the DFG under Germany’s Excellence Strategy EXC- 2181/1 - 390900948 (the Heidelberg Excellence Cluster STRUCTURES).

Appendix A. Usage changes from DoFun 2

This section lists differences between DoFun 2 and 3 and is intended for users already familiar with the former. New users can skip this section.

Appendix A.1. Quick fact sheet on how to update to DoFun 3

| Task                        | Description                                                                 |
|-----------------------------|------------------------------------------------------------------------------|
| Field definitions           | Fields need to be explicitly declared before any calculations with setFields[]. |
| Sign conventions            | Vertices are defined now as the positive derivative of the effective action which leads to additional minus signs in diagrams. The old behavior can be restored by setting $signConvention=1$ before any derivations. |
| Derivatives                 | All derivatives are now left-derivatives. This may affect signs of fermionic vertices. |
| Algebraic expressions       | The order of the resulting field arguments of propagators and vertices might be different now. When converting the symbolic into algebraic expressions, the definitions of propagators and vertices might thus need to be adapted. |

Appendix A.2. Types of fields and setFields[]

Fields have an explicit type now. They can be (real) bosons, complex fields or fermions. To have a clear connection between fields and their anti-fields, the latter have the types anti-complex field and anti-fermionic, respectively. The field type can be obtained with fieldType[]. Before doing any calculations, the field type has to be declared with setFields[]. It also sets other properties like if they are commuting or anti-commuting, which can be checked with cFieldQ[] or grassmannQ[], respectively.

Appendix A.3. Sign conventions

- The definition of vertices changed compared to DoFun 2. They are defined now as

\[
\Gamma^{i_1...i_n} := \Gamma_{j=0}^{i_1...i_n} = \frac{\delta^n \Gamma[\Phi]}{\delta \Phi_{i_1} \ldots \delta \Phi_{i_n}} \bigg|_{\Phi = \Phi_{phys}}. \tag{A.1}
\]

This is determined by the default value of $\text{signConventional}=-1$. It can be reset to 1 to recover the old behavior.

- For Grassmann-valued fields only left-derivatives are used. This can lead to different signs compared to using left- and right-derivatives.
Appendix B. New functions

Various new functions were added. The ones accessible for the user are listed below:

- **setFields[]**: Defines properties of fields, see Sec. Appendix A.2.
- **doCO[]**: Derive equation for the correlation function of a composite operator.
- **getVertexNumbers[], getDiagramType[], extractDiagramType[] and groupDiagrams[]**: Tools to classify and extract diagrams. Known diagram types are stored in diagramTypes, which can be extended by definitions of the user. For example, all diagrams of triangle type can be extracted from the expression exp by

  \[\text{extractDiagramType}[\text{exp}, \text{"triangle"}]\]

Currently the following diagrams are defined: oneLoop, tadpole, sunset, squint, triangle3, swordfish3, box, triangle4, swordfish4, fivePoint4
- **sortCanonical[]**: Puts fields in a canonical order as required for diagram identification. Replaces the function orderFermions[].
- **getSigns[], sf[]**: Signs from permuting fields are determined with getSigns[] using the information stored in the auxiliary function sf[].
- **getConnected[], getDisconnected[], connectedQ[], disconnectedQ[]**: Extracts (dis)connected diagrams.
- **getNon1PI[], get1PI[], onePIQ[]**: Extracts 1PI/non-1PI diagrams.

Appendix C. Limitations and disclaimer

*DoFun* was carefully tested. Nevertheless we cannot guarantee that the program is free of flaws. However, we encourage everybody who finds a bug to report it on GitHub via [https://github.com/markusqh/DoFun/issues](https://github.com/markusqh/DoFun/issues).

At the moment of publication of this article, we know of the following limitations with respect to diagram identification and plotting expressions. The symbolic and algebraic results, though, are correct.

- Identification of diagrams only works up to two-loop. It should be noted that graph identification is a non-trivial problem in general. We decided not to put too much effort into this, because in relevant cases the identifications can still be done manually. In practice, we think the only relevant case are equations of composite operators. Identification can also fail when mixed propagators appear.
- *Mathematica* 12.0.0 introduced some changes in plotting graphs which either introduced a bug or removed a certain feature on purpose which was used in *DoFun* 2.0. Thus, it may cause problems to plot diagrams with more than two propagators connecting the same vertices. A warning message is printed if this happens and the styles of the propagators may be incorrect.

References

[1] S. Wolfram, The Mathematica Book, Wolfram Media and Cambridge University Press, 2004.
[2] R. Harlander, M. Steinhauser, Prog. Part. Nucl. Phys. 43 (1999) 167–228. doi:10.1016/S0146-6410(99)00095-2 [arXiv:hep-ph/9812357](https://arxiv.org/abs/hep-ph/9812357).
[3] U. Baur, Int. J. Mod. Phys. E17 (2008) 826–844. doi:10.1142/S0218301308010192 [arXiv:hep-ph/0701164](https://arxiv.org/abs/hep-ph/0701164).
[4] G. Luisoni, S. Poslavsky, Y. Schroder, J. Phys. Conf. Ser. 762 (2016) 012077. doi:10.1088/1742-6596/762/1/012077 [arXiv:1604.03370](https://arxiv.org/abs/1604.03370).
[28] B. Ruijl, T. Ueda, J. Vermaseren (2017). arXiv:1707.06453.

[29] M. Wiebusch, Comput. Phys. Commun. 195 (2015) 172–190. doi:10.1016/j.cpc.2015.04.022 arXiv:1412.6102.

[30] R. Mertig, M. Bohm, A. Denner, Comput. Phys. Commun. 64 (1991) 345–359. doi:10.1016/0010-4655(91)90130-D.

[31] V. Shtabovenko, R. Mertig, F. Orellana, Comput. Phys. Commun. 207 (2016) 432–444. doi:10.1016/j.cpc.2016.06.008 arXiv:1601.01167.

[32] V. Shtabovenko, Comput. Phys. Commun. 218 (2017) 48–65. doi:10.1016/j.cpc.2017.04.014 arXiv:1611.06793.

[33] R. Alkofer, M. Q. Huber, K. Schwenzer, Eur. Phys. J. C62 (2009) 761–781. doi:10.1140/epjc/s10052-009-1066-3 arXiv:0812.4045.

[34] M. Q. Huber, K. Schwenzer, R. Alkofer, Eur. Phys. J. C68 (2010) 581–600. doi:10.1140/epjc/s10052-010-1371-x arXiv:0904.1873.

[35] M. Q. Huber, R. Alkofer, S. P. Sorella, Phys. Rev. D81 (2010) 065003. doi:10.1103/PhysRevD.81.065003 arXiv:0910.5604.

[36] L. Fister, R. Alkofer, K. Schwenzer, Phys. Lett. B688 (2010) 237–243. doi:10.1016/j.physletb.2010.04.001 arXiv:1003.1668.

[37] V. Macher, A. Maas, R. Alkofer, Int. J. Mod. Phys. A27 (2012) 1250098. doi:10.1142/S0217751X12500984 arXiv:1106.5381.

[38] N. Alkofer, R. Alkofer, Phys. Lett. B702 (2011) 158–163. doi:10.1016/j.physletb.2011.06.073 arXiv:1102.2753.

[39] M. Q. Huber, A. Maas, L. von Smekal, JHEP 1211 (2012) 035. doi:10.1007/JHEP11(2012)035 arXiv:1207.0222.

[40] M. Q. Huber, L. von Smekal, JHEP 1304 (2013) 149. doi:10.1007/JHEP04(2013)149 arXiv:1211.6092.

[41] A. Blum, M. Q. Huber, M. Mitter, L. von Smekal, Phys. Rev. D 89 (2014) 061703(R). doi:10.1103/PhysRevD.89.061703 arXiv:1401.0713.

[42] J. Braun, L. Fister, J. M. Pawlowski, F. Rennecke, Phys. Rev. D94 (2016) 034016. doi:10.1103/PhysRevD.94.034016 arXiv:1412.1045.

[43] M. Mitter, J. M. Pawlowski, N. Strodthoff, Phys. Rev. D91 (2015) 054035. doi:10.1103/PhysRevD.91.054035 arXiv:1411.7978.

[44] M. Q. Huber, D. R. Campagnari, H. Reinhardt, Phys.Rev. D91 (2015) 025014. doi:10.1103/PhysRevD.91.025014 arXiv:1410.4766.

[45] A. K. Cyrol, M. Q. Huber, L. von Smekal, Eur. Phys. J. C75 (2015) 102. doi:10.1140/epjc/s10052-015-3312-1 arXiv:1408.5409.

[46] M. Q. Huber, L. von Smekal, JHEP 1406 (2014) 015. doi:10.1007/JHEP06(2014)015 arXiv:1404.3642.

[47] F. Rennecke, Phys. Rev. D92 (2015) 076012. doi:10.1103/PhysRevD.92.076012 arXiv:1504.03585.

[48] M. Q. Huber, Phys. Rev. D91 (2015) 085018. doi:10.1103/PhysRevD.91.085018 arXiv:1502.04057.

[49] M. Q. Huber, Phys. Rev. D93 (2016) 085033. doi:10.1103/PhysRevD.93.085033 arXiv:1602.02038.
[50] A. K. Cyrol, L. Fister, M. Mitter, J. M. Pawlowski, N. Strodthoff, Phys. Rev. D94 (2016) 054005. doi:10.1103/PhysRevD.94.054005 arXiv:1605.01856

[51] M. Q. Huber, Eur. Phys. J. C77 (2017) 733. doi:10.1140/epjc/s10052-017-5310-y arXiv:1709.05848

[52] A. K. Cyrol, M. Mitter, J. M. Pawlowski, N. Strodthoff, Phys. Rev. D97 (2018) 054006. doi:10.1103/PhysRevD.97.054006 arXiv:1803.10092

[53] L. Corell, A. K. Cyrol, M. Mitter, J. M. Pawlowski, N. Strodthoff, SciPost Phys. 5 (2018) 066. doi:10.21468/SciPostPhys.5.6.066 arXiv:1803.10092

[54] M. Q. Huber, EPJ Web Conf. 137 (2017) 07009. doi:10.1051/epjconf/201713707009 arXiv:1611.06136

[55] A. K. Cyrol, M. Mitter, J. M. Pawlowski, N. Strodthoff, Phys. Rev. D97 (2018) 054015. doi:10.1103/PhysRevD.97.054015 arXiv:1706.06326

[56] R. Contant, M. Q. Huber, Phys. Rev. D96 (2017) 074002. doi:10.1103/PhysRevD.96.074002 arXiv:1611.00943

[57] M. Leonhardt, M. Pospiech, B. Schallmo, J. Braun, C. Drischler, K. Hebeler, A. Schwenk (2019). arXiv:1907.05814

[58] J. Braun, M. Leonhardt, M. Pospiech (2019). arXiv:1909.12727

[59] O. Hajizadeh, M. Q. Huber, A. Maas, J. M. Pawlowski (2019). arXiv:1909.12796

[60] R. Contant, M. Q. Huber (2019). arXiv:1909.12796

[61] N. Strodthoff, Phys. Rev. D95 (2017) 076002. doi:10.1103/PhysRevD.95.076002 arXiv:1611.05036

[62] J. M. Pawlowski, N. Strodthoff, N. Wink, Phys. Rev. D98 (2018) 074008. doi:10.1103/PhysRevD.98.074008 arXiv:1711.07444

[63] J. Braun, M. Leonhardt, M. Pospiech, Phys. Rev. D96 (2017) 076003. doi:10.1103/PhysRevD.96.076003 arXiv:1705.00074

[64] J. Braun, M. Leonhardt, M. Pospiech, Phys. Rev. D97 (2018) 076010. doi:10.1103/PhysRevD.97.076010 arXiv:1801.08338

[65] J. Eser, F. Divotgey, M. Mitter, D. H. Rischke, Phys. Rev. D98 (2018) 014024. doi:10.1103/PhysRevD.98.014024 arXiv:1804.01787

[66] R. Alkofer, A. Maas, W. A. Mian, M. Mitter, J. París-López, J. M. Pawlowski, N. Wink, Phys. Rev. D99 (2019) 054029. doi:10.1103/PhysRevD.99.054029 arXiv:1810.07955

[67] F. Divotgey, J. Eser, M. Mitter, Phys. Rev. D99 (2019) 054023. doi:10.1103/PhysRevD.99.054023 arXiv:1901.02472

[68] T. Denz, J. M. Pawlowski, M. Reichert, Eur. Phys. J. C78 (2018) 336. doi:10.1140/epjc/s10052-018-5806-0 arXiv:1612.07315

[69] L. Janssen, H. Gies, Phys. Rev. D86 (2012) 105007. doi:10.1103/PhysRevD.86.105007 arXiv:1208.3327

[70] D. Brizuela, J. M. Martin-Garcia, G. A. Mena Marugan, Gen. Rel. Grav. 41 (2009) 2415–2431. doi:10.1007/s10714-009-0773-2 arXiv:0807.0824

[71] R. Kubo, J. Phys. Soc. Jap. 12 (1957) 570–586. doi:10.1143/JPSJ.12.570

[72] M. Haas, Spectral functions in finite temperature SU(3) gauge theory and applications to transport phenomena, 2014. URL: http://archiv.ub.uni-heidelberg.de/volltextserver/17875/ Ph.D. Thesis, University of Heidelberg.