

# **CHIRON v0.53 Manual and User Guide**

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Manual version of June 2015

## **Abstract**

This manual and user guide describes the classes and functions contained in the ChPT program collection CHIRONv0.53 which includes the numerical library `jnumlib` and the ChPT routine library `chiron`.

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# 1 Introduction

This is the manual and user guide for the Chiral Perturbation Theory package **CHIRON** v0.53. It also defines the functions included in a more extended fashion as compared to the published short description [1]. There is obviously a large overlap with that publication. The numerical routines are described in Sect. 4. The remaining sections are devoted to the **chiron** library.

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Kheiron, *Χείρων*, or Chiron, was the wisest and eldest of the Centaurs, half-horse men of Greek mythology. His name comes from the Greek word for hand (Kheir) which is also the origin of the word chiral which is his name was deemed appropriate for this package [3].

## 2 Guidelines

### 2.1 Main comments

Most of these routines were produced during and after scientific research. They are licensed under the GPL v2 or later, see App. A, [4] or the file **COPYING** in the main directory, so you have very strong rights in using and modifying them. However, please respect the guidelines as described in the file **GUIDELINES** in the main directory. A summary of these is

- Citations are important in the academic world so when using these please both cite the relevant **CHIRON** publication [1] and the papers where the work itself was done as quoted in the different chapters.
- Suspected bugs, proposed fixes and suggestions should preferably be communicated to the author(s) so they can be added in future releases.
- If you distribute modified versions, please indicate clearly the modifications in the source and at the point of distributions. However, the preferred way to introduce changes is via future releases.
- To make published results reproducible, the exact versions of the code that were used should be kept. This includes the values of all parameters used including the precisions.

### 2.2 Some caution for use

These routines have been used and tested in a ChPT environment using units in powers of GeV. Typical accuracies are set by default to relevant and obtainable values for that case.

In addition, there are often special cases where the routines might not work, often due to 0/0 or large cancelations.

Similar comments apply to the special functions included. They are sufficiently accurate for the purposes they were used for originally and usually return values with a precision close to double precision but this is not guaranteed.

In some cases, the large formulas have inherently large cancelations. This might lead to degrading of precision in unexpected places. Use common (scientific) sense to judge the quality of the results.

Finally, there are a number of internal functions and extensions already present in the source code but not yet documented in this manual. These might change and have not been tested as well as the documented ones. In particular interfaces etc. might change.

## 3 Files, installation and testroutines

The package can be downloaded from [5]. There are ready to install libraries there for some cases, but in general it is better to compile it for your own system. C++ can have a large overhead in calling classes and functions compared to FORTRAN. Therefore always compile the library with optimization. The interfaces are as much as possible defined with the keyword `const` to allow the compiler to optimize more efficiently.

### 3.1 Files

The gzipped tarred file (`chiron.vvvv.tar.gz`) will produce a directory `chiron.vvvv` with a number of subdirectories. `vvvv` is version information. The created directory is called the main directory in the remainder.

The main directory contains the files `COPYING`, `INSTRUCTIONS`, `GUIDELINES` and a `Makefile`. The subdirectory `doc` contains the documentation. The latest published article about CHIRON, this manual (`manual.tex`), a list of files (`filelist.txt`) and a summary of things added since earlier versions (`Changelog.vvv.to.www.txt`).

The subdirectory `lib` will after compiling contain the compiled libraries `libbnumlib.a` and `libchiron.a`.

The subdirectory `include` contains all the needed header files. The subdirectory `src` contains the source files. `test` contains the testing and example programs. `testoutputs` contains the output the testprograms should produce.

Typically for each subject `xxx` there are files `xxx.h`, `xxx.cc`, `testxxx.cc` and `testxxx.dat` in the respective directories.

There are a few extra files around as well. These typically contain inputs needed or large sets of constants.

## 3.2 Installation

The main steps are to run `make` in the main directory. This should produce the files `libjbnlib.a` and `libchiron.a` and also copy them to the `lib` subdirectory. You might have to change the variables `CC`, `CFLAGS` and `CFLAGTESTS`. `CC` should specify the C++ compiler and the options to be used for everything. `CFLAGS` can be used to specify additional options in compiling the libraries and `CFLAGTESTS` to specify additional options for the testing programs.

“`make clean`” can be used to remove many of the files created during compiling.

The actual installation is by putting the contents of the `include` directory somewhere in the include path of your compiler and the two files `libjbnlib.a` and `libchiron.a` somewhere in the library path. For many C++ compilers the paths are given in the environment variables `CPLUS_INCLUDE_PATH` and `LIBRARY_PATH` respectively.

## 3.3 testroutines

For every file `xxx.h` and `xxx.cc` included for `chiron` there is a testing/example code `testxxx.cc` in the subdirectory `test`. These can be compiled using “`make testxxx`” in the main directory. Executing the resulting file `a.out` should then produce output identical (up to the precision specified and possible randomly generated cases) to the file `testxxx.dat` in the subdirectory `testoutputs`.

# 4 jbnlib

## 4.1 Complex numbers

Complex numbers are defined via the standard C++ library and an abbreviation provided as

```
typedef std::complex<double> dcomplex;
```

All variables declared complex will be of the this type and referred to as `dcomplex` in the remainder.

## 4.2 Special functions

### 4.2.1 jbdli2

```
dcomplex jbdli2(const dcomplex x)
```

Returns the complex dilogarithm or Spence function defined by

$$\mathrm{Li}_2(x) = - \int_0^1 dt \frac{\log(1 - xt)}{t}, \quad (1)$$

where it converges and analytic continuation. Cut defined on the positive real axis from 1 to  $\infty$ . Uses the properties of the dilogarithm to transform the argument and then the Bernoulli series as described in [6].

Defined in `jbnunlib.h` and implemented in `jbdli2.cc`.

## 4.2.2 Bessel functions

### 4.2.2.1 `jbdbesi0`

`double jbdbesi0(const double x)`

Returns the modified Bessel function  $I_0$  for real values of the argument. A simple port to C++ of CERNLIB[7] routine DBESI0.

Defined in `jbnunlib.h`, implemented in `jbdbesik.cc`.

### 4.2.2.2 `jbdbesi1`

`double jbdbesi1(const double x)`

Returns the modified Bessel function  $I_1$  for real values of the argument. A simple port to C++ of CERNLIB[7] routine DBESI1.

Defined in `jbnunlib.h`, implemented in `jbdbesik.cc`.

### 4.2.2.3 `jbdbesk0`

`double jbdbesk0(const double x)`

Returns the modified Bessel function  $K_0$  for real values of the argument. A simple port to C++ of CERNLIB[7] routine DBESK0.

Defined in `jbnunlib.h`, implemented in `jbdbesik.cc`.

### 4.2.2.4 `jbdbesk1`

`double jbdbesk1(const double x)`

Returns the modified Bessel function  $K_1$  for real values of the argument. A simple port to C++ of CERNLIB[7] routine DBESK1.

Defined in `jbnunlib.h`, implemented in `jbdbesik.cc`.

### 4.2.2.5 `jbdbesk2`

`double jbdbesk2(const double x)`

Returns the modified Bessel function  $K_2$  for real values of the argument. Uses the recursion relations for Bessel functions and `jbdbesk0` and `jbdbesk1`.

Defined in `jbnunlib.h`, implemented in `jbdbesik.cc`.

### 4.2.2.6 `jbdbesk3`

`double jbdbesk3(const double x)`

Returns the modified Bessel function  $K_3$  for real values of the argument. Uses the recursion relations for Bessel functions and `jbdbesk0` and `jbdbesk1`.

Defined in `jbnunlib.h`, implemented in `jbdbesik.cc`.

#### 4.2.2.7 jbdbesk4

`double jbdbesk4(const double x)`

Returns the modified Bessel function  $K_4$  for real values of the argument. Uses the recursion relations for Bessel functions and `jbdbesk0` and `jbdbesk1`.

Defined in `jbnumlib.h`, implemented in `jbdbesik.cc`.

### 4.2.3 Theta and related functions

#### 4.2.3.1 jbdtheta30

`double jbdtheta30(const double q)`

Returns the value of the function

$$\theta_{30}(q) = 1 + 2 \sum_{n=1,\infty} q^{(n^2)} = \sum_{n=-\infty,\infty} q^{(n^2)}. \quad (2)$$

This function is related to the third Jacobi theta function. For small  $q$  the summation in (2) is used directly. For larger  $q$  the identity

$$\theta_{30}(q) = \sqrt{\frac{\lambda}{\pi}} \theta_{30}(e^{-\lambda}) \quad (3)$$

with  $\lambda = \pi^2/|\log(q)|$  is used instead. This is related to the modular invariance for the higher dimensional case. Precision can be judged by comparing the two series to each other. Same idea as used in the CERNLIB[7] routine `DTHETA`.

Defined in `jbnumlib.h`, implemented in `jbdtheta30.cc`.

#### 4.2.3.2 jbdtheta30m1

`double jbdtheta30m1(const double q)`

Returns the value of the function

$$\theta_{30}(q) - 1 = 2 \sum_{n=1,\infty} q^{(n^2)} = \sum_{n \in \mathbb{Z}, n \neq 0} q^{(n^2)}. \quad (4)$$

Implementation as for `jbdtheta30` but without the 1. Especially for small  $q$  often needed to keep accuracy in the finite volume applications in ChPT.

Defined in `jbnumlib.h`, implemented in `jbdtheta30m1.cc`.

#### 4.2.3.3 jbdtheta32

`double jbdtheta32(const double q)`

Returns the value of the function

$$\theta_{32}(q) = 2 \sum_{n=1,\infty} q^{(n^2)} = \sum_{n=-\infty,\infty} n^2 q^{(n^2)} = q \frac{d}{dq} \theta_{30}(q). \quad (5)$$

For small  $q$  the summation in (5) is used directly. For larger  $q$  the derivative of the right-hand-side of the identity (3) is used.

Defined in `jbnlib.h`, implemented in `jbdtheta32.cc`.

#### 4.2.3.4 jbdtheta34

`double jbdtheta34(const double q)`

Returns the value of the function

$$\theta_{34}(q) = \sum_{n=1,\infty} n^4 q^{(n^2)} = \sum_{n=-\infty,\infty} n^4 q^{(n^2)} = \left( q \frac{d}{dq} \right)^2 \theta_{30}(q). \quad (6)$$

For small  $q$  the summation in (6) is used directly. For larger  $q$  the appropriate derivative of the right-hand-side of the identity (3) is used.

Defined in `jbnlib.h`, implemented in `jbdtheta34.cc`.

#### 4.2.3.5 jbdtheta3

`double jbdtheta3(const double u, const double q)`

Returns the value of the function

$$\theta_3(u, q) = 1 + 2 \sum_{n=1,\infty} q^{(n^2)} \cos(2\pi n u) = \sum_{n=-\infty,\infty} q^{(n^2)} e^{i2\pi n u}. \quad (7)$$

For small  $q$  the summation in (7) is used directly. For larger  $q$  the expansion after using the relation

$$\theta_3(u, q) = \sqrt{\pi/|\log(q)|} \exp(-\pi^2 u^2/|\log(q)|) \theta_3(-iu\pi/|\log(q)|, \exp(-\pi^2/|\log(q)|)) \quad (8)$$

is used.

Defined in `jbnlib.h`, implemented in `jbdtheta3.cc`.

#### 4.2.3.6 jbdderivutheta3

`double jbdderivutheta3(const double u, const double q)`

Returns the value of the function

$$\frac{\partial}{\partial u} \theta_3(u, q) = -4\pi \sum_{n=1,\infty} q^{(n^2)} \sin(2\pi n u) = i2\pi \sum_{n=-\infty,\infty} q^{(n^2)} e^{i2\pi n u}. \quad (9)$$

For small  $q$  the summation in (9) is used directly. For larger  $q$  the appropriate derivative of the relation (8) is used.

Defined in `jbnlib.h`, implemented in `jbderivutheta3.cc`.

#### 4.2.3.7 jbdderiv2utheta3

`double jbdderiv2utheta3(const double u, const double q)`

Returns the value of the function

$$\frac{\partial^2}{\partial u^2} \theta_3(u, q) = -8\pi^2 \sum_{n=1, \infty} q^{(n^2)} \cos(2\pi n u) = -4\pi^2 \sum_{n=-\infty, \infty} q^{(n^2)} e^{i2\pi n u}. \quad (10)$$

For small  $q$  the summation in (10) is used directly. For larger  $q$  the appropriate derivative of the relation (8) is used.

Defined in `jbnlib.h`, implemented in `jbderiv2utheta3.cc`.

#### 4.2.3.8 jbdtheta2d0

`double jbdtheta2d0(const double a, const double b, const double c)`

Returns the value of the function

$$\theta_0^{(2)}(a, b, c) = \sum_{n_1, n_2 = -\infty, \infty} e^{-an_1^2 - bn_2^2 - c(n_1 - n_2)^2}. \quad (11)$$

There are many higher-dimensional generalizations of the Jacobi theta functions. The modular invariance properties of these are discussed in App. B of [8] and are used in the evaluation to speed up the calculation. It should be noted that  $\theta_0^{(2)}(a, b, c)$  is fully symmetric in  $a, b, c$ .

Defined in `jbnlib.h` and implemented in `jbtheta2d0.cc`.

#### 4.2.3.9 jbdtheta2d0m1

`double jbdtheta2d0m1(const double a, const double b, const double c)`

Returns the value of the function

$$\theta_0^{(2)}(a, b, c) - 1 = \sum_{n_1, n_2 = -\infty, \infty} e^{-an_1^2 - bn_2^2 - c(n_1 - n_2)^2} - 1 = \sum_{\substack{n_1, n_2 \in \mathbb{Z} \\ (n_1, n_2) \neq (0, 0)}} e^{-an_1^2 - bn_2^2 - c(n_1 - n_2)^2} - 1. \quad (12)$$

Method as in `jbtheta2d0` but the 1 removed, more accurate for small  $a, b, c$  as often needed in finite volume ChPT.

Defined in `jbnlib.h` and implemented in `jbtheta2d0m1.cc`.

#### 4.2.3.10 jbdtheta2d02

`double jbdtheta2d02(const double a, const double b, const double c)`

Returns the value of the function

$$\theta_{02}^{(2)}(a, b, c) = \sum_{n_1, n_2 = -\infty, \infty} n_1^2 e^{-an_1^2 - bn_2^2 - c(n_1 - n_2)^2} = -\frac{\partial}{\partial a} \theta_0^{(2)}(a, b, c). \quad (13)$$

It should be noted that  $\theta_{02}^{(2)}(a, b, c)$  is symmetric in  $b, c$ . Method similar to `jbtheta2d0`.

Defined in `jbnlib.h` and implemented in `jbtheta2d02.cc`.

## 4.3 Integration routines

### 4.3.1 One dimension, real

The interface of these routines is identical so they can be simply interchanged. For most problems the speed decreases as `jbdquad15`, `jbdquad21`, `jbdgauss2`, `jbdgauss` but this is somewhat dependent on the function integrated and the precision requested.

The routines do not use the endpoints so an integrable singularity at the endpoint can be done but an integrand transformation that removes the singularity will lead to a much better performance.

An example program that shows the relative speeds is in `testintegralsreal.cc`.

#### 4.3.1.1 `jbdgauss`

`double jbdgauss(f,a,b,eps)`

`f: double (*f)(const double x)` The double precision function to be integrated over.

`a,b,eps: const double`

`a`: Lower limit of integration.

`b`: Upper limit of integration.

`eps`: Precision attempted to be reached: relative precision if absolute value of the integral is above 1, otherwise absolute precision.

Subroutine translated from the CERNLIB[7] routine `DGAUSS`. Uses 8 and 16 point Gaussian rules with the 16 point for the estimate and the difference for the error estimate. Adaptive with a subdivision strategy.

Defined in `jbnmllib.h`, implemented in `jbdgauss.cc`.

#### 4.3.1.2 `jbdgauss2`

`double jbdgauss2(f,a,b,eps)`

`f: double (*f)(const double x)` The double precision function to be integrated over.

`a,b,eps: const double`

`a`: Lower limit of integration.

`b`: Upper limit of integration.

`eps`: Precision attempted to be reached: relative precision if absolute value of the integral is above 1, otherwise absolute precision.

Uses 8 and 16 point Gaussian rules with the 16 point for the estimate and the difference for the error estimate. Adaptive with a subdivision strategy. Very similar to `jbdgauss` but the subdivision strategy is more appropriate for high precision.

Defined in `jbnmllib.h`, implemented in `jbdgauss2.cc`.

#### 4.3.1.3 `jbdquad15`

`double jbdquad15(f,a,b,eps)`

`f: double (*f)(const double x)` The double precision function to be integrated over.

**a,b,eps: const double**

**a:** Lower limit of integration.

**b:** Upper limit of integration.

**eps:** Precision attempted to be reached: relative precision if absolute value of the integral is above 1, otherwise absolute precision.

Uses 15 point Gauss-Kronrod rule for the estimate and the difference with the embedded 7 point Gauss rule for the error estimate. Adaptive with a subdivision strategy appropriate for high precision.

Defined in `jbdnumlib.h`, implemented in `jbdquad15.cc`.

#### 4.3.1.4 `jbdquad21`

**double jbdquad21(f,a,b,eps)**

**f: double (\*f)(const double x)** The double precision function to be integrated over.

**a,b,eps: const double**

**a:** Lower limit of integration.

**b:** Upper limit of integration.

**eps:** Precision attempted to be reached: relative precision if absolute value of the integral is above 1, otherwise absolute precision.

Uses 21 point Gauss-Kronrod rule for the estimate and the difference with the embedded 10 point Gauss rule for the error estimate. Adaptive with a subdivision strategy appropriate for high precision.

Defined in `jbdnumlib.h`, implemented in `jbdquad21.cc`.

### 4.3.2 One dimension, real with singularity

The interface of these routines is identical so they can be simply interchanged. For most problems the speed decreases as `jbdquad15` or `jbdquad21`, `jbdgauss2`, `jbdgauss` but this is somewhat dependent on the function integrated and the precision requested.

An example program that shows the relative speeds is in `testintegralsrealsingular.cc`.

#### 4.3.2.1 `jbdcauch`

**double jbdcauch(f,a,b,s,eps)**

**f: double (\*f)(const double x)** The double precision function to be integrated over.

**a,b,s,eps: const double**

**a:** Lower limit of integration.

**b:** Upper limit of integration.

**s:** Place of the singularity.

**eps:** Precision attempted to be reached: relative precision if absolute value of the integral is above 1, otherwise absolute precision.

Subroutine translated from the CERNLIB[7] routine `DCAUCH`. Uses 8 and 16 point Gaussian rules with the 16 point for the estimate and the difference for the error estimate. Adaptive

with a subdivision strategy. Integrates symmetrically around the singularity so it returns the integral in the sense of the principal value prescription. Uses `jbdgauss`.

Defined in `jbnlib.h`, implemented in `jbdcauch.cc`.

#### 4.3.2.2 `jbdcauch2`

`double jbdcauch2(f,a,b,s,eps)`

`f: double (*f)(const double x)` The double precision function to be integrated over.

`a,b,s,eps: const double`

`a`: Lower limit of integration.

`b`: Upper limit of integration.

`s`: Place of the singularity.

`eps`: Precision attempted to be reached: relative precision if absolute value of the integral is above 1, otherwise absolute precision.

Subroutine translated from the CERNLIB[7] routine `DCAUCH`. Uses 8 and 16 point Gaussian rules with the 16 point for the estimate and the difference for the error estimate. Adaptive with a subdivision strategy more suitable for high precision. Integrates symmetrically around the singularity so it returns the integral in the sense of the principal value prescription. Uses `jbdgauss2`.

Defined in `jbnlib.h`, implemented in `jbdcauch2.cc`.

#### 4.3.2.3 `jbdsing15`

`double jbdsing15(f,a,b,s,eps)`

`f: double (*f)(const double x)` The double precision function to be integrated over.

`a,b,s,eps: const double`

`a`: Lower limit of integration.

`b`: Upper limit of integration.

`s`: Place of the singularity.

`eps`: Precision attempted to be reached: relative precision if absolute value of the integral is above 1, otherwise absolute precision.

Subroutine similar to `jbdcauch2` but uses a Gauss-Kronrod 15 point rule for the estimate and the difference with the embedded 7 point Gauss rule for the error estimate. Adaptive with a subdivision strategy more suitable for high precision. Integrates symmetrically around the singularity so it returns the integral in the sense of the principal value prescription. Uses `jbdquad15`.

Defined in `jbnlib.h`, implemented in `jbdsing15.cc`.

#### 4.3.2.4 `jbdsing21`

`double jbdsing21(f,a,b,s,eps)`

`f: double (*f)(const double x)` The double precision function to be integrated over.

`a,b,s,eps: const double`

`a`: Lower limit of integration.

**b:** Upper limit of integration.

**s:** Place of the singularity.

**eps:** Precision attempted to be reached: relative precision if absolute value of the integral is above 1, otherwise absolute precision.

Subroutine similar to `jbdcauch2` but uses a Gauss-Kronrod 21 point rule for the estimate and the difference with the embedded 10 point Gauss rule for the error estimate. Adaptive with a subdivision strategy more suitable for high precision. Integrates symmetrically around the singularity so it returns the integral in the sense of the principal value prescription. Uses `jbdquad21`.

Defined in `jbnlib.h`, implemented in `jbdsing21.cc`.

### 4.3.3 One dimension, complex

The interface of these routines is identical so they can be simply interchanged. For most problems the speed decreases as `jbwquad15` or `jbwquad21` or `jbwgauss2`, `jbwgauss` but this is somewhat dependent on the function integrated and the precision requested.

An example program that shows the relative speeds is in `testintegralscomplex.cc`.

#### 4.3.3.1 jbwgauss

`dcomplex jbwgauss(f,a,b,eps)`

**f:** `dcomplex (*f)(const dcomplex x)` The complex double precision function to be integrated over.

**a,b:** `const dcomplex`

**a:** Lower endpoint of integration.

**b:** Upper endpoint of integration.

**eps:** `const double` Precision attempted to be reached: relative precision if absolute value of the integral is above 1, otherwise absolute precision.

Subroutine translated from the CERNLIB[7] routine `WGAUSS`. Uses 8 and 16 point Gaussian rules with the 16 point for the estimate and the difference for the error estimate. Adaptive with a subdivision strategy. The integration is the lineintegral over the straight line between **a** and **b**.

Defined in `jbnlib.h`, implemented in `jbwgauss.cc`.

#### 4.3.3.2 jbwgauss2

`dcomplex jbwgauss2(f,a,b,eps)`

**f:** `dcomplex (*f)(const dcomplex x)` The complex double precision function to be integrated over.

**a,b:** `const dcomplex`

**a:** Lower endpoint of integration.

**b:** Upper endpoint of integration.

**eps:** `const double` Precision attempted to be reached: relative precision if absolute value of the integral is above 1, otherwise absolute precision.

Subroutine translated from the CERNLIB[7] routine **WGAUSS**. Uses 8 and 16 point Gaussian rules with the 16 point for the estimate and the difference for the error estimate. Adaptive with a subdivision strategy better suited for high precision. The integration is the lineintegral over the straight line between **a** and **b**.  
Defined in **jbnunlib.h**, implemented in **jbwgauss2.cc**.

#### 4.3.3.3 jbwquad15

**dcomplex jbwquad15(f,a,b,eps)**

**f: dcomplex (\*f)(const dcomplex x)** The complex double precision function to be integrated over.

**a,b: const dcomplex**

**a:** Lower endpoint of integration.

**b:** Upper endpoint of integration.

**eps: const double** Precision attempted to be reached: relative precision if absolute value of the integral is above 1, otherwise absolute precision.

Subroutinre similar to **jbwgauss2** but uses a 15 point Gauss-Kronrod rule for the estimate and the difference with the embedded 7 point Gauss rule for the error estimate. Adaptive with a subdivision strategy better suited for high precision. The integration is the lineintegral over the straight line between **a** and **b**.

Defined in **jbnunlib.h**, implemented in **jbwquad15.cc**.

#### 4.3.3.4 jbwquad21

**dcomplex jbwquad21(f,a,b,eps)**

**f: dcomplex (\*f)(const dcomplex x)** The complex double precision function to be integrated over.

**a,b: const dcomplex**

**a:** Lower endpoint of integration.

**b:** Upper endpoint of integration.

**eps: const double** Precision attempted to be reached: relative precision if absolute value of the integral is above 1, otherwise absolute precision.

Subroutinre similar to **jbwgauss2** but uses a 21 point Gauss-Kronrod rule for the estimate and the difference with the embedded 10 point Gauss rule for the error estimate. Adaptive with a subdivision strategy better suited for high precision. The integration is the lineintegral over the straight line between **a** and **b**.

Defined in **jbnunlib.h**, implemented in **jbwquad21.cc**.

### 4.3.4 Two dimensions, real

#### 4.3.4.1 jbdad2

**double jbdad2(f,a,b,releps, relerr, ifail)**

**f:** double (\*f)(double x[]) The double precision function to be integrated over,  $x[0]$  and  $x[1]$  contain the values of the two variables to be integrated over.  
**a:** double a[]  $a[0]$  and  $a[1]$  are the lower limits of integration.  
**b:** double b[]  $b[0]$  and  $b[1]$  are the upper limits of integration.  
**releps:** const double requested relative precision of the integral.  
**relerr:** double & returns the obtained relative precision via a reference.  
**ifail:** int & returns an integer. Zero indicates success, if not zero the routine did not obtain the requested precision..  
 The function does a two dimensional integration over a hypercube. The underlying routine is `jbdadm1` which is a simple port to C++ of the CERNLIB[7] routine `DADMUL`. This in turn was based on [9].  
 Defined in `jbn1lib.h`, implemented in `jbdadm1.cc`.

### 4.3.5 Three dimensions, real

#### 4.3.5.1 jbdad3

**double jbdad3(f,a,b,releps, relerr, ifail)**  
**f:** double (\*f)(double x[]) The double precision function to be integrated over,  $x[0]$ ,  $x[1]$  and  $x[2]$  contain the values of the three variables to be integrated over.  
**a:** double a[]  $a[0]$ ,  $a[1]$  and  $a[2]$  are the lower limits of integration.  
**b:** double b[]  $b[0]$ ,  $b[1]$  and  $b[2]$  are the upper limits of integration.  
**releps:** const double requested relative precision of the integral.  
**relerr:** double & returns the obtained relative precision via a reference.  
**ifail:** int & returns an integer. Zero indicates success, if not zero the routine did not obtain the requested precision..  
 The function does a three dimensional integration over a hypercube. The underlying routine is `jbdadm1` which is a simple port to C++ of the CERNLIB[7] routine `DADMUL`. This in turn was based on [9].  
 Defined in `jbn1lib.h`, implemented in `jbdadm1.cc`.

## 5 Chiral Perturbation Theory

The classic papers introducing ChPT are [10, 11, 12]. References to lectures and introductions can be found in [13]. A review at two-loop order is [14]. The notation used here correspond to the notation introduced by Gasser and Leutwyler,  $B, F, l_i^r, B_0$  [11] and  $F_0 L_i^r$  [12] for the two and three flavour case. In general the decay constants are defined with a normalization of  $F_\pi \approx 92$  MeV. The coupling constants in the higher order Lagrangians are usually referred to as low-energy constants (LECs). Power counting is the usual dimensional counting with orders referred to as  $p^n$  with alternatively  $p^2$  or lowest-order (LO),  $p^4$  or next-to-leading-order (NLO) and  $p^6$  or next-to-next-to-leading order (NNLO).

## 6 Data structures

This section describes a number of classes to deal with input parameters and LECs. The default value mechanism of C++ is used to give them initial values if not specified. These are visible below as “=value” in the definitions.

### 6.1 Three flavour ChPT

#### 6.1.1 Class: physmass

```
physmass(mpiin=0.135,mkin=0.495,metain=0.548,fpiin=0.0922,muin=0.77)
```

```
mpiin,mkin,metain,fpiin,muin:  const double
```

```
Private data: double mpi,mk,meta,fpi,mu
```

Physical quantities: pion, kaon and eta mass, pion-decay constant and subtraction scale  $\mu$ .

Relevant physical case: three flavour ChPT, isospin limit.

Input member functions:

```
void setmpi(const double mpiin=0.135)
```

```
void setmk(const double mkin=0.495)
```

```
void setmeta(const double metain=0.548)
```

```
void setfpi(const double fpiin=0.0922)
```

```
void setmu(const double muiin=0.77)
```

Output member functions exist in two varieties. Those that return all or a subset of values using references or those that return one value as the function value.

```
void out(double &mpiout, double &mkout, double &metaout, double &fpiout,  
         double &muout)
```

```
double getmpi(void)
```

```
double getmk(void)
```

```
double getmeta(void)
```

```
double getfpi(void)
```

```
double getmu(void)
```

Operators defined: <<, >> and ==.

<< and >> are defined such that output and input streams work as expected. The input stream should be exactly in the format provided by the output stream.

== checks for equality within relative precision of  $10^{-7}$ . An error will occur if any of the data members is zero.

Defined in `inputs.h`, implemented in `inputs.cc`, examples of use in `testinputs.cc`.

### 6.1.2 Class: lomass

```
lomass(mp0in=0.135, mk0in=0.495, f0in=0.090, muin=0.77)
```

```
mp0in,mk0in,f0in,muin:  const double
```

```
lomass(const quarkmass mass)
```

```
Private data: double mp0,mk0,f0,mu
```

Physical quantities: lowest order pion mass, lowest order kaon mass, lowest order pion-decay constant and subtraction scale  $\mu$ .

Relevant physical case: three flavour ChPT, isospin limit.

The constructor from a `quarkmass` is provided such that conversions can be used.

Input member functions:

```
void setmp0(const double mp0in=0.135) void setmk0(const double mk0in=0.495)
```

```
void setf0(const double f0in=0.09) void setmu(const double muin=0.77)
```

Output member functions exist in two varieties. Those that return all or a subset of values using references or those that return one value as the function value.

```
void out(double &mp0out, double &mk0out, double &f0out, double &muout)
```

```
double getmp0(void)
```

```
double getmk0(void)
```

```
double getf0(void)
```

```
double getmu(void)
```

Operators defined: `<<`, `>>` and `==`.

`<<` and `>>` are defined such that output and input streams work as expected. The input stream should be exactly in the format provided by the output stream.

`==` checks for equality within relative precision of  $10^{-7}$ . An error will occur if any of the data members is zero.

Defined in `inputs.h`, implemented in `inputs.cc`, examples of use in `testinputs.cc`.

### 6.1.3 Class: quarkmass

```
quarkmass(B0mhatin=0.01, B0msin=0.25, f0in=0.090, muin=0.77)
```

```
B0mhatin,B0msin,f0in,muin:  const double
```

```
quarkmass(const lomass mass)
```

```
Private data: double B0mhat,B0ms,f0,mu
```

Physical quantities:  $B_0\hat{m}$ ,  $B_0m_s$ , lowest order pion-decay constant and subtraction scale  $\mu$ .

The quantities  $B_0\hat{m}$  and  $B_0m_s$  are the LEC  $B_0$  [12] multiplied by the up-down quark mass and strange quark mass respectively. These are independent of the QCD scale. The lowest order pion and kaon masses are given by  $m_{\pi LO} = \sqrt{2B_0\hat{m}}$  and  $m_{K LO} = \sqrt{B_0(\hat{m} + m_s)}$

Relevant physical case: three flavour ChPT, isospin limit.

The constructor from a lomass is provided such that conversions can be used.

Input member functions:

```
void setB0mhat(const double B0mhatin=0.01)
void setB0ms(const double B0msin=0.25)
void setf0(const double f0in=0.09)
void setmu(const double muin=0.77)
```

Output member functions exist in two varieties. Those that return all or a subset of values using references or those that return one value as the function value.

```
void out(double &B0mhatout, double &B0msout, double &f0out, double &muout)
double getB0mhat(void)
double getB0ms(void)
double getf0(void)
double getmu(void)
```

Operators defined: <<, >> and ==.

<< and >> are defined such that output and input streams work as expected. The input stream should be exactly in the format provided by the output stream.

== checks for equality within relative precision of  $10^{-7}$ . An error will occur if any of the data members is zero.

Defined in `inputs.h`, implemented in `inputs.cc`, examples of use in `testinputs.cc`.

#### 6.1.4 NLO LECs: Class Li

```
Li(l1r=0.,l2r=0.,l3r=0.,l4r=0.,l5r=0.,l6r=0.,l7r=0.,l8r=0.,l9r=0.,l10r=0.,
   h1r=0.,h2r=0.,mu=0.77,Name="nameless Li")
```

const double: l1r,...,l10r,h1r,h2r,mu

const string: Name

Private data: double L1r,L2r,L3r,L4r,L5r,L6r,L7r,L8r,L9r,L10r,H1r,H2r,mu and string name

Physical quantities the 12 LECs,  $L_i^r, H_i^r$  (of which two are so-called contact terms) of three-flavour ChPT as introduced in [12] and the subtraction scale  $\mu$ .

Relevant physical case: three flavour ChPT

Input member functions:

```
void setli(const int n, const double lin)
void setli(const double lin, const int n)
```

Set the value of the LECs with index  $n$ .  $n = 11, 12$  correspond to  $H_1^r, H_2^r$ .

```
setmu(const double muin)
```

Sets the scale  $\mu$  to the value muin. This does *not* change the LECs, for that use `changescale`.

```
setname(const string namein)
```

Sets the name of the set of LECs.

Output member functions:

`double out(const int n)` returns the value of the n'th LEC.

`void out` exists in many varieties, 13 double references and a string returning all private data, 13 double references returning all LECS and the subtraction scale, 12 double references returning all LECs, 11 double references returning  $L_1^r, \dots, L_{10}^r$  and the subtraction scale and 10 double references returning  $L_1^r, \dots, L_{10}^r$ .

`void changescale(const double newmu)`

This changes the subtraction scale to the new value given by `muin` and changes the LECs according to the running derived in [12].

Operators defined: `<<`, `>>`, `+`, `-` and `*`.

`<<` and `>>` are defined such that output and input streams work as expected. The input stream should be exactly in the format provided by the output stream.

`*` allows to multiply an `Li` by a `double` in either order. The resulting value has all LECs multiplied by the value of the `double`.

`+` and `-` allow to add or subtract set of LECs. The resulting value of all LECs is the sum respectively the difference. A warning is printed of the scales are different.

Extra functions:

`Li Lirandom(void)`

`Li LirandomlargeNc(void)`

`Li LirandomlargeNc2(void)`

These return a set of random NLO LECs. The values are uniformly distributed between  $\pm 1/(16\pi^2)$  for `Lirandom`. `LirandomlargeNc` does the same except that it leaves  $L_4^r, L_6^r$  and  $L_7^r$  zero. `LirandomlargeNc2` does the same but  $L_4^r, L_6^r$  and  $L_7^r$  get a random value between  $\pm(1/3)/(16\pi^2)$ . The random numbers are generated using the system generator `rand()` so initializing using something like `srand(time(0))`. These latter functions were used in the random walks in the  $L_i^r$  in [15].

Defined in `Li.h`, implemented in `Li.cc`, examples of use in `testLi.cc`.

In the subdirectory `test` there is a file `LiCiBE14.dat` that contains the last fit of the LECs [16].

### 6.1.5 NNLO LECs: Class Ci

`Ci(Cr, mu=0.77, Name="nameless Ci")`

`Ci(mu=0.77, Name="nameless Ci")`

`const double: mu`

`const string: Name`

Private data: `double Cr[95]`, `mu` and `string name`

Physical quantities the 94 LECs,  $C_i^r$  (of which four are so-called contact terms) of three-flavour ChPT as introduced in [17, 18] and the subtraction scale  $\mu$ . The  $C_i^r$  are the dimensionless version. Scale to the dimensionfull version with appropriate powers of  $F_0$  but in practice normally with  $F_\pi$ .

Relevant physical case: three flavour ChPT

Input member functions:

`void setci(const int n, const double lin)`

`void setci(const double lin, const int n)`

Set the value of the LECs with index  $n$ .

`setmu(const double muin)`

Sets the scale  $\mu$  to the value `muin`. This does *not* change the LECs, for that use `changescale`.

`setname(const string namein)` Sets the name of the set of LECs.

Output member functions:

`double out(const int n)` returns the value of the  $n$ 'th LEC.

`void out` exists in many varieties, with a `double Ci` [95], a double reference and a string returning all private data, a `double Ci` [95], a double reference returning all LECS and the subtraction scale, and a `double Ci` [95] returning the LECs only.

`void changescale(const double newmu, Li & Liin)`

`void changescale(Li & Liin, const double newmu)`

This changes the subtraction scale to the new value given by `muin` and changes the LECs according to the running derived in [18]. Note that it changes the scale of the values of the NLO LECs  $L_i^r$  in `Liin` as well.

Operators defined: `<<`, `>>`, `+`, `-` and `*`.

`<<` and `>>` are defined such that output and input streams work as expected. The input stream should be exactly in the format provided by the output stream.

`*` allows to multiply a `Ci` by a `double` in either order. The resulting value has all LECs multiplied by the value of the `double`.

`+` and `-` allow to add or subtract set of LECs. The resulting value of all LECs is the sum respectively the difference. A warning is printed if the scales are different.

Extra functions:

`Ci Cirandom(void)`

`Ci CirandomlargeNc(void)`

`Ci CirandomlargeNc2(void)`

These return a set of random NNLO LECs. The values are uniformly distributed between  $\pm 1/(16\pi^2)^2$  for `Cirandom`. `CirandomlargeNc` does the same except that it leaves all LECs that are not single trace terms zero. `CirandomlargeNc2` does the same but the non-single-trace terms get a LEC with a random value between  $\pm(1/3)/(16\pi^2)^2$ . The random numbers are generated using the system generator `rand()` so initializing using something like `srand(time(0))`. These latter functions were used in the random walks in the  $C_i^r$  in [15].

Defined in `Ci.h`, implemented in `Ci.cc`, examples of use in `testCi.cc`.

## 6.2 $n_F$ flavour ChPT

### 6.2.1 Class: quarkmassnf

```
quarkmassnf(f0in=0.090, muin=0.77, nqin=3)
quarkmassnf(const vector<double> B0mqin,f0in=0.090, muin=0.77)
const double: f0in,muin
const int: nfin
const vector<double> B0mqin
Private data: vector<double> B0mq,double f0,mu, int nq.
```

Physical quantities:  $B_0 m_i$  quark masses multiplied by  $B_0$ , lowest order (pion-)decay constant and subtraction scale  $\mu$ . The quantities  $B_0 m_i$  are the  $n_q = \mathbf{nq}$  quark masses multiplied by the LEC  $B_0$  [12],  $B_0$  for the relevant number of quarks  $n_F$ . These are independent of the QCD scale. The lowest order charged kaon mass is given by  $m_{KLO} = \sqrt{B_0(m_u + m_s)}$ . Relevant physical case:  $n_F$  flavour ChPT, possibly partially quenched where we need  $n_q$  different quark masses. The masses are referred to as 1,...,nq (i.e. the counting does not start with 0).

```
void setB0mq(const double B0miin,const int i)
void setB0mq(const int i, const double B0miin=0.)
void setB0mq(const vector<double> B0mqin)
void setf0(const double f0in=0.09)
void setmu(const double muin=0.77)
```

Output member functions exist in two varieties. Those that return all or a subset of values using references or those that return one value as the function value.

```
void out(vector<double> &B0mq) const;
void out(vector<double> &B0mq, double &f0out, double &muout) const;
void out(vector<double> &B0mq, double &f0out, double &muout, int &nq) const;
int getnq(void) const; vector<double> getB0mq(void) const; double getB0mq(const
int i) const; double getf0(void) const; double getmu(void) const;
```

Operators defined: <<, >> and ==.

<< and >> are defined such that output and input streams work as expected. The input stream should be exactly in the format provided by the output stream.

== checks for equality within relative precision of  $10^{-7}$ . An error will occur if any of the data members is zero.

Defined in `inputsnf.h`, implemented in `inputsnf.cc`, examples of use in `testinputsnf.cc`.

### 6.2.2 NLO LECs: Class Linf

```
Linf(l1r=0.,l2r=0.,l3r=0.,l4r=0.,l5r=0.,l6r=0.,l7r=0.,l8r=0.,l9r=0.,l10r=0.,
    l11r=0.,h1r=0.,h2r=0.,mu=0.77,Name="nameless Linf",const int nfin=3)
const double: l1r,...,l11r,h1r,h2r,mu
const string: Name
```

`const int: nfin`

Private data: `double L1r,L2r,L3r,L4r,L5r,L6r,L7r,L8r,L9r,L10r,L11r,H1r,H2r,mu,`  
`int nf` and `string name`

Physical quantities the 12 LECs,  $L_{i=1,10}^r, H_i^r$  (of which two are so-called contact terms) and the extra equation of motion term LEC  $L_{11}^r$  of  $n_F$ -flavour ChPT as introduced in [18] and the subtraction scale  $\mu$ . The extra constant  $L_{11}^r$  is added to be able to deal with two-flavour partially quenched ChPT.

Relevant physical case:  $n_F$  flavour ChPT and partially quenched ChPT

Input member functions:

`void setnf(const int nfin)`

`void setli(const int n, const double lin)`

`void setli(const double lin, const int n)`

Set the value of the LECs with index  $n$ .  $n = 12, 13$  correspond to  $H_1^r, H_2^r$ .

`setmu(const double muin)`

Sets the scale  $\mu$  to the value `muin`. This does *not* change the LECs, for that use `changescale`.

`setname(const string namein)` Sets the name of the set of LECs.

Output member functions:

`double out(const int n)` returns the value of the  $n$ 'th LEC.

`void out` exists in many varieties, 15 double references, a string and an integer returning all private data, 15 double references and an integer returning all LECs and the subtraction scale and the number of flavours, 13 double references and an integer returning all LECs and  $n_F$ , 12 double and an integer references returning  $L_1^r, \dots, L_{11}^r$  and the subtraction scale and the number of flavours, 11 double and an integer references returning  $L_1^r, \dots, L_{11}^r$  and the number of flavours, and 11 double references returning  $L_1^r, \dots, L_{11}^r$ .

`void changescale(const double newmu)`

This changes the subtraction scale to the new value given by `muin` and changes the LECs according to the running derived in [12].

Operators defined: `<<`, `>>`, `+`, `-` and `*`.

`<<` and `>>` are defined such that output and input streams work as expected. The input stream should be exactly in the format provided by the output stream.

`*` allows to multiply an `Li` by a `double` in either order. The resulting value has all LECs multiplied by the value of the `double`.

`+` and `-` allow to add or subtract set of LECs. The resulting value of all LECs is the sum respectively the difference. A warning is printed if the scales are different.

Extra functions:

`Linfrandom(void)`

This returns a set of random NLO LECs. The values are uniformly distributed between  $\pm 1/(16\pi^2)$ . The random numbers are generated using the system generator `rand()` so initializing using something like `srand(time(0))`.

Defined in `Linf.h`, implemented in `Linf.cc`, examples of use in `testLinf.cc`.

### 6.2.3 NNLO LECs: Class Ki

```
Ki(Kr, mu=0.77, Name="nameless Ci", nfin=3)
Ci(mu=0.77, Name="nameless Ci")
const double: mu
const string: Name
const int: nfin
```

Private data: double `Kr[116]`, `mu`, `int nf` and `string name`

Physical quantities the 115 LECs,  $K_i^r$  (of which three are so-called contact terms) of  $n_F$ -flavour ChPT as introduced in [17, 18] and the subtraction scale  $\mu$ . The  $K_i^r$  are the dimensionless version. Scale to the dimensionfull version with appropriate powers of  $F_0$  but in practice normally with  $F_\pi$ .

Relevant physical case:  $n_F$  flavour ChPT

Input member functions:

```
void setki(const int n, const double kin)
void setki(const double kin, const int n)
Set the value of the LECs with index  $n$ .
setmu(const double muin)
```

Sets the scale  $\mu$  to the value `muin`. This does *not* change the LECs, for that use `changescale`.

```
setname(const string namein) Sets the name of the set of LECs.
```

Output member functions:

`double out(const int n)` returns the value of the  $n$ 'th LEC.

`void out` exists in many varieties, with a `double Kit[116]`, a double reference and a string returning all private data, a `double Kit[116]`, a double reference returning all LECs and the subtraction scale, and a `double Kit[116]` returning the LECs only.

```
void changescale(const double newmu, Linf & Liin)
void changescale(Linf & Liin, const double newmu)
```

This changes the subtraction scale to the new value given by `muin` and changes the LECs according to the running derived in [18]. Note that it changes the scale of the values of the NLO LECs  $L_i^r$  in `Liin` as well.

Operators defined: `<<`, `>>`, `+`, `-` and `*`.

`<<` and `>>` are defined such that output and input streams work as expected. The input stream should be exactly in the format provided by the output stream.

`*` allows to multiply a `Ci` by a `double` in either order. The resulting value has all LECs multiplied by the value of the `double`.

`+` and `-` allow to add or subtract set of LECs. The resulting value of all LECs is the sum

respectively the difference. A warning is printed if the scales are different.

Extra functions:

`Ki Kirandom(void)`

This returns a set of random NNLO LECs. The values are uniformly distributed between  $\pm 1/(16\pi^2)^2$ . The random numbers are generated using the system generator `rand()` so initializing using something like `srand(time(0))`.

Defined in `Ki.h`, implemented in `Ki.cc`, examples of use in `testKi.cc`.

## 7 Loop integrals

Loop integrals are done with dimensional regularization and we use the standard ChPT variant of  $\overline{MS}$ . At one-loop order it was defined in [11, 12]. The definition at two-loop order can be found in [18].

We define for subtraction purposes:

$$d = 4 - 2\epsilon, \quad C = \ln(4\pi) + 1 - \gamma, \quad \lambda_0 = \frac{1}{\epsilon} + C, \quad \lambda_1 = \lambda_0 + C, \quad \lambda_2 = \lambda_0^2 + C^2. \quad (14)$$

The  $d$ -dimensional Feynman integrals do not depend directly on the subtraction scale. However, renormalization will always introduce the correct dependence. We define the one-loop integrals multiplied by an extra factor of  $\mu^{2\epsilon}$  and the two-loop integrals with an extra factor of  $\mu^{4\epsilon}$ . This introduces the  $\mu$  dependence in the expressions given below. References are to places where the integrals are defined and/or the method used elaborated.

### 7.1 Tadpole or one-propagator integrals

These are defined by

$$A(n, m^2) = \frac{\mu^{4-d}}{i} \int \frac{d^d q}{(2\pi)^d} \frac{1}{(q^2 - m^2)^n},$$

$$A(m^2, \mu^2) = A(1, m^2), \quad B(m^2, \mu^2) = A(2, m^2), \quad C(m^2, \mu^2) = A(3, m^2). \quad (15)$$

The expansions in  $\epsilon$  are given by, see e.g. [19],

$$\begin{aligned} A(m^2, \mu^2) &= \frac{\lambda_0 m^2}{16\pi^2} + \overline{A}(m^2, \mu^2) + \epsilon A^\epsilon(m^2, \mu^2) + \mathcal{O}(\epsilon^2), \\ B(m^2, \mu^2) &= \frac{\lambda_0}{16\pi^2} + \overline{B}(m^2, \mu^2) + \epsilon B^\epsilon(m^2, \mu^2) + \mathcal{O}(\epsilon^2), \\ C(m^2, \mu^2) &= \overline{C}(m^2, \mu^2) + \epsilon C^\epsilon(m^2, \mu^2) + \mathcal{O}(\epsilon^2). \end{aligned} \quad (16)$$

The  $\mathcal{O}(\epsilon)$  terms are further expanded as

$$A^\epsilon(m^2, \mu^2) = \frac{m^2}{16\pi^2} \left( \frac{1}{2} C^2 - C \log \frac{m^2}{\mu^2} \right) + \overline{A}^\epsilon(m^2, \mu^2),$$

$$\begin{aligned}
B^\epsilon(m^2, \mu^2) &= \frac{1}{16\pi^2} \left( \frac{1}{2} C^2 - C \log \frac{m^2}{\mu^2} - C \right) + \bar{B}^\epsilon(m^2, \mu^2), \\
C^\epsilon(m^2, \mu^2) &= \frac{1}{16\pi^2} \left( -\frac{C}{2m^2} \right) + \bar{C}^\epsilon(m^2, \mu^2).
\end{aligned} \tag{17}$$

The analytical expressions are

$$\begin{aligned}
\bar{A}(m^2, \mu^2) &= \frac{-m^2}{16\pi^2} \log \frac{m^2}{\mu^2} & \bar{A}^\epsilon(m^2, \mu^2) &= \frac{m^2}{16\pi^2} \left( \frac{1}{2} + \frac{\pi^2}{12} + \frac{1}{2} \log^2 \frac{m^2}{\mu^2} \right), \\
\bar{B}(m^2, \mu^2) &= \frac{1}{16\pi^2} \left( -1 - \log \frac{m^2}{\mu^2} \right) & \bar{B}^\epsilon(m^2, \mu^2) &= \frac{1}{16\pi^2} \left( \frac{1}{2} + \frac{\pi^2}{12} + \frac{1}{2} \log^2 \frac{m^2}{\mu^2} + \log \frac{m^2}{\mu^2} \right), \\
\bar{C}(m^2, \mu^2) &= \frac{1}{16\pi^2} \frac{-1}{2m^2} & \bar{C}^\epsilon(m^2, \mu^2) &= \frac{1}{16\pi^2} \left( \frac{1}{2m^2} + \frac{1}{2m^2} \log \frac{m^2}{\mu^2} \right),
\end{aligned} \tag{18}$$

double Ab(const double msq, const double mu2): returns  $\bar{A}(m^2, \mu^2)$ .  
double Bb(const double msq, const double mu2): returns  $\bar{B}(m^2, \mu^2)$ .  
double Cb(const double msq, const double mu2): returns  $\bar{C}(m^2, \mu^2)$ .  
double Abeps(const double msq, const double mu2): returns  $\bar{A}^\epsilon(m^2, \mu^2)$ .  
double Bbeps(const double msq, const double mu2): returns  $\bar{B}^\epsilon(m^2, \mu^2)$ .  
double Cbeps(const double msq, const double mu2): returns  $\bar{C}^\epsilon(m^2, \mu^2)$ .  
double Ab(const int n, const double msq, const double mu2): returns  $\bar{A}(m^2, \mu^2)$ ,  $\bar{B}(m^2, \mu^2)$ ,  $\bar{C}(m^2, \mu^2)$  for  $n = 1, 2, 3$ .

Defined in `oneloopintegrals.h`, implemented in `oneloopintegrals.cc`, examples of use in `testoneloopintegrals.cc`.

## 7.2 Bubbles or two-propagator integrals

### 7.2.1 Definitions

We first define the abbreviation

$$\langle X \rangle = \frac{\mu^{4-d}}{i} \int \frac{d^d q}{(2\pi)^d} \frac{X}{(q^2 - m_1^2)((q-p)^2 - m_2^2)}. \tag{19}$$

The bubble integrals themselves are defined by, see e.g. [20],

$$\begin{aligned}
B(m_1^2, m_2^2, p^2, \mu^2) &= \langle 1 \rangle, \\
B_\mu(m_1^2, m_2^2, p, \mu^2) &= \langle q_\mu \rangle = p_\mu B_1(m_1^2, m_2^2, p^2, \mu^2), \\
B_{\mu\nu}(m_1^2, m_2^2, p, \mu^2) &= \langle q_\mu q_\nu \rangle = p_\mu p_\nu B_{21}(m_1^2, m_2^2, p^2, \mu^2) + g_{\mu\nu} B_{22}(m_1^2, m_2^2, p^2, \mu^2), \\
B_{\mu\nu\rho}(m_1^2, m_2^2, p, \mu^2) &= \langle q_\mu q_\nu q_\rho \rangle = p_\mu p_\nu p_\rho B_{31}(m_1^2, m_2^2, p^2, \mu^2) \\
&\quad + (g_{\mu\nu} p_\rho + g_{\mu\rho} p_\nu + g_{\rho\nu} p_\mu) B_{32}(m_1^2, m_2^2, p^2, \mu^2).
\end{aligned} \tag{20}$$

The methods of [21] can be used to deduce the relations

$$\begin{aligned}
B_1(m_1^2, m_2^2, p^2, \mu^2) &= -\frac{1}{2p^2} (A(m_1^2, \mu^2) - A(m_2^2, \mu^2) + (m_2^2 - m_1^2 - p^2)B(m_1^2, m_2^2, p^2, \mu^2)) , \\
B_{22}(m_1^2, m_2^2, p^2, \mu^2) &= \frac{1}{2(d-1)} \left( A(m_2^2, \mu^2) + 2m_1^2 B(m_1^2, m_2^2, p^2, \mu^2) \right. \\
&\quad \left. + (m_2^2 - m_1^2 - p^2)B_1(m_1^2, m_2^2, p^2, \mu^2) \right) , \\
B_{21}(m_1^2, m_2^2, p^2, \mu^2) &= \frac{1}{p^2} (A(m_2^2, \mu^2) + m_1^2 B(m_1^2, m_2^2, p^2, \mu^2) - dB_{22}(m_1^2, m_2^2, p^2, \mu^2)) . \quad (21)
\end{aligned}$$

This allows to rewrite all in terms of  $B(m_1^2, m_2^2, p^2, \mu^2)$ . These relations are used for the analytical evaluations given below.

The final evaluation is done by using a Feynman parameter  $x$  to combine the propagators and use the results for the tadpoles. The  $x$  integral needed can be done analytically or numerically.

The functions are then all expanded in terms of  $\epsilon$ . The arguments of the various Bubble integrals are not written out.

$$\begin{aligned}
B &= \frac{\lambda_0}{16\pi^2} + \bar{B} + \epsilon B^\epsilon + \mathcal{O}(\epsilon^2) , \\
B_1 &= \frac{\lambda_0}{16\pi^2} \frac{1}{2} + \bar{B}_1 + \epsilon B_1^\epsilon + \mathcal{O}(\epsilon^2) , \\
B_{21} &= \frac{\lambda_0}{16\pi^2} \frac{1}{3} + \bar{B}_{21} + \epsilon B_{21}^\epsilon + \mathcal{O}(\epsilon^2) , \\
B_{22} &= \frac{\lambda_0}{16\pi^2} \left( \frac{m_1^2}{4} + \frac{m_2^2}{4} - \frac{p^2}{12} \right) + \bar{B}_{22} + \epsilon B_{22}^\epsilon + \mathcal{O}(\epsilon^2) , \\
B_{31} &= \frac{\lambda_0}{16\pi^2} \frac{1}{4} + \bar{B}_{31} + \epsilon B_{31}^\epsilon + \mathcal{O}(\epsilon^2) , \\
B_{32} &= \frac{\lambda_0}{16\pi^2} \left( \frac{m_1^2}{12} + \frac{m_2^2}{6} - \frac{p^2}{24} \right) + \bar{B}_{32} + \epsilon B_{32}^\epsilon + \mathcal{O}(\epsilon^2) , \quad (22)
\end{aligned}$$

### 7.2.2 Analytical implementation

The functions in this section are all implemented fully analytically.

const double: msq, m1sq, m2sq, psq, mu2 these are  $m^2, m_1^2, m_2^2, p^2, \mu^2$ .

dcomplex Bb(m1sq, m2sq, psq, mu2): returns  $\bar{B}(m_1^2, m_2^2, p^2, \mu^2)$

dcomplex Bb(msq, psq, mu2): returns  $\bar{B}(m^2, m^2, p^2, \mu^2)$  using the simpler equal mass formula.

dcomplex B1b(m1sq, m2sq, psq, mu2): returns  $\bar{B}_1(m_1^2, m_2^2, p^2, \mu^2)$

dcomplex B21b(m1sq, m2sq, psq, mu2): returns  $\bar{B}_{21}(m_1^2, m_2^2, p^2, \mu^2)$

dcomplex B22b(m1sq, m2sq, psq, mu2): returns  $\bar{B}_{22}(m_1^2, m_2^2, p^2, \mu^2)$

dcomplex B22b(msq, psq, mu2): returns  $\bar{B}_{22}(m^2, m^2, p^2, \mu^2)$  using the simpler equal mass

formula.

Defined in `oneloopintegrals.h`, implemented in `oneloopintegrals.cc`, examples of use in `testoneloopintegrals.cc`.

### 7.2.3 Numerical implementation

The functions in this section are all implemented using a numerical complex integration over  $x$ . The integration routine used can be specified using the macro `WINTEGRAL` which defaults to `jbwgauss`. Any of the complex integration routines of `jbnumlib` can be used instead.

```
const double: m1sq, m2sq, psq, mu2 these are  $m_1^2, m_2^2, p^2, \mu^2$ .
dcomplex Bbnum(m1sq, m2sq, psq, mu2): returns  $\overline{B}(m_1^2, m_2^2, p^2, \mu^2)$ 
dcomplex B1bnum(m1sq, m2sq, psq, mu2): returns  $\overline{B}(m_1^2, m_2^2, p^2, \mu^2)$ 
dcomplex B21bnum(m1sq, m2sq, psq, mu2): returns  $\overline{B}_{21}(m_1^2, m_2^2, p^2, \mu^2)$ 
dcomplex B22bnum(m1sq, m2sq, psq, mu2): returns  $\overline{B}_{22}(m_1^2, m_2^2, p^2, \mu^2)$ 
dcomplex B31bnum(m1sq, m2sq, psq, mu2): returns  $\overline{B}_{31}(m_1^2, m_2^2, p^2, \mu^2)$ 
dcomplex B32bnum(m1sq, m2sq, psq, mu2): returns  $\overline{B}_{32}(m_1^2, m_2^2, p^2, \mu^2)$ 
```

The precision of the numerical integration can be set and obtained:

```
void setprecisiononeloopintegrals(const double eps) sets the precision to eps.
double getprecisiononeloopintegrals(void) returns the present precision. The default is 1e-10.
```

Defined in `oneloopintegrals.h`, implemented in `oneloopintegrals.cc`, examples of use in `testoneloopintegrals.cc`:

## 7.3 Sunset integrals

### 7.3.1 Definition

We first define the abbreviation

$$\langle\langle X \rangle\rangle = \left( \frac{\mu^{4-d}}{i} \right) \int \frac{d^d r}{(2\pi)^d} \frac{d^d s}{(2\pi)^d} \frac{X}{(r^2 - m_1^2)(s^2 - m_2^2)((r+s-p)^2 - m_3^2)}. \quad (23)$$

The sunset integrals themselves are defined by

$$\begin{aligned} H(m_1^2, m_2^2, m_3^2, p^2, \mu^2) &= \langle\langle 1 \rangle\rangle, \\ H_\mu(m_1^2, m_2^2, m_3^2, p, \mu^2) &= \langle\langle r_\mu \rangle\rangle = p_\mu H_1(m_1^2, m_2^2, m_3^2, p^2, \mu^2), \\ H_{\mu\nu}(m_1^2, m_2^2, m_3^2, p, \mu^2) &= \langle\langle r_\mu r_\nu \rangle\rangle = p_\mu p_\nu H_{21}(m_1^2, m_2^2, m_3^2, p^2, \mu^2) \\ &\quad + g_{\mu\nu} H_{22}(m_1^2, m_2^2, m_3^2, p^2, \mu^2), \\ H_{\mu\nu\rho}(m_1^2, m_2^2, m_3^2, p, \mu^2) &= \langle\langle r_\mu r_\nu r_\rho \rangle\rangle = p_\mu p_\nu p_\rho H_{31}(m_1^2, m_2^2, m_3^2, p^2, \mu^2) \end{aligned}$$

$$+ (g_{\mu\nu}p_\rho + g_{\mu\rho}p_\nu + g_{\rho\nu}p_\mu) H_{32}(m_1^2, m_2^2, m_3^2, p^2, \mu^2). \quad (24)$$

The needed integrals with  $s_\mu$  replacing some of the  $r_\mu$  in the definitions can be related to those without  $s_\mu$  as descibed in [19]. The evaluation of these sunsetintegrals has been done in [19]. Further references can be found there.

We extract the parts the divergent parts and the parts containing  $C$  via

$$\begin{aligned} H(m_1^2, m_2^2, m_3^2, p^2, \mu^2) = & \frac{1}{(16\pi^2)^2} \left[ (\lambda_2/2) (m_1^2 + m_2^2 + m_3^2) + (\lambda_1/2) (m_1^2 (1 - \log(m_1^2/\mu^2)) \right. \\ & + m_2^2 (1 - \log(m_2^2/\mu^2)) + m_3^2 (1 - \log(m_3^2/\mu^2)) - (p^2/2)) \Big] \\ & + H^F(m_1^2, m_2^2, m_3^2, p^2, \mu^2) + \mathcal{O}(\epsilon), \end{aligned} \quad (25)$$

$$\begin{aligned} H_1(m_1^2, m_2^2, m_3^2, p^2, \mu^2) = & \frac{1}{(16\pi^2)^2} \left[ (\lambda_2/4) (m_2^2 + m_3^2) + (\lambda_1/8) (2m_1^2 \right. \\ & + m_2^2 (1 - 4\log(m_2^2/\mu^2)) + m_3^2 (1 - 4\log(m_3^2/\mu^2)) - (2p^2/3)) \Big] \\ & + H_1^F(m_1^2, m_2^2, m_3^2, p^2, \mu^2) + \mathcal{O}(\epsilon), \end{aligned} \quad (26)$$

$$\begin{aligned} H_{21}(m_1^2, m_2^2, m_3^2, p^2, \mu^2) = & \frac{1}{(16\pi^2)^2} \left[ (\lambda_2/6) (m_2^2 + m_3^2) + (\lambda_1/36) (3m_1^2 \right. \\ & + m_2^2 (2 - 12\log(m_2^2/\mu^2)) + m_3^2 (2 - 12\log(m_3^2/\mu^2)) \\ & - (3p^2/2)) \Big] + H_{21}^F(m_1^2, m_2^2, m_3^2, p^2, \mu^2) + \mathcal{O}(\epsilon), \end{aligned} \quad (27)$$

$$\begin{aligned} H_{31}(m_1^2, m_2^2, m_3^2, p^2, \mu^2) = & \frac{1}{(16\pi^2)^2} \left[ (\lambda_2/8) (m_2^2 + m_3^2) + (\lambda_1/96) (4m_1^2 \right. \\ & + m_2^2 (3 - 24\log(m_2^2/\mu^2)) + m_3^2 (3 - 24\log(m_3^2/\mu^2)) \\ & - (12p^2/5)) \Big] + H_{31}^F(m_1^2, m_2^2, m_3^2, p^2, \mu^2) + \mathcal{O}(\epsilon), \end{aligned} \quad (28)$$

The routines for the sunset integrals calculate the value at  $p^2 = 0$  and the derivative there analytically. The remainder is then calculated with a rather smoot integral valid below threshold for the **double hh** functions and with a dispersive method for the **dcomplex zhh** functions. The latter is valid above and below threshold. The functions returning the derivative w.r.t.  $p^2$  calculate the value at  $p^2 = 0$  analytically and the remainder via a numerical integration as above.

### 7.3.2 Functions

The integration routines needed can be set using the macro **DINTEGRAL** for the real integration, default is **jbdgauss**, and **SINTEGRAL** for the real integration with a singularity, default is **jbdcauch**. Any of the similar routines in **jbnunlib** can be used instead.

**const double:** **m1sq, m2sq, m3sq, psq, mu2:** these are  $m_1^2, m_2^2, m_3^2, p^2, \mu^2$ .

n	1	2	3	4	5	6	7	8
i	1	2	1	1	2	2	1	2
j	1	1	2	1	2	1	2	2
k	1	1	1	2	1	2	2	2

Table 1: The relation between the value of  $n$  and the powers  $i, j, k$  of the three propagators.

Valid below threshold:

double hh(m1sq, m2sq, m3sq, psq, mu2) returns  $H^F(m_1^2, m_2^2, m_3^2, p^2, \mu^2)$   
double hh1(m1sq, m2sq, m3sq, psq, mu2) returns  $H_1^F(m_1^2, m_2^2, m_3^2, p^2, \mu^2)$   
double hh21(m1sq, m2sq, m3sq, psq, mu2) returns  $H_{21}^F(m_1^2, m_2^2, m_3^2, p^2, \mu^2)$   
double hh31(m1sq, m2sq, m3sq, psq, mu2) returns  $H_{31}^F(m_1^2, m_2^2, m_3^2, p^2, \mu^2)$   
double hhd(m1sq, m2sq, m3sq, psq, mu2) returns  $(\partial/\partial p^2)H^F(m_1^2, m_2^2, m_3^2, p^2, \mu^2)$   
double hh1d(m1sq, m2sq, m3sq, psq, mu2) returns  $(\partial/\partial p^2)H_1^F(m_1^2, m_2^2, m_3^2, p^2, \mu^2)$   
double hh21d(m1sq, m2sq, m3sq, psq, mu2) returns  $(\partial/\partial p^2)H_{21}^F(m_1^2, m_2^2, m_3^2, p^2, \mu^2)$

Valid above and below threshold:

dcomplex zhh(m1sq, m2sq, m3sq, psq, mu2) returns  $H^F(m_1^2, m_2^2, m_3^2, p^2, \mu^2)$   
dcomplex zhh1(m1sq, m2sq, m3sq, psq, mu2) returns  $H_1^F(m_1^2, m_2^2, m_3^2, p^2, \mu^2)$   
dcomplex zhh21(m1sq, m2sq, m3sq, psq, mu2) returns  $H_{21}^F(m_1^2, m_2^2, m_3^2, p^2, \mu^2)$   
dcomplex zhh31(m1sq, m2sq, m3sq, psq, mu2) returns  $H_{31}^F(m_1^2, m_2^2, m_3^2, p^2, \mu^2)$   
dcomplex zhhd(m1sq, m2sq, m3sq, psq, mu2) returns  $(\partial/\partial p^2)H^F(m_1^2, m_2^2, m_3^2, p^2, \mu^2)$   
dcomplex zhh1d(m1sq, m2sq, m3sq, psq, mu2) returns  $(\partial/\partial p^2)H_1^F(m_1^2, m_2^2, m_3^2, p^2, \mu^2)$   
dcomplex zhh21d(m1sq, m2sq, m3sq, psq, mu2) returns  $(\partial/\partial p^2)H_{21}^F(m_1^2, m_2^2, m_3^2, p^2, \mu^2)$

void setprecisionsunsetintegrals(const double eps) sets the precision to `eps`.  
double getprecisionsunsetintegrals(void) returns the present precision. The default is `1e-10`.

Defined in `unsetintegrals.h`, implemented in `unsetintegrals.cc`, examples of use in `testunsetintegrals.cc`:

## 7.4 Sunsetintegrals with different powers of propagators

### 7.4.1 Definition

We first define the abbreviation

$$\langle\langle X \rangle\rangle_n = \left( \frac{\mu^{4-d}}{i} \right) \int \frac{d^d r}{(2\pi)^d} \frac{d^d s}{(2\pi)^d} \frac{X}{(r^2 - m_1^2)^i (s^2 - m_2^2)^j ((r+s-p)^2 - m_3^2)^k}. \quad (29)$$

The translation of  $n$  to values for  $i, j, k$  is given in Tab. 1. The sunset integrals themselves

are defined by

$$\begin{aligned}
H(n, m_1^2, m_2^2, m_3^2, p^2, \mu^2) &= \langle \langle 1 \rangle \rangle_n, \\
H_\mu(n, m_1^2, m_2^2, m_3^2, p, \mu^2) &= \langle \langle r_\mu \rangle \rangle_n = p_\mu H_1(n, m_1^2, m_2^2, m_3^2, p^2, \mu^2), \\
H_{\mu\nu}(n, m_1^2, m_2^2, m_3^2, p, \mu^2) &= \langle \langle r_\mu r_\nu \rangle \rangle_n = p_\mu p_\nu H_{21}(n, m_1^2, m_2^2, m_3^2, p^2, \mu^2) \\
&\quad + g_{\mu\nu} H_{22}(n, m_1^2, m_2^2, m_3^2, p^2, \mu^2). \tag{30}
\end{aligned}$$

The needed integrals with  $s_\mu$  replacing some of the  $r_\mu$  in the definitions can be related to those without  $s_\mu$  as described in [22, 23, 24, 25]. The evaluation of these sunset integrals is by the generalization of the methods of [19]. Further references can be found there.

The divergent parts and the parts containing  $C$  via taking derivatives w.r.t. masses of (25). We thus define the functions  $H_i^F(n, m_1^2, m_2^2, m_3^2, p^2, \mu^2)$  for all cases above,  $i = 0(\text{blank}), 1, 21$ .

The routines for the sunset integrals calculate the value at  $p^2 = 0$  and the derivative there analytically. The remainder is then calculated with a rather smooth integral valid below threshold for the `double hh` functions. The functions returning the derivative w.r.t.  $p^2$  calculate the value at  $p^2 = 0$  analytically and the remainder via a numerical integration as above.

An added addition here is that case where the Kahlen function

$$\lambda(m_1^2, m_2^2, m_3^2) = \sqrt{(m_1^2 - m_2^2 - m_3^2)^2 - 4m_2^2 m_3^2}$$

vanishes, is treated correctly.

## 7.4.2 Functions

The integration routines needed can be set using the macro `DINTEGRAL` for the real integration, default is `jbdgauss`. Any of the similar routines in `jbnlib` can be used instead.

`const int n`: the integer  $n$  labelling the powers of the propagators as defined in Tab. 1.  
`const double: m1sq, m2sq, m3sq, psq, mu2`: these are  $m_1^2, m_2^2, m_3^2, p^2, \mu^2$ .

Valid below threshold:

`double hh(n, m1sq, m2sq, m3sq, psq, mu2)` returns  $H^F(n, m_1^2, m_2^2, m_3^2, p^2, \mu^2)$   
`double hh1(n, m1sq, m2sq, m3sq, psq, mu2)` returns  $H_1^F(n, m_1^2, m_2^2, m_3^2, p^2, \mu^2)$   
`double hh21(n, m1sq, m2sq, m3sq, psq, mu2)` returns  $H_{21}^F(n, m_1^2, m_2^2, m_3^2, p^2, \mu^2)$   
`double hhd(n, m1sq, m2sq, m3sq, psq, mu2)` returns  $(\partial/\partial p^2)H^F(n, m_1^2, m_2^2, m_3^2, p^2, \mu^2)$   
`double hh1d(n, m1sq, m2sq, m3sq, psq, mu2)` returns  $(\partial/\partial p^2)H_1^F(n, m_1^2, m_2^2, m_3^2, p^2, \mu^2)$   
`double hh21d(n, m1sq, m2sq, m3sq, psq, mu2)` returns  $(\partial/\partial p^2)H_{21}^F(n, m_1^2, m_2^2, m_3^2, p^2, \mu^2)$

`void setprecisionquenchedsunsetintegrals(const double eps)` sets the precision to `eps`.

`double getprecisionquenchedsunsetintegrals(void)` returns the present precision. The

default is 1e-10.

Defined in `quenchedsunsetintegrals.h`, implemented in `quenchedsunsetintegrals.cc`, examples of use in `testquenchedsunsetintegrals.cc`:

## 7.5 Finite volume tadpole integrals

### 7.5.1 Definitions

The methods used for these are derived in detail in [8], references to earlier literature can be found there. The integrals used here are given in the Minkowski conventions as defined in [26]. All of the integrals are available with two different methods, one using a summation over Bessel function and the other an integral over a Jacobi theta function. The versions included at present are using periodic boundary conditions, all three spatial sizes of the same length  $L$  and the time direction of infinite extent.

The tadpole integrals  $A$  and  $A_{\mu\nu}$  are defined as

$$\left\{ \tilde{A}^V(m^2, L, \mu^2), \tilde{A}_{\mu\nu}^V(m^2, L, \mu^2) \right\} = \frac{\mu^{4-d}}{i} \int_V \frac{d^d r}{(2\pi)^d} \frac{\{1, r_\mu r_\nu\}}{(r^2 - m^2)}. \quad (31)$$

The  $B$  tadpole integrals are the same but with a doubled propagator,  $C$  tadpoles are with a tripled propagator and  $D$  tadpoles with a quadrupled propagator. The subscript  $V$  on the integral indicates that the integral is a discrete sum over the three spatial components and an integral over the remainder. The size of the spatial directions is  $L$ .

At finite volume, there are more Lorentz-structures possible. The tensor  $t_{\mu\nu}$ , the spatial part of the Minkowski metric  $g_{\mu\nu}$ , is needed for these. The functions for  $\tilde{A}_{\mu\nu}^V$  are

$$\tilde{A}_{\mu\nu}^V(m^2, L, \mu^2) = g_{\mu\nu} \tilde{A}_{22}^V(m^2, L, \mu^2) + t_{\mu\nu} \tilde{A}_{23}^V(m^2, L, \mu^2). \quad (32)$$

Similar definitions are relevant for the  $B, C, D$  tadpoles. In infinite volume  $A_{22}$  is related to  $A$  and  $A_{23}$  vanishes. The relations in finite volume is given by

$$d\tilde{A}_{22}^V(m^2, L, \mu^2) + 3\tilde{A}_{23}^V(m^2, L, \mu^2) = m^2 \tilde{A}^V(m^2, L, \mu^2). \quad (33)$$

The relations for the other cases are:

$$\begin{aligned} d\tilde{B}_{22}^V(m^2, L, \mu^2) + 3\tilde{B}_{23}^V(m^2, L, \mu^2) &= m^2 \tilde{B}^V(m^2, L, \mu^2) + \tilde{A}^V(m^2, L, \mu^2), \\ d\tilde{C}_{22}^V(m^2, L, \mu^2) + 3\tilde{C}_{23}^V(m^2, L, \mu^2) &= m^2 \tilde{C}^V(m^2, L, \mu^2) + \tilde{B}^V(m^2, L, \mu^2), \\ d\tilde{D}_{22}^V(m^2, L, \mu^2) + 3\tilde{D}_{23}^V(m^2, L, \mu^2) &= m^2 \tilde{D}^V(m^2, L, \mu^2) + \tilde{C}^V(m^2, L, \mu^2). \end{aligned} \quad (34)$$

The full integrals are now split in the infinite volume part which was defined earlier in Sect. 7.1 and the finite volume remainder as

$$\tilde{A}^V(m^2, L, \mu^2) = \frac{\lambda_0 m^2}{16\pi^2} + \bar{A}(m^2, \mu^2) + \bar{A}^V(m^2, L) + \epsilon \left( A^\epsilon(m^2, \mu^2) + A^{V\epsilon}(m^2, L, \mu^2) \right) + \mathcal{O}(\epsilon^2),$$

$$\begin{aligned}
\tilde{B}^V(m^2, L, \mu^2) &= \frac{\lambda_0}{16\pi^2} + \bar{B}(m^2, \mu^2) + \bar{B}^V(m^2, L) + \epsilon (B^\epsilon(m^2, \mu^2) + B^{V\epsilon}(m^2, L, \mu^2)) + \mathcal{O}(\epsilon^2), \\
\tilde{C}^V(m^2, L, \mu^2) &= \bar{C}(m^2, \mu^2) + \bar{C}^V(m^2, L) + \epsilon (C^\epsilon(m^2, \mu^2) + C^{V\epsilon}(m^2, L, \mu^2)) + \mathcal{O}(\epsilon^2), \\
\tilde{D}^V(m^2, L, \mu^2) &= \bar{D}(m^2, \mu^2) + \bar{D}^V(m^2, L) + \epsilon (D^\epsilon(m^2, \mu^2) + D^{V\epsilon}(m^2, L, \mu^2)) + \mathcal{O}(\epsilon^2), \\
\tilde{A}_{22}^V(m^2, L, \mu^2) &= \frac{\lambda_0 m^4}{4(16\pi^2)} + \bar{A}_{22}(m^2, \mu^2) + \bar{A}_{22}^V(m^2, L) + \epsilon (A_{22}^\epsilon(m^2, \mu^2) + A_{22}^{V\epsilon}(m^2, L, \mu^2)) \\
\tilde{B}_{22}^V(m^2, L, \mu^2) &= \frac{\lambda_0 m^2}{2(16\pi^2)} + \bar{B}_{22}(m^2, \mu^2) + \bar{B}_{22}^V(m^2, L) + \epsilon (B_{22}^\epsilon(m^2, \mu^2) + B_{22}^{V\epsilon}(m^2, L, \mu^2)) \\
\tilde{C}_{22}^V(m^2, L, \mu^2) &= \frac{\lambda_0}{4(16\pi^2)} + \bar{C}_{22}(m^2, \mu^2) + \bar{C}_{22}^V(m^2, L) + \epsilon (C_{22}^\epsilon(m^2, \mu^2) + C_{22}^{V\epsilon}(m^2, L, \mu^2)) \\
\tilde{D}_{22}^V(m^2, L, \mu^2) &= \bar{D}_{22}(m^2, \mu^2) + \bar{D}_{22}^V(m^2, L) + \epsilon (D_{22}^\epsilon(m^2, \mu^2) + D_{22}^{V\epsilon}(m^2, L, \mu^2)) + \mathcal{O}(\epsilon^2), \\
\tilde{A}_{23}^V(m^2, L, \mu^2) &= \bar{A}_{23}^V(m^2, \mu^2) + \epsilon A_{22}^{V\epsilon}(m^2, L) + \mathcal{O}(\epsilon^2). \\
\tilde{B}_{23}^V(m^2, L, \mu^2) &= \bar{B}_{23}^V(m^2, \mu^2) + \epsilon B_{22}^{V\epsilon}(m^2, L) + \mathcal{O}(\epsilon^2). \\
\tilde{C}_{23}^V(m^2, L, \mu^2) &= \bar{C}_{23}^V(m^2, \mu^2) + \epsilon C_{22}^{V\epsilon}(m^2, L) + \mathcal{O}(\epsilon^2). \\
\tilde{D}_{23}^V(m^2, L, \mu^2) &= \bar{D}_{23}^V(m^2, \mu^2) + \epsilon D_{22}^{V\epsilon}(m^2, L) + \mathcal{O}(\epsilon^2).
\end{aligned} \tag{35}$$

### 7.5.2 Functions

The integration routines needed can be set using the macro `DINTEGRAL` for the real integration, default is `jbdgauss`. Any of the similar routines in `jbnunlib` can be used instead.

`const double: msq, L : msq` is  $m^2$  and `L` is the size  $L$  of the spatial dimension.

Evaluated with theta functions:

`double AbVt(msq, L):` returns  $\bar{A}^V(m^2, L)$ .  
`double A22bVt(msq, L):` returns  $\bar{A}_{22}^V(m^2, L)$ .  
`double A23bVt(msq, L):` returns  $\bar{A}_{23}^V(m^2, L)$ .  
`double BbVt(msq, L):` returns  $\bar{B}^V(m^2, L)$ .  
`double B22bVt(msq, L):` returns  $\bar{B}_{22}^V(m^2, L)$ .  
`double B23bVt(msq, L):` returns  $\bar{B}_{23}^V(m^2, L)$ .  
`double CbVt(msq, L):` returns  $\bar{C}^V(m^2, L)$ .  
`double C22bVt(msq, L):` returns  $\bar{C}_{22}^V(m^2, L)$ .  
`double C23bVt(msq, L):` returns  $\bar{C}_{23}^V(m^2, L)$ .  
`double DbVt(msq, L):` returns  $\bar{D}^V(m^2, L)$ .  
`double D22bVt(msq, L):` returns  $\bar{D}_{22}^V(m^2, L)$ .  
`double D23bVt(msq, L):` returns  $\bar{D}_{23}^V(m^2, L)$ .

Evaluated with Bessel functions:

```

double AbVb(msq,L): returns  $\overline{A}^V(m^2, L)$ .
double A22bVb(msq,L): returns  $\overline{A}_{22}^V(m^2, L)$ .
double A23bVb(msq,L): returns  $\overline{A}_{23}^V(m^2, L)$ .
double BbVb(msq,L): returns  $\overline{B}^V(m^2, L)$ .
double B22bVb(msq,L): returns  $\overline{B}_{22}^V(m^2, L)$ .
double B23bVb(msq,L): returns  $\overline{B}_{23}^V(m^2, L)$ .
double CbVb(msq,L): returns  $\overline{C}^V(m^2, L)$ .
double C22bVb(msq,L): returns  $\overline{C}_{22}^V(m^2, L)$ .
double C23bVb(msq,L): returns  $\overline{C}_{23}^V(m^2, L)$ .
double DbVb(msq,L): returns  $\overline{D}^V(m^2, L)$ .
double D22bVb(msq,L): returns  $\overline{D}_{22}^V(m^2, L)$ .
double D23bVb(msq,L): returns  $\overline{D}_{23}^V(m^2, L)$ .

```

The last letter indicates whether they are computed with the theta function or Bessel function method. The results were checked by comparing against each other and by comparing when possible with the independent Bessel function implementation done in [27].

```

void setprecisionfinitevolumeoneloop(const double Abacc=1e-10,
    const double Bbacc=1e-9, const bool printout=true)

```

sets the precision for the finite volume integrals evaluated with theta function to Abacc for the tadpole integrals, Bbacc for the bubble integrals. The last variable printout is a logical variable which can be set to true or false, default is false. Default values are those indicated.

```

void setprecisionfinitevolumeoneloopb(const int maxsum=100,
    const double Bbacc=1e-5, const bool printout=true)

```

sets the precision for the finite volume integrals evaluated with Bessel functions. The first argument indicates how far the sum over Bessel functions is taken. Maximum at present is 1000. The second argument gives the precision of the numerical integration for the bubble integrals. Defined in `finitevolumeoneloopintegrals.h`, implemented in `finitevolumeoneloopintegrals.cc`, examples of use in `testfinitevolumeoneloopintegrals.cc`.

## 7.6 Finite volume bubble integrals

### 7.6.1 Definitions

The methods used for these are derived in detail in [8], references to earlier literature can be found there. The integrals used here are given in the Minkowski conventions as defined in [26]. All of the integrals are available with two different methods, one using a summation over Bessel function and the other an integral over a Jacobi theta function. The versions included at present are using periodic boundary conditions, all three spatial sizes of the same length  $L$  and the time direction of infinite extent.

The bubble integrals  $B$ ,  $B_\mu$  and  $B_{\mu\nu}$  are defined as

$$\left\{ \tilde{B}^V, \tilde{B}_\mu^V, \tilde{B}_{\mu\nu}^V \right\} (m_1^2, m_2^2, p, L, \mu^2) = \frac{\mu^{4-d}}{i} \int_V \frac{d^d r}{(2\pi)^d} \frac{\{1, r_\mu, r_\mu r_\nu\}}{(r^2 - m_1^2)^{n_1} ((p-r)^2 - m_1^2)^{n_2}}. \quad (36)$$

The subscript  $V$  on the integral indicates that the integral is a discrete sum over the three spatial components and an integral over the remainder. The size of the spatial directions is  $L$ .

At finite volume, there are more Lorentz-structures possible. The tensor  $t_{\mu\nu}$ , the spatial part of the Minkowski metric  $g_{\mu\nu}$ , is needed for these. In addition, the functions can in principle depend on the components of the vector  $p$  as well, not only via  $p^2$ .

The functions themselves are split in the infinite volume part discussed in Sect. 7.2 and a finite volume part via

$$\tilde{B}^V = \frac{\lambda_0}{16\pi^2} + \overline{B}(m^2, \mu^2) + \overline{B}^V(m^2, L) + \epsilon (B^\epsilon + B^{V\epsilon}) + \mathcal{O}(\epsilon^2), \quad (37)$$

where all functions have as argument  $(m_1^2, m_2^2, p, L, \mu^2)$ .

## 7.6.2 Functions

The integration routines needed can be set using the macro `DINTEGRAL` for the real integration, default is `jbdgauss`.

```
void setprecisionfinitevolumeoneloop(const double Abacc=1e-10,
    const double Bbacc=1e-9, const bool printout=true) sets the precision for the fi-
nite volume integrals evaluated with theta function to Abacc for the tadpole integrals,
Bbacc for the bubble integrals. The last variable printout is a logical variable which can
be set to true or false, default is false. Default values are those indicated.
```

```
void setprecisionfinitevolumeoneloopb(const int maxsum=100,
    const double Bbacc=1e-5, const bool printout=true) sets the precision for the fi-
nite volume integrals evaluated with Bessel functions. The first argument indicates how far
the sum over Bessel functions is taken. Maximum at present is 1000. The second argument
gives the precision of the numerical integration for the bubble integrals.
```

Defined in `finitevolumeoneloopintegrals.h`, implemented in `finitevolumeoneloop-
integrals.cc`, examples of use in `testfinitevolumeoneloopintegrals.cc`.

### 7.6.2.1 $p = 0$ and periodic boundary conditions

`const double: m1sq, m2sq, L, mu2.` These correspond to  $msq, m_1^2, m_2^2, L, \mu^2$ .  $L$  is the size of the finite dimensions.

Evaluated with theta functions:

`double BbVt(m1sq,m2sq,L):` returns  $\overline{B}^V(m_1^2, m_2^2, p=0, L, \mu^2)$

`double BbVt(msq,L):` returns  $\overline{B}^V(m^2, m^2, p=0, L, \mu^2)$

Evaluated with Bessel functions:

`double BbVb(m1sq,m2sq,L):` return  $\overline{B}^V(m_1^2, m_2^2, p=0, L, \mu^2)$

`double BbVb(msq,L):` returns  $\overline{B}^V(m^2, m^2, p=0, L, \mu^2)$

## 7.7 Finite volume sunset integrals

### 7.7.1 Definitions

The sunset integrals are defined with

$$\langle\langle X \rangle\rangle_V = \frac{\mu^{8-2d}}{i^2} \int_V \frac{d^d r}{(2\pi)^d} \frac{d^d 1}{(2\pi)^d} \frac{\{1, r_\mu, r_\mu r_\nu\}}{(r^2 - m_1^2)(s^2 - m_2^2)((r+s-p)^2 - m_3^2)}. \quad (38)$$

The subscript  $V$  indicates that the spatial dimensions are a discrete sum rather than an integral. The conventions correspond to those in infinite volume of [19] and of Sect. 7.3. Integrals with the other momentum  $s$  in the numerator are related using the relations shown in [19] which remain valid at finite volume in the cms frame [8].

In the cms frame we define the functions<sup>1</sup>

$$\begin{aligned} \tilde{H}_\mu^V &= \langle\langle X \rangle\rangle_V \\ \tilde{H}_\mu^V &= \langle\langle r_\mu \rangle\rangle_V = p_\mu \tilde{H}_1^V \\ \tilde{H}_{\mu\nu}^V &= \langle\langle r_\mu r_\nu \rangle\rangle_V = p_\mu p_\nu \tilde{H}_{21}^V + g_{\mu\nu} \tilde{H}_{22}^V + t_{\mu\nu} \tilde{H}_{27}^V. \end{aligned} \quad (39)$$

The arguments of all functions in the cms frame are  $(m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ . These functions satisfy in finite volume [8],

$$\begin{aligned} \tilde{H}_1^V + \tilde{H}_1^V(m_2^2, m_3^2, m_1^2, p^2, L, \mu^2) + \tilde{H}_1^V(m_3^2, m_1^2, m_2^2, p^2, L, \mu^2) &= \tilde{H}^V, \\ p^2 \tilde{H}_{21}^V + d \tilde{H}_{22}^V + 3 \tilde{H}_{27}^V - m_1^2 H &= \tilde{A}^V(m_2^2) \tilde{A}^V(m_3^2). \end{aligned} \quad (40)$$

The arguments of the sunset functions in the relations, if not mentioned explicitly, are  $(m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .

We split the functions in an infinite volume part,  $H_i$ , and a finite volume correction,  $H_i^V$ , with  $\tilde{H}_i^V = H_i + H_i^V$ . The infinite volume part has been discussed above. For the finite volume parts we define

$$H^V = \frac{\lambda_0}{16\pi^2} \left( \overline{A}^V(m_1^2) + \overline{A}^V(m_2^2) + \overline{A}^V(m_3^2) \right) + \frac{1}{16\pi^2} \left( A^{V\epsilon}(m_1^2) + A^{V\epsilon}(m_2^2) + A^{V\epsilon}(m_3^2) \right)$$

---

<sup>1</sup>In the cms frame, after the reduction to four dimensions,  $t_{\mu\nu} = g_{\mu\nu} - p_\mu p_\nu / p^2$  but the separation appears naturally in the calculation [8]. In addition, it avoids singularities in the limit  $p \rightarrow 0$ .

$$\begin{aligned}
& + H^{VF} + \mathcal{O}(\epsilon), \\
H_1^V &= \frac{\lambda_0}{16\pi^2} \frac{1}{2} \left( \overline{A}^V(m_2^2) + \overline{A}^V(m_3^2) \right) + \frac{1}{16\pi^2} \frac{1}{2} (A^{V\epsilon}(m_2^2) + A^{V\epsilon}(m_3^2)) + H_1^{VF} + \mathcal{O}(\epsilon), \\
H_{21}^V &= \frac{\lambda_0}{16\pi^2} \frac{1}{3} \left( \overline{A}^V(m_2^2) + \overline{A}^V(m_3^2) \right) + \frac{1}{16\pi^2} \frac{1}{3} (A^{V\epsilon}(m_2^2) + A^{V\epsilon}(m_3^2)) + H_{21}^{VF} + \mathcal{O}(\epsilon), \\
H_{27}^V &= \frac{\lambda_0}{16\pi^2} \left( \overline{A}_{23}^V(m_1^2) + \frac{1}{3} \overline{A}_{23}^V(m_2^2) + \frac{1}{3} \overline{A}_{23}^V(m_3^2) \right) \\
& + \frac{1}{16\pi^2} \left( A_{23}^{V\epsilon}(m_1^2) + \frac{1}{3} A_{23}^{V\epsilon}(m_2^2) + \frac{1}{3} A_{23}^{V\epsilon}(m_3^2) \right) + H_{27}^{VF} + \mathcal{O}(\epsilon). \tag{41}
\end{aligned}$$

The finite parts are defined differently from the infinite volume case in [19]. The parts with  $A^{V\epsilon}$  are removed here as well.

The functions  $H_i^{VF}$  can be computed with the methods of [8]. They are obtained by adding the parts labeled with  $G$  and  $H$  in Sect. 4.3 and the part of Sect. 4.4 in [8]. The derivatives w.r.t.  $p^2$  can be treated using a simple adaptation of that method.

The method for evaluation works only below threshold. The numerical evaluation is rather slow. Playing with the precision settings for the specific case you need is very strongly recommended.

### 7.7.2 Functions

`const double: m1sq,m2sq,m3sq,psq,L,mu2`. These correspond to  $m_1^2, m_2^2, m_3^2, p^2, L, \mu^2$ .

Evaluation using theta functions:

```

double hhVt(m1sq,m2sq,m3sq,psq,L,mu2): returns  $H^{VF}(m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .
double hh1Vt(m1sq,m2sq,m3sq,psq,L,mu2): returns  $H_1^{VF}(m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .
double hh21Vt(m1sq,m2sq,m3sq,psq,L,mu2): returns  $H_{21}^{VF}(m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .
double hh22Vt(m1sq,m2sq,m3sq,psq,L,mu2): returns  $H_{22}^{VF}(m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .
double hh27Vt(m1sq,m2sq,m3sq,psq,L,mu2): returns  $H_{27}^{VF}(m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .
double hhdVt(m1sq,m2sq,m3sq,psq,L,mu2): returns  $(\partial/\partial p^2)H^{VF}(m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .
double hh1dVt(m1sq,m2sq,m3sq,psq,L,mu2): returns  $(\partial/\partial p^2)H_1^{VF}(m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .
double hh21dVt(m1sq,m2sq,m3sq,psq,L,mu2): returns  $(\partial/\partial p^2)H_{21}^{VF}(m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .
double hh22dVt(m1sq,m2sq,m3sq,psq,L,mu2): returns  $(\partial/\partial p^2)H_{22}^{VF}(m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .
double hh27dVt(m1sq,m2sq,m3sq,psq,L,mu2): returns  $(\partial/\partial p^2)H_{27}^{VF}(m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .

```

Evaluation using Bessel functions:

```

double hhVb(m1sq,m2sq,m3sq,psq,L,mu2): returns  $H^{VF}(m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .
double hh1Vb(m1sq,m2sq,m3sq,psq,L,mu2): returns  $H_1^{VF}(m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .
double hh21Vb(m1sq,m2sq,m3sq,psq,L,mu2): returns  $H_{21}^{VF}(m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .
double hh22Vb(m1sq,m2sq,m3sq,psq,L,mu2): returns  $H_{22}^{VF}(m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .
double hh27Vb(m1sq,m2sq,m3sq,psq,L,mu2): returns  $H_{27}^{VF}(m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .
double hhdVb(m1sq,m2sq,m3sq,psq,L,mu2): returns  $(\partial/\partial p^2)H^{VF}(m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .
double hh1dVb(m1sq,m2sq,m3sq,psq,L,mu2): returns  $(\partial/\partial p^2)H_1^{VF}(m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .

```

```
double hh21dVb(m1sq,m2sq,m3sq,psq,L,mu2): returns  $(\partial/\partial p^2)H_{21}^{VF}(m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .
double hh22dVb(m1sq,m2sq,m3sq,psq,L,mu2): returns  $(\partial/\partial p^2)H_{22}^{VF}(m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .
double hh27dVb(m1sq,m2sq,m3sq,psq,L,mu2): returns  $(\partial/\partial p^2)H_{27}^{VF}(m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .
```

For all cases discussed both methods, via Bessel or (generalized) Jacobi theta functions, give the same results. The derivatives w.r.t.  $p^2$  for all the integrals were compared with taking a numerical derivative.

Note that the sunset functions at finite volume call the tadpole integrals evaluated with the same method. Do not forget to set precision for those as well.

```
void setprecisionfinitevolumesunsett(const double racc=1e-5,
    const double rsacc=1e-4,const bool printout=true)
```

The double values `sunsetracc` and `sunsetrsacc` set the accuracies of the numerical integration needed when one or two loop-momenta “feel” the finite volume. Default values are `1e-5` and `1e-4` respectively. The bool variable `printout` defaults to `true` and sets whether the setting is printed.

```
void setprecisionfinitevolumesunsetb(const int maxsum1=100,
    const int maxsum2=40,racc=1e-5,rsacc=1e-4,printout)
```

The integers `maxsum1` and `maxsum2` give how far the sum over Bessel functions is used for the case with one or two loop momenta “feeling” the finite volume. The first is maximum 1000, the second maximum 40 in the present implementation. In the latter case a triple sum is needed, hence the much lower upper bound. The double values `sunsetracc` and `sunsetrsacc` set the accuracies of the numerical integration which is still needed after the sum for both cases.

For most applications it makes sense to have a higher precision for the case with one loop momentum quantized, i.e. `racc` smaller than `rsacc`.

Defined in `finitevolumesunsetintegrals.h`, implemented in `finitevolumesunsetintegrals.cc` and examples of use in `testfinitevolumesunsetintegrals.cc`

## 7.8 Finite volume sunsetintegrals with different powers of propagators

### 7.8.1 Definitions

The sunset integrals with different powers of momenta are defined with

$$\langle\langle X \rangle\rangle_{nV} = \frac{\mu^{8-2d}}{i^2} \int_V \frac{d^d r}{(2\pi)^d} \frac{d^d 1}{(2\pi)^d} \frac{\{1, r_\mu, r_\mu r_\nu\}}{(r^2 - m_1^2)^i (s^2 - m_2^2)^j ((r + s - p)^2 - m_3^2)^k}. \quad (42)$$

The subscript  $V$  indicates that the spatial dimensions are a discrete sum rather than an integral. The translation of  $n$  to the powers  $i, j, k$  is given in Tab. 1. In the cms frame we define the functions<sup>2</sup>

$$\begin{aligned}\tilde{H}_\mu^V &= \langle\langle X \rangle\rangle_{nV} \\ \tilde{H}_\mu^V &= \langle\langle r_\mu \rangle\rangle_{nV} = p_\mu \tilde{H}_1^V \\ \tilde{H}_{\mu\nu}^V &= \langle\langle r_\mu r_\nu \rangle\rangle_{nV} = p_\mu p_\nu \tilde{H}_{21}^V + g_{\mu\nu} \tilde{H}_{22}^V + t_{\mu\nu} \tilde{H}_{27}^V.\end{aligned}\tag{43}$$

The arguments of all functions in the cms frame are  $(n, m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .

We split the functions in an infinite volume part,  $H_i$ , and a finite volume correction,  $H_i^V$ , with  $\tilde{H}_i^V = H_i + H_i^V$ . The infinite volume part has been discussed above. Note that the functions in the section are defined with the derivative w.r.t.  $m_i^2$  for the propagators with mass  $m_i^2$ . For the finite volume parts we define the subtraction as before in (41), i.e. we subtract the  $A^{V\epsilon}, B^{V\epsilon}$  parts.

The functions  $H_i^{VF}$  can be computed with the methods of [8]. They are obtained by adding the parts labeled with  $G$  and  $H$  in Sect. 4.3 and the part of Sect. 4.4 in [8]. The derivatives w.r.t.  $p^2$  can be treated using a simple adaptation of that method.

The method for evaluation works only below threshold. The numerical evaluation is rather slow. Playing with the precision settings for the specific case you need is very strongly recommended.

### 7.8.2 Functions

`const int n` The propagator cases as given in Tab. 1.

`const double: m1sq, m2sq, m3sq, psq, L, mu2.` These correspond to  $m_1^2, m_2^2, m_3^2, p^2, L, \mu^2$ .

Evaluation using theta functions:

`double hhVt(n, m1sq, m2sq, m3sq, psq, L, mu2):` returns  $H^{VF}(n, m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .  
`double hh1Vt(n, m1sq, m2sq, m3sq, psq, L, mu2):` returns  $H_1^{VF}(n, m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .  
`double hh21Vt(n, m1sq, m2sq, m3sq, psq, L, mu2):` returns  $H_{21}^{VF}(n, m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .  
`double hh22Vt(n, m1sq, m2sq, m3sq, psq, L, mu2):` returns  $H_{22}^{VF}(n, m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .  
`double hh27Vt(n, m1sq, m2sq, m3sq, psq, L, mu2):` returns  $H_{27}^{VF}(n, m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .  
`double hhdVt(n, m1sq, m2sq, m3sq, psq, L, mu2):` returns  $(\partial/\partial p^2)H^{VF}(n, m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .  
`double hh1dVt(n, m1sq, m2sq, m3sq, psq, L, mu2):` returns  $(\partial/\partial p^2)H_1^{VF}(n, m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .  
`double hh21dVt(n, m1sq, m2sq, m3sq, psq, L, mu2):` returns  $(\partial/\partial p^2)H_{21}^{VF}(n, m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .  
`double hh22dVt(n, m1sq, m2sq, m3sq, psq, L, mu2):` returns  $(\partial/\partial p^2)H_{22}^{VF}(n, m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .  
`double hh27dVt(n, m1sq, m2sq, m3sq, psq, L, mu2):` returns  $(\partial/\partial p^2)H_{27}^{VF}(n, m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .

Evaluation using Bessel functions:

`double hhVb(n, m1sq, m2sq, m3sq, psq, L, mu2):` returns  $H^{VF}(n, m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .  
`double hh1Vb(n, m1sq, m2sq, m3sq, psq, L, mu2):` returns  $H_1^{VF}(n, m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .

---

<sup>2</sup>In the cms frame  $t_{\mu\nu} = g_{\mu\nu} - p_\mu p_\nu / p^2$  but the separation appears naturally in the calculation [8]. In addition, it avoids singularities in the limit  $p \rightarrow 0$ .

```

double hh21Vb(n,m1sq,m2sq,m3sq,psq,L,mu2): returns  $H_{21}^{VF}(n, m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .
double hh22Vb(n,m1sq,m2sq,m3sq,psq,L,mu2): returns  $H_{22}^{VF}(n, m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .
double hh27Vb(n,m1sq,m2sq,m3sq,psq,L,mu2): returns  $H_{27}^{VF}(n, m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .
double hhdVb(n,m1sq,m2sq,m3sq,psq,L,mu2): returns  $(\partial/\partial p^2)H^{VF}(n, m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .
double hh1dVb(n,m1sq,m2sq,m3sq,psq,L,mu2): returns  $(\partial/\partial p^2)H_1^{VF}(n, m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .
double hh21dVb(n,m1sq,m2sq,m3sq,psq,L,mu2): returns  $(\partial/\partial p^2)H_{21}^{VF}(n, m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .
double hh22dVb(n,m1sq,m2sq,m3sq,psq,L,mu2): returns  $(\partial/\partial p^2)H_{22}^{VF}(n, m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .
double hh27dVb(n,m1sq,m2sq,m3sq,psq,L,mu2): returns  $(\partial/\partial p^2)H_{27}^{VF}(n, m_1^2, m_2^2, m_3^2, p^2, L, \mu^2)$ .

```

For all cases discussed both methods, via Bessel or (generalized) Jacobi theta functions, give the same results. The derivatives w.r.t.  $p^2$  for all the integrals were compared with taking a numerical derivative.

Note that the sunset functions at finite volume call the tadpole integrals evaluated with the same method. Do not forget to set precision for those as well.

```

void setprecisionfinitevolumesunsett(const double racc=1e-5,
    const double rsacc=1e-4,const bool printout=true)

```

The double values `sunsetracc` and `sunsetrsacc` set the accuracies of the numerical integration needed when one or two loop-momenta “feel” the finite volume. Default values are `1e-5` and `1e-4` respectively. The bool variable `printout` defaults to `true` and sets whether the setting is printed.

```

void setprecisionfinitevolumesunsetb(const int maxsum1=100,
    const int maxsum2=40,racc=1e-5,rsacc=1e-4,printout)

```

The integers `maxsum1` and `maxsum2` give how far the sum over Bessel functions is used for the case with one or two loop momenta “feeling” the finite volume. The first is maximum 1000, the second maximum 40 in the present implementation. In the latter case a triple sum is needed, hence the much lower upper bound. The double values `sunsetracc` and `sunsetrsacc` set the accuracies of the numerical integration which is still needed after the sum for both cases.

For most applications it makes sense to have a higher precision for the case with one loop momentum quantized, i.e. `racc` smaller than `rsacc`.

Defined in `finitevolumesunsetintegrals.h`, implemented in `finitevolumesunsetintegrals.cc` and examples of use in `testfinitevolumesunsetintegrals.cc`

## 8 Three flavour isospin conserving results

### 8.1 Masses, decay constants and vacuum-expectation-values: in physical

The exansions in this subsection are defined in terms of the physical masses,  $m_\pi, m_K, m_\eta$  and the physical pion decay constant  $F_\pi$ .

#### 8.1.1 Masses

The masses of the pion, kaon and eta at two-loops in three flavour ChPT were evaluated in [19]. The pion and eta mass were done earlier with a different subtraction scheme and a different way to perform the sunset integrals in [28].

The expressions for the physical masses for  $a = \pi, K, \eta$  are given by

$$m_{a\text{phys}}^2 = m_{a0}^2 + m_a^{2(4)} + m_a^{2(6)}. \quad (44)$$

The superscripts indicate the order of the diagrams in  $p$  that each contribution comes from. The lowest order masses are

$$m_{\pi 0}^2 = 2B_0\hat{m}, \quad m_{K 0}^2 = B_0(\hat{m} + m_s), \quad m_{\eta 0}^2 = \frac{2}{3}(\hat{m} + 2m_2). \quad (45)$$

The higher order contributions are split in the parts depending on the NLO LECs  $L_i^r$ , on the NNLO LECs  $C_i^r$  and the remainder as

$$m_a^{2(4)} = m_{aL}^{2(4)} + m_{aR}^{2(4)}, \quad m_a^{2(6)} = m_{aL}^{2(6)} + m_{aC}^{2(6)} + m_{aR}^{2(6)}. \quad (46)$$

The expressions for these can be found in [19] and on [13]. Note that when combining these with results from other sources one should be sure to use a compatible LO and NLO.

Pion mass:

```
double mpi4(phymass,Li) returns  $m_\pi^{2(4)}$ 
double mpi4L(phymass,Li) returns  $m_{\pi L}^{2(4)}$ 
double mpi4R(phymass,Li) returns  $m_{\pi R}^{2(4)}$ 
double mpi6(phymass,Li,Ci) returns  $m_\pi^{2(6)}$ 
double mpi6L(phymass,Li) returns  $m_{\pi L}^{2(6)}$ 
double mpi6C(phymass,Ci) returns  $m_{\pi C}^{2(6)}$ 
double mpi6R(phymass) returns  $m_{\pi R}^{2(6)}$ 
```

Kaon mass:

```
double mk4(phymass,Li) returns  $m_K^{2(4)}$ 
double mk4L(phymass,Li) returns  $m_{KL}^{2(4)}$ 
double mk4R(phymass,Li) returns  $m_{KR}^{2(4)}$ 
```

double mk6(phymass,Li,Ci) returns  $m_K^{2(6)}$   
double mk6L(phymass,Li) returns  $m_{KL}^{2(6)}$   
double mk6C(phymass,Ci) returns  $m_{KC}^{2(6)}$   
double mk6R(phymass) returns  $m_{KR}^{2(6)}$

Eta mass:

double meta4(phymass,Li) returns  $m_\eta^{2(4)}$   
double meta4L(phymass,Li) returns  $m_{\eta L}^{2(4)}$   
double meta4R(phymass,Li) returns  $m_{\eta R}^{2(4)}$   
double meta6(phymass,Li,Ci) returns  $m_\eta^{2(6)}$   
double meta6L(phymass,Li) returns  $m_{\eta L}^{2(6)}$   
double meta6C(phymass,Ci) returns  $m_{\eta C}^{2(6)}$   
double meta6R(phymass) returns  $m_{\eta R}^{2(6)}$

The functions are defined in `massesdecayvev.h`, implemented in `massesdecayvev.cc` and examples of use are in `testmassdecayvev.cc`.

### 8.1.2 Decay constants

The decay constants of the pion, kaon and eta at two-loops in three flavour ChPT were obtained in [19]. The pion and eta decay constants were done earlier with a different subtraction scheme and a different way to perform the sunset integrals in [28].

The expressions for the decay constants for  $a = \pi, K, \eta$  are given by

$$F_{a \text{ phys}} = F_0 \left( 1 + F_a^{(4)} + F_a^{(6)} \right) . \quad (47)$$

The superscripts indicate the order of the diagrams in  $p$  that each contribution comes from.  $F_0$  denotes the decay constant in the three-flavour chiral limit. The expressions were originally derived in [19], but note the description in the erratum of [29]. The expressions corrected for the error can be found in the website [13]. The normalization is such that  $F_\pi \approx 92$  MeV.

The contributions themselves are divided into the parts depending on the NLO LECs  $L_i^r$ , on the NNLO LECs  $C_i^r$  and the remainder as

$$F_a^{(4)} = F_{aL}^{(4)} + F_{aR}^{(4)}, \quad F_a^{(6)} = F_{aL}^{(6)} + F_{aC}^{(6)} + F_{aR}^{(6)}. \quad (48)$$

For the  $\eta$  the decay constant has been defined with the octet axial-vector current.

Pion decay constant:

double fpi4(phymass,Li) returns  $F_\pi^{(4)}$   
double fpi4L(phymass,Li) returns  $F_{\pi L}^{(4)}$   
double fpi4R(phymass,Li) returns  $F_{\pi R}^{(4)}$

```

double fpi6(phymass,Li,Ci) returns  $F_{\pi}^{(6)}$ 
double fpi6L(phymass,Li) returns  $F_{\pi L}^{(6)}$ 
double fpi6C(phymass,Ci) returns  $F_{\pi C}^{(6)}$ 
double fpi6R(phymass) returns  $F_{\pi R}^{(6)}$ 

```

Kaon decay constant:

```

double fk4(phymass,Li) returns  $F_K^{(4)}$ 
double fk4L(phymass,Li) returns  $F_{KL}^{(4)}$ 
double fk4R(phymass,Li) returns  $F_{KR}^{(4)}$ 
double fk6(phymass,Li,Ci) returns  $F_K^{(6)}$ 
double fk6L(phymass,Li) returns  $F_{KL}^{(6)}$ 
double fk6C(phymass,Ci) returns  $F_{KC}^{(6)}$ 
double fk6R(phymass) returns  $F_{KR}^{(6)}$ 

```

Eta decay constant:

```

double feta4(phymass,Li) returns  $F_{\eta}^{(4)}$ 
double feta4L(phymass,Li) returns  $F_{\eta L}^{(4)}$ 
double feta4R(phymass,Li) returns  $F_{\eta R}^{(4)}$ 
double feta6(phymass,Li,Ci) returns  $F_{\eta}^{(6)}$ 
double feta6L(phymass,Li) returns  $F_{\eta L}^{(6)}$ 
double feta6C(phymass,Ci) returns  $F_{\eta C}^{(6)}$ 
double feta6R(phymass) returns  $F_{\eta R}^{(6)}$ 

```

The functions are defined in `massesdecayvev.h`, implemented in `massesdecayvev.cc` and examples of use are in `testmassdecayvev.cc`.

### 8.1.3 getfpimeta

A problem that occurs in trying to compare to lattice QCD is that many of the routines are written in terms of the physical pion decay constant and physical masses. In particular, the eta mass is treated as physical. One thus needs a consistent eta mass and pion decay constant when varying the input pion and kaon mass. This assumes we have fitted the LECs  $L_i^r$  and  $C_i^r$  with a known set of  $m_{\pi}, m_K, m_{\eta}, F_{\pi}$ .

With that input we can obtain an eta mass and pion decay constant with as input values the original `Liin`, `Ciin` and the `massin`. The formulas used are (46) and (48) up to order  $p^6$  and  $p^4$ . The solution is obtained by iteration and stops when six digits of precision are reached. This method was used in [26] to obtain the consistent set of masses and decay constants used there.

```

phymass getfpimeta6(const double mpiin, const double mkin,
  const phymass massin, const Li Liin, const Ci Ciin)

```

returns a `physmass` containing `mpiin`, `mk` and the calculated compatible `meta`, `fpi` with the formulas including order  $p^6$ , i.e. to NNLO.

```
physmass getfpimeta4(const double mpiin, const double mk,
    const physmass massin, const Li Liin)
```

returns a `physmass` containing `mpiin`, `mk` and the calculated compatible `meta`, `fpi` with the formulas including order  $p^4$ , i.e. to NLO.

The functions are defined in `getfpimeta.h`, implemented in `getfpimeta.cc` and examples of use are in `testgetfpimeta.cc`.

#### 8.1.4 Vacuum-expectation-values

The corrections to the vacuum expectation values (vevs)  $\langle 0|\bar{q}q|0\rangle$  for up, down and strange quarks in the isospin limit were calculated at two-loops in three flavour ChPT in [29]. The expression for the up and down quark vev are identical since we are in the isospin limit.

We write the expressions in a form analogous to the decay constant treatment:

$$\langle 0|\bar{q}q|0\rangle_{a\text{phys}} = -F_0^2 B_0 \left(1 + \langle 0|\bar{q}q|0\rangle_a^{(4)} + \langle 0|\bar{q}q|0\rangle_a^{(6)}\right). \quad (49)$$

The superscripts indicate the order of the diagrams in  $p$  that each contribution comes from. The lowest order values are  $-F_0^2 B_0$ .

Note that the vevs are not directly measurable quantities. They depend on exactly the way the scalar densities are defined in QCD. ChPT can be used for them when a massindependent, chiral symmetry respecting subtraction scheme is used.  $\overline{MS}$  in QCD satisfies this, but there are other possibilities. Even within a scheme,  $B_0$  and the quark masses depend on the QCD subtraction scale  $\mu_{\text{QCD}}$  in such a way that  $B_0 m_q$  is independent of it. The higher order corrections in this case also depend on the LECs for fully local counterterms,  $H_1^r, H_2^r$  at order  $p^4$  and  $C_{91}^r, \dots, C_{94}^r$  at  $p^6$ . When the scalar density is fully defined, measuring these quantities in e.g. lattice QCD and comparing with the ChPT expressions is a well defined procedure.

The contributions at the different orders themselves are split in the parts depending on the NLO LECs  $L_i^r$ , on the NNLO LECs  $C_i^r$  and the remainder as

$$\begin{aligned} \langle 0|\bar{q}q|0\rangle_a^{(4)} &= \langle 0|\bar{q}q|0\rangle_{aL}^{(4)} + \langle 0|\bar{q}q|0\rangle_{aR}^{(4)}, \\ \langle 0|\bar{q}q|0\rangle_a^{(6)} &= \langle 0|\bar{q}q|0\rangle_{aL}^{(6)} + \langle 0|\bar{q}q|0\rangle_{aC}^{(6)} + \langle 0|\bar{q}q|0\rangle_{aR}^{(6)}. \end{aligned} \quad (50)$$

These are defined for  $q = u, s$ .

$\langle 0|\bar{q}q|0\rangle_{u\text{phys}}$ :

```
double qqup4(physmass, Li) returns  $\langle 0|\bar{q}q|0\rangle_u^{(4)}$ 
double qqup4L(physmass, Li) returns  $\langle 0|\bar{q}q|0\rangle_{uL}^{(4)}$ 
double qqup4R(physmass) returns  $\langle 0|\bar{q}q|0\rangle_{uR}^{(4)}$ 
double qqup6(physmass, Li, Ci) returns  $\langle 0|\bar{q}q|0\rangle_u^{(6)}$ 
double qqup6L(physmass, Li) returns  $\langle 0|\bar{q}q|0\rangle_{uL}^{(6)}$ 
```

double qqup6C(phymass,Li) returns  $\langle 0|\bar{q}q|0\rangle_{uC}^{(6)}$   
double qqup6R(phymass) returns  $\langle 0|\bar{q}q|0\rangle_{uR}^{(6)}$

$\langle 0|\bar{q}q|0\rangle_{s\text{phys}}$ :

double qqstrange4(phymass,Li) returns  $\langle 0|\bar{q}q|0\rangle_s^{(4)}$   
double qqstrange4L(phymass,Li) returns  $\langle 0|\bar{q}q|0\rangle_{sL}^{(4)}$   
double qqstrange4R(phymass) returns  $\langle 0|\bar{q}q|0\rangle_{sR}^{(4)}$   
double qqstrange6(phymass,Li,Ci) returns  $\langle 0|\bar{q}q|0\rangle_s^{(6)}$   
double qqstrange6L(phymass,Li) returns  $\langle 0|\bar{q}q|0\rangle_{sL}^{(6)}$   
double qqstrange6C(phymass,Li) returns  $\langle 0|\bar{q}q|0\rangle_{sC}^{(6)}$   
double qqstrange6R(phymass) returns  $\langle 0|\bar{q}q|0\rangle_{sR}^{(6)}$

The functions are defined in `massesdecayvev.h`, implemented in `massesdecayvev.cc` and examples of use are in `testmassesdecayvev.cc`

## 8.2 Masses, decay constants and vacuum-expectation-values: in lowest order

The exansions in this subsection are defined in terms of the lowest order masses,  $m_{\pi 0}, m_{K 0}, m_{\eta} = \sqrt{(4m_{K 0}^2 - m_{\pi 0}^2)}/3$  and the lowest order, or chiral limit, pion decay constant  $F_0$ .

### 8.2.1 Masses: in lowest order

The masses of the pion, kaon and eta at two-loops in three flavour ChPT were evaluated in [19]. The pion and eta mass were done earlier with a different subtraction scheme and a different way to perform the sunset integrals in [28].

The expressions for the physical masses for  $a = \pi, K, \eta$  are given by

$$m_{a\text{phys}}^2 = m_{a0}^2 + m_a^{2(4)0} + m_a^{2(6)0}. \quad (51)$$

The superscripts indicate the order of the diagrams in  $p$  that each contribution comes from and the extra 0 that it is defined in terms of lowest-order quantities.

The lowest order masses are

$$m_{\pi 0}^2 = 2B_0\hat{m}, \quad m_{K 0}^2 = B_0(\hat{m} + m_s), \quad m_{\eta 0}^2 = \frac{2}{3}(\hat{m} + 2m_2). \quad (52)$$

The higher order contributions are split in the parts depending on the NLO LECs  $L_i^r$ , on the NNLO LECs  $C_i^r$  and the remainder as

$$m_a^{2(4)0} = m_{aL}^{2(4)0} + m_{aR}^{2(4)0}, \quad m_a^{2(6)0} = m_{aL}^{2(6)0} + m_{aC}^{2(6)0} + m_{aR}^{2(6)0}. \quad (53)$$

The expressions for were derived during the work for [19] and on [13]. Note that when combining these with results from other sources one should be sure to use a compatible

LO and NLO.

Pion mass:

```
double mpi4lo(lomass,Li) returns  $m_{\pi}^{2(4)0}$ 
double mpi4Llo(lomass,Li) returns  $m_{\pi L}^{2(4)0}$ 
double mpi4Rlo(lomass,Li) returns  $m_{\pi R}^{2(4)0}$ 
double mpi6lo(lomass,Li,Ci) returns  $m_{\pi}^{2(6)0}$ 
double mpi6Llo(lomass,Li) returns  $m_{\pi L}^{2(6)0}$ 
double mpi6Clo(lomass,Ci) returns  $m_{\pi C}^{2(6)0}$ 
double mpi6Rlo(lomass) returns  $m_{\pi R}^{2(6)0}$ 
```

Kaon mass:

```
double mk4lo(lomass,Li) returns  $m_K^{2(4)0}$ 
double mk4Llo(lomass,Li) returns  $m_{K L}^{2(4)0}$ 
double mk4Rlo(lomass,Li) returns  $m_{K R}^{2(4)0}$ 
double mk6lo(lomass,Li,Ci) returns  $m_K^{2(6)0}$ 
double mk6Llo(lomass,Li) returns  $m_{K L}^{2(6)0}$ 
double mk6Clo(lomass,Ci) returns  $m_{K C}^{2(6)0}$ 
double mk6Rlo(lomass) returns  $m_{K R}^{2(6)0}$ 
```

Eta mass:

```
double meta4lo(lomass,Li) returns  $m_{\eta}^{2(4)0}$ 
double meta4Llo(lomass,Li) returns  $m_{\eta L}^{2(4)0}$ 
double meta4Rlo(lomass,Li) returns  $m_{\eta R}^{2(4)0}$ 
double meta6lo(lomass,Li,Ci) returns  $m_{\eta}^{2(6)0}$ 
double meta6Llo(lomass,Li) returns  $m_{\eta L}^{2(6)0}$ 
double meta6Clo(lomass,Ci) returns  $m_{\eta C}^{2(6)0}$ 
double meta6Rlo(lomass) returns  $m_{\eta R}^{2(6)0}$ 
```

The functions are defined in `massesdecayvevlo.h`, implemented in `massesdecayvevlo.cc` and examples of use are in `testmassdecayvevlo.cc`.

### 8.2.2 Decay constants: in lowest order

The decay constants of the pion, kaon and eta at two-loops in three flavour ChPT were obtained in [19]. The pion and eta decay constants were done earlier with a different subtraction scheme and a different way to perform the sunset integrals in [28].

The expressions for the decay constants for  $a = \pi, K, \eta$  are given by

$$F_{a\text{phys}} = F_0 \left( 1 + F_a^{(4)0} + F_a^{(6)0} \right) . \quad (54)$$

The superscripts indicate the order of the diagrams in  $p$  that each contribution comes from.

The extra 0 indicates that the expansion is in terms of lowest-order quantities.  $F_0$  denotes the decay constant in the three-flavour chiral limit. The expressions were originally derived during the work for [19] and can be found in the website [13]. The normalization is such that  $F_\pi \approx 92$  MeV.

The contributions themselves are divided into the parts depending on the NLO LECs  $L_i^r$ , on the NNLO LECs  $C_i^r$  and the remainder as

$$F_a^{(4)0} = F_{aL}^{(4)0} + F_{aR}^{(4)0}, \quad F_a^{(6)0} = F_{aL}^{(6)0} + F_{aC}^{(6)0} + F_{aR}^{(6)0}. \quad (55)$$

For the  $\eta$  the decay constant has been defined with the octet axial-vector current.

Pion decay constant:

```
double fpi4lo(lomass,Li) returns  $F_\pi^{(4)0}$ 
double fpi4Llo(lomass,Li) returns  $F_{\pi L}^{(4)0}$ 
double fpi4Rlo(lomass,Li) returns  $F_{\pi R}^{(4)0}$ 
double fpi6lo(lomass,Li,Ci) returns  $F_\pi^{(6)0}$ 
double fpi6Llo(lomass,Li) returns  $F_{\pi L}^{(6)0}$ 
double fpi6Clo(lomass,Ci) returns  $F_{\pi C}^{(6)0}$ 
double fpi6Rlo(lomass) returns  $F_{\pi R}^{(6)0}$ 
```

Kaon decay constant:

```
double fk4lo(lomass,Li) returns  $F_K^{(4)0}$ 
double fk4Llo(lomass,Li) returns  $F_{KL}^{(4)0}$ 
double fk4Rlo(lomass,Li) returns  $F_{KR}^{(4)0}$ 
double fk6lo(lomass,Li,Ci) returns  $F_K^{(6)0}$ 
double fk6Llo(lomass,Li) returns  $F_{KL}^{(6)0}$ 
double fk6Clo(lomass,Ci) returns  $F_{KC}^{(6)0}$ 
double fk6Rlo(lomass) returns  $F_{KR}^{(6)0}$ 
```

Eta decay constant:

```
double feta4lo(lomass,Li) returns  $F_\eta^{(4)0}$ 
double feta4Llo(lomass,Li) returns  $F_{\eta L}^{(4)0}$ 
double feta4Rlo(lomass,Li) returns  $F_{\eta R}^{(4)0}$ 
double feta6lo(lomass,Li,Ci) returns  $F_\eta^{(6)0}$ 
double feta6Llo(lomass,Li) returns  $F_{\eta L}^{(6)0}$ 
double feta6Clo(lomass,Ci) returns  $F_{\eta C}^{(6)0}$ 
double feta6Rlo(lomass) returns  $F_{\eta R}^{(6)0}$ 
```

The functions are defined in `massesdecayvevlo.h`, implemented in `massesdecayvevlo.cc` and examples of use are in `testmassdecayvevlo.cc`.

### 8.2.3 Vacuum-expectation-values: in lowest order

The corrections to the vacuum expectation values (vevs)  $\langle 0|\bar{q}q|0\rangle$  for up, down and strange quarks in the isospin limit were calculated at two-loops in three flavour ChPT in [29]. The expression for the up and down quark vev are identical since we are in the isospin limit. We write the expressions in a form analogous to the decay constant treatment:

$$\langle 0|\bar{q}q|0\rangle_{a\text{phys}} = -F_0^2 B_0 \left( 1 + \langle 0|\bar{q}q|0\rangle_a^{(4)0} + \langle 0|\bar{q}q|0\rangle_a^{(6)0} \right). \quad (56)$$

The superscripts indicate the order of the diagrams in  $p$  that each contribution comes from. The extra 0 indicates that the expansion is defined in terms of lowest-order quantities. The lowest order values are  $-F_0^2 B_0$ .

Note that the vevs are not directly measurable quantities. They depend on exactly the way the scalar densities are defined in QCD. ChPT can be used for them when a massindependent, chiral symmetry respecting subtraction scheme is used.  $\overline{MS}$  in QCD satisfies this, but there are other possibilities. Even within a scheme,  $B_0$  and the quark masses depend on the QCD subtraction scale  $\mu_{\text{QCD}}$  in such a way that  $B_0 m_q$  is independent of it. The higher order corrections in this case also depend on the LECs for fully local counterterms,  $H_1^r, H_2^r$  at order  $p^4$  and  $C_{91}^r, \dots, C_{94}^r$  at  $p^6$ . When the scalar density is fully defined, measuring these quantities in e.g. lattice QCD and comparing with the ChPT expressions is a well defined procedure.

The contributions at the different orders themselves are split in the parts depending on the NLO LECs  $L_i^r$ , on the NNLO LECs  $C_i^r$  and the remainder as

$$\begin{aligned} \langle 0|\bar{q}q|0\rangle_a^{(4)0} &= \langle 0|\bar{q}q|0\rangle_{aL}^{(4)0} + \langle 0|\bar{q}q|0\rangle_{aR}^{(4)0}, \\ \langle 0|\bar{q}q|0\rangle_a^{(6)0} &= \langle 0|\bar{q}q|0\rangle_{aL}^{(6)0} + \langle 0|\bar{q}q|0\rangle_{aC}^{(6)0} + \langle 0|\bar{q}q|0\rangle_{aR}^{(6)0}. \end{aligned} \quad (57)$$

These are defined for  $q = u, s$ .

$\langle 0|\bar{q}q|0\rangle_{u\text{phys}}$ :

```
double qqup4lo(lomass,Li) returns  $\langle 0|\bar{q}q|0\rangle_u^{(4)0}$ 
double qqup4Llo(lomass,Li) returns  $\langle 0|\bar{q}q|0\rangle_{uL}^{(4)0}$ 
double qqup4Rlo(lomass) returns  $\langle 0|\bar{q}q|0\rangle_{uR}^{(4)0}$ 
double qqup6lo(lomass,Li,Ci) returns  $\langle 0|\bar{q}q|0\rangle_u^{(6)0}$ 
double qqup6Llo(lomass,Li) returns  $\langle 0|\bar{q}q|0\rangle_{uL}^{(6)0}$ 
double qqup6Clo(lomass,Li) returns  $\langle 0|\bar{q}q|0\rangle_{uC}^{(6)0}$ 
double qqup6Rlo(lomass) returns  $\langle 0|\bar{q}q|0\rangle_{uR}^{(6)0}$ 
```

$\langle 0|\bar{q}q|0\rangle_{s\text{phys}}$ :

```
double qqstrange4lo(lomass,Li) returns  $\langle 0|\bar{q}q|0\rangle_s^{(4)0}$ 
double qqstrange4Llo(lomass,Li) returns  $\langle 0|\bar{q}q|0\rangle_{sL}^{(4)0}$ 
double qqstrange4Rlo(lomass) returns  $\langle 0|\bar{q}q|0\rangle_{sR}^{(4)0}$ 
double qqstrange6lo(lomass,Li,Ci) returns  $\langle 0|\bar{q}q|0\rangle_s^{(6)0}$ 
```

```
double qqstrange6Llo(lomass,Li) returns  $\langle 0|\bar{q}q|0\rangle_{sL}^{(6)0}$ 
double qqstrange6Clo(lomass,Li) returns  $\langle 0|\bar{q}q|0\rangle_{sC}^{(6)0}$ 
double qqstrange6Rlo(lomass) returns  $\langle 0|\bar{q}q|0\rangle_{sR}^{(6)0}$ 
```

The functions are defined in `massesdecayvevlo.h`, implemented in `massesdecayvevlo.cc` and examples of use are in `testmassesdecayvevlo.cc`

### 8.3 Masses and decay constants at finite volume: in physical

The expressions treated in this section have been derived in [26]. A general remark is that care should be taken to set the precision in the loop integrals sufficiently high. For the one-loop integrals setting it very high is usually no problem. For the sunset integrals the evaluation can become very slow. It is strongly recommended to play around with the settings and compare the outputs for the two ways to evaluate the integral. The theta and Bessel function evaluation approach the correct answer differently. For most cases it is possible to have `rsacc` set smaller than `racc`.

For many applications it is useful to calculate the very time consuming parts, those labeled `6RV`, once and store them. They only depend nontrivially on the masses and size of the finite volume. The decay constant dependence is very simple, an overall factor at each order, and there is no dependence on the NLO LECs  $L_i^r$ .

The results presented in this section are with periodic boundary conditions and an infinite extension in the time direction. They are also restricted to the case where the particle is at rest, i.e.  $\vec{p} = 0$ .

#### 8.3.1 Masses at finite volume: in physical

The finite volume corrections to the masses squared<sup>3</sup> are defined as the difference of the mass squared in finite volume and in infinite volume:

$$\begin{aligned}\Delta^V m_a^2 &= m_a^{2V} - m_a^{2V=\infty} = m_a^{2V(4)} + m_a^{2V(6)} . \\ m_a^{2V(6)} &= m_{aL}^{2V(6)} + m_{aR}^{2V(6)} .\end{aligned}\tag{58}$$

These definitions are for  $a = \pi, K, \eta$ .

Pion mass (theta function method):

```
double mpi4Vt(const physmass massin,const double L) returns  $m_\pi^{2V(4)}$ .
double mpi6Vt(const physmass massin,const Li Liin,const double L) returns  $m_\pi^{2V(6)}$ .
double mpi6VLt(const physmass massin,const Li Liin,const double L) returns  $m_{\pi L}^{2V(6)}$ .
double mpi6VRt(const physmass massin,const double L) returns  $m_{\pi R}^{2V(6)}$ .
```

---

<sup>3</sup>Note that in other papers the corrections to the mass itself are sometimes quoted.

Pion mass (Bessel function method):

```
double mpi4Vb(const physmass massin, const double L) returns  $m_\pi^{2V(4)}$  .
double mpi6Vb(const physmass massin, const Li Liin, const double L) returns  $m_\pi^{2V(6)}$  .
double mpi6VLb(const physmass massin, const Li Liin, const double L) returns  $m_{\pi L}^{2V(6)}$  .
double mpi6VRb(const physmass massin, const double L) returns  $m_{\pi R}^{2V(6)}$  .
```

Kaon mass (theta function method):

```
double mk4Vt(const physmass massin, const double L) returns  $m_K^{2V(4)}$  .
double mk6Vt(const physmass massin, const Li Liin, const double L) returns  $m_K^{2V(6)}$  .
double mk6VLt(const physmass massin, const Li Liin, const double L) returns  $m_{KL}^{2V(6)}$  .
double mk6VRt(const physmass massin, const double L) returns  $m_{KR}^{2V(6)}$  .
```

Kaon mass (Bessel function method):

```
double mk4Vb(const physmass massin, const double L) returns  $m_K^{2V(4)}$  .
double mk6Vb(const physmass massin, const Li Liin, const double L) returns  $m_K^{2V(6)}$  .
double mk6VLb(const physmass massin, const Li Liin, const double L) returns  $m_{KL}^{2V(6)}$  .
double mk6VRb(const physmass massin, const double L) returns  $m_{KR}^{2V(6)}$  .
```

Eta mass (theta function method):

```
double meta4Vt(const physmass massin, const double L) returns  $m_\eta^{2V(4)}$  .
double meta6Vt(const physmass massin, const Li Liin, const double L) returns  $m_\eta^{2V(6)}$  .
double meta6VLt(const physmass massin, const Li Liin, const double L) returns  $m_{\eta L}^{2V(6)}$  .
double meta6VRt(const physmass massin, const double L) returns  $m_{\eta R}^{2V(6)}$  .
```

Eta mass (Bessel function method):

```
double meta4Vb(const physmass massin, const double L) returns  $m_\eta^{2V(4)}$  .
double meta6Vb(const physmass massin, const Li Liin, const double L) returns  $m_\eta^{2V(6)}$  .
double meta6VLb(const physmass massin, const Li Liin, const double L) returns  $m_{\eta L}^{2V(6)}$  .
double meta6VRb(const physmass massin, const double L) returns  $m_{\eta R}^{2V(6)}$  .
```

All these are defined in `massdecayvevV.h` and implemented in `massdecayvevV.h`. Examples of use are in `testmassdecayvevV.cc`.

### 8.3.2 Decay constants at finite volume: in physical

The finite volume corrections to the decay constants are defined as the difference of the decay constant in finite volume and in infinite volume:

$$\begin{aligned}\Delta^V F_a &= F_a^V - F_a^{V=\infty} = F_a^{V(4)} + F_a^{V(6)} . \\ F_a^{V(6)} &= F_{aL}^{V(6)} + F_{aR}^{V(6)} .\end{aligned}\tag{59}$$

These definitions are for  $a = \pi, K, \eta$ . Note that the correction is defined to the value of the decay constant, not divided by the the lowest order decay constant as in (47). The eta decay constant is defined with the octet axial current.

Pion decay constant (theta function method):

```
double fpi4Vt(const physmass massin,const double L) returns  $F_\pi^{V(4)}$ .
double fpi6Vt(const physmass massin,const Li Liin,const double L) returns  $F_\pi^{V(6)}$ .
double fpi6VLt(const physmass massin,const Li Liin,const double L) returns  $F_{\pi L}^{V(6)}$ .
double fpi6VRt(const physmass massin,const double L) returns  $F_{\pi R}^{V(6)}$ .
```

Pion decay constant (Bessel function method):

```
double fpi4Vb(const physmass massin,const double L) returns  $F_\pi^{V(4)}$ .
double fpi6Vb(const physmass massin,const Li Liin,const double L) returns  $F_\pi^{V(6)}$ .
double fpi6VLb(const physmass massin,const Li Liin,const double L) returns  $F_{\pi L}^{V(6)}$ .
double fpi6VRb(const physmass massin,const double L) returns  $F_{\pi R}^{V(6)}$ .
```

Kaon decay constant (theta function method):

```
double fk4Vt(const physmass massin,const double L) returns  $F_K^{V(4)}$ .
double fk6Vt(const physmass massin,const Li Liin,const double L) returns  $F_K^{V(6)}$ .
double fk6VLt(const physmass massin,const Li Liin,const double L) returns  $F_{K L}^{V(6)}$ .
double fk6VRt(const physmass massin,const double L) returns  $F_{K R}^{V(6)}$ .
```

Kaon decay constant (Bessel function method):

```
double fk4Vb(const physmass massin,const double L) returns  $F_K^{V(4)}$ .
double fk6Vb(const physmass massin,const Li Liin,const double L) returns  $F_K^{V(6)}$ .
double fk6VLb(const physmass massin,const Li Liin,const double L) returns  $F_{K L}^{V(6)}$ .
double fk6VRb(const physmass massin,const double L) returns  $F_{K R}^{V(6)}$ .
```

Eta decay constant (theta function method):

```
double feta4Vt(const physmass massin,const double L) returns  $F_\eta^{V(4)}$ .
double feta6Vt(const physmass massin,const Li Liin,const double L) returns  $F_\eta^{V(6)}$ .
double feta6VLt(const physmass massin,const Li Liin,const double L) returns  $F_{\eta L}^{V(6)}$ .
double feta6VRt(const physmass massin,const double L) returns  $F_{\eta R}^{V(6)}$ .
```

Eta decay constant (Bessel function method):

```
double feta4Vb(const physmass massin,const double L) returns  $F_\eta^{V(4)}$ .
double feta6Vb(const physmass massin,const Li Liin,const double L) returns  $F_\eta^{V(6)}$ .
double feta6VLb(const physmass massin,const Li Liin,const double L) returns  $F_{\eta L}^{V(6)}$ .
double feta6VRb(const physmass massin,const double L) returns  $F_{\eta R}^{V(6)}$ .
```

All these are defined in `massdecayvevV.h` and implemented in `massdecayvevV.h`. Examples of use are in `testmassdecayvevV.cc`.

## 8.4 Masses and decay constants at finite volume: in lowest order

The expressions treated in this section have been derived in [26]. A general remark is that care should be taken to set the precision in the loop integrals sufficiently high. For the one-loop integrals setting it very high is usually no problem. For the sunset integrals the evaluation can become very slow. It is strongly recommended to play around with the settings and compare the outputs for the two ways to evaluate the integral. The theta and Bessel function evaluation approach the correct answer differently. For most cases it is possible to have `rsacc` set smaller than `racc`.

For many applications it is useful to calculate the very time consuming parts, those labeled `6RV`, once and store them. They only depend nontrivially on the masses and size of the finite volume. The decay constant dependence is very simple, an overall factor at each order, and there is no dependence on the NLO LECs  $L_i^r$ .

The results presented in this section are with periodic boundary conditions and an infinite extension in the time direction. They are also restricted to the case where the particle is at rest, i.e.  $\vec{p} = 0$ .

### 8.4.1 Masses at finite volume: in lowest order

The finite volume corrections to the masses squared<sup>4</sup> are defined as the difference of the mass squared in finite volume and in infinite volume:

$$\begin{aligned}\Delta^V m_a^2 &= m_a^{2V} - m_a^{2V=\infty} = m_a^{2V(4)0} + m_a^{2V(6)0} . \\ m_a^{2V(6)0} &= m_{aL}^{2V(6)0} + m_{aR}^{2V(6)0} .\end{aligned}\tag{60}$$

These definitions are for  $a = \pi, K, \eta$ .

Pion mass (theta function method):

```
double mpi4loVt(const lomass massin, const double L) returns  $m_\pi^{2V(4)0}$ .
double mpi6loVt(const lomass massin, const Li Liin, const double L) returns  $m_\pi^{2V(6)0}$ .
double mpi6LloVt(const lomass massin, const Li Liin, const double L) returns  $m_{\pi L}^{2V(6)0}$ .
double mpi6RloVt(const lomass massin, const double L) returns  $m_{\pi R}^{2V(6)0}$ .
```

Pion mass (Bessel function method):

```
double mpi4loVb(const lomass massin, const double L) returns  $m_\pi^{2V(4)0}$ .
double mpi6loVb(const lomass massin, const Li Liin, const double L) returns  $m_\pi^{2V(6)0}$ .
double mpi6LloVb(const lomass massin, const Li Liin, const double L) returns  $m_{\pi L}^{2V(6)0}$ .
```

---

<sup>4</sup>Note that in other papers the corrections to the mass itself are sometimes quoted.

double mpi6RloVb(const lomass massin, const double L) returns  $m_{\pi R}^{2V(6)0}$ .

Kaon mass (theta function method):

double mk4loVt(const lomass massin, const double L) returns  $m_K^{2V(4)0}$ .  
double mk6loVt(const lomass massin, const Li Liin, const double L) returns  $m_K^{2V(6)0}$ .  
double mk6LloVt(const lomass massin, const Li Liin, const double L) returns  $m_{KL}^{2V(6)0}$ .  
double mk6RloVt(const lomass massin, const double L) returns  $m_{KR}^{2V(6)0}$ .

Kaon mass (Bessel function method):

double mk4loVb(const lomass massin, const double L) returns  $m_K^{2V(4)0}$ .  
double mk6loVb(const lomass massin, const Li Liin, const double L) returns  $m_K^{2V(6)0}$ .  
double mk6LloVb(const lomass massin, const Li Liin, const double L) returns  $m_{KL}^{2V(6)0}$ .  
double mk6RloVb(const lomass massin, const double L) returns  $m_{KR}^{2V(6)0}$ .

Eta mass (theta function method):

double meta4loVt(const lomass massin, const double L) returns  $m_\eta^{2V(4)0}$ .  
double meta6loVt(const lomass massin, const Li Liin, const double L) returns  $m_\eta^{2V(6)0}$ .  
double meta6LloVt(const lomass massin, const Li Liin, const double L) returns  $m_{\eta L}^{2V(6)0}$ .  
double meta6RloVt(const lomass massin, const double L) returns  $m_{\eta R}^{2V(6)0}$ .

Eta mass (Bessel function method):

double meta4loVb(const lomass massin, const double L) returns  $m_\eta^{2V(4)0}$ .  
double meta6loVb(const lomass massin, const Li Liin, const double L) returns  $m_\eta^{2V(6)0}$ .  
double meta6LloVb(const lomass massin, const Li Liin, const double L) returns  $m_{\eta L}^{2V(6)0}$ .  
double meta6RloVb(const lomass massin, const double L) returns  $m_{\eta R}^{2V(6)0}$ .

All these are defined in `massdecayvevloV.h` and implemented in `massdecayvevloV.h`.  
Examples of use are in `testmassdecayvevloV.cc`.

#### 8.4.2 Decay constants at finite volume: in lowest order

The finite volume corrections to the decay constants are defined as the difference of the decay constant in finite volume and in infinite volume:

$$\begin{aligned}\Delta^V F_a &= F_a^V - F_a^{V=\infty} = F_0 (F_a^{V(4)0} + F_a^{V(6)0}) . \\ F_a^{V(6)0} &= F_{aL}^{V(6)0} + F_{aR}^{V(6)0} .\end{aligned}\tag{61}$$

Note that this is a different normalization compared to the expressions in terms of physical masses and the physical  $F_\pi$ . This was done to have the same normalization as the partially quenched results. These definitions are for  $a = \pi, K, \eta$ . The correction is defined to the value of the decay constant divided by the the lowest order decay constant as in (47). The

eta decay constant is defined with the octet axial current.

Pion decay constant (theta function method):

```
double fpi4loVt(const lomass massin,const double L) returns  $F_{\pi}^{V(4)0}$ .
double fpi6loVt(const lomass massin,const Li Liin,const double L) returns  $F_{\pi}^{V(6)0}$ .
double fpi6LloVt(const lomass massin,const Li Liin,const double L) returns  $F_{\pi L}^{V(6)0}$ .
double fpi6RloVt(const lomass massin,const double L) returns  $F_{\pi R}^{V(6)0}$ .
```

Pion decay constant (Bessel function method):

```
double fpi4loVb(const lomass massin,const double L) returns  $F_{\pi}^{V(4)0}$ .
double fpi6loVb(const lomass massin,const Li Liin,const double L) returns  $F_{\pi}^{V(6)0}$ .
double fpi6LloVb(const lomass massin,const Li Liin,const double L) returns  $F_{\pi L}^{V(6)0}$ .
double fpi6RloVb(const lomass massin,const double L) returns  $F_{\pi R}^{V(6)0}$ .
```

Kaon decay constant (theta function method):

```
double fk4loVt(const lomass massin,const double L) returns  $F_K^{V(4)0}$ .
double fk6loVt(const lomass massin,const Li Liin,const double L) returns  $F_K^{V(6)0}$ .
double fk6LloVt(const lomass massin,const Li Liin,const double L) returns  $F_{KL}^{V(6)0}$ .
double fk6RloVt(const lomass massin,const double L) returns  $F_{KR}^{V(6)0}$ .
```

Kaon decay constant (Bessel function method):

```
double fk4loVb(const lomass massin,const double L) returns  $F_K^{V(4)0}$ .
double fk6loVb(const lomass massin,const Li Liin,const double L) returns  $F_K^{V(6)0}$ .
double fk6LloVb(const lomass massin,const Li Liin,const double L) returns  $F_{KL}^{V(6)0}$ .
double fk6RloVb(const lomass massin,const double L) returns  $F_{KR}^{V(6)0}$ .
```

Eta decay constant (theta function method):

```
double feta4loVt(const lomass massin,const double L) returns  $F_{\eta}^{V(4)0}$ .
double feta6loVt(const lomass massin,const Li Liin,const double L) returns  $F_{\eta}^{V(6)0}$ .
double feta6LloVt(const lomass massin,const Li Liin,const double L) returns  $F_{\eta L}^{V(6)0}$ .
double feta6RloVt(const lomass massin,const double L) returns  $F_{\eta R}^{V(6)0}$ .
```

Eta decay constant (Bessel function method):

```
double feta4loVb(const lomass massin,const double L) returns  $F_{\eta}^{V(4)0}$ .
double feta6loVb(const lomass massin,const Li Liin,const double L) returns  $F_{\eta}^{V(6)0}$ .
double feta6LloVb(const lomass massin,const Li Liin,const double L) returns  $F_{\eta L}^{V(6)0}$ .
double feta6RloVb(const lomass massin,const double L) returns  $F_{\eta R}^{V(6)0}$ .
```

All these are defined in massdecayvevloV.h and implemented in massdecayvevloV.h.  
Examples of use are in testmassdecayvevloV.cc.

## 9 Three flavour partially quenched results

This section contains the routines used for the partially quenched results with three sea quark flavours of [22, 24, 25]. The formulas used are analytically equivalent to those in the published papers, but are longer and avoid some of the 0/0 problems that can appear.

Do not forget to set the precision for the needed sunset integrals with

`setprecisionquenchedsunsetintegral`.

The interface is always defined with the  $n_F$  flavour NLO and NNLO LECs `Lin` and `Ki` with  $n_F = 3$ . The routines also expect a `quarkmassnf` with precisely the number of quark masses needed for each case.

The reason why the quarkmasses are alternatively lowest-order meson masses are used is that in these cases there are very many physical masses compared to the number of quark masses. There would thus have been a very large ambiguity in expressing the results in physical masses.

The inputs used are  $Bm_1 = m_{11}^2/2$ ,  $Bm_2 = m_{11}^2/2$ ,  $Bm_3 = m_{33}^2/2$ ,  $Bm_4 = m_{44}^2/2$ ,  $Bm_5 = m_{55}^2/2$ ,  $Bm_6 = m_{66}^2/2$ .

We give the cases for equal or different valence quark mass, cases `v1` or `v2`, and one, two or three different sea quark masses, cases `s1`, `s2`, `s3` for always three sea flavours, case `nf3`. For the one sea mass case we have  $Bm_4 = Bm_5 = Bm_6$  and for the two sea mass case  $Bm_4 = Bm_5$ .

The quark masses The masses are labelled starting with `m` and the decay constants starting with `f`. `f0` is  $F_0$  the three flavour chiral limit decay constant and `mu` is the subtraction scale  $\mu$ .

For the finite volume cases the names have an additional `V` and a `b` or `t` depending on whether the Bessel function or the theta function method is used for the finite volume integrals. `L` is the spatial extent of the finite directions.

### 9.1 Masses

The expansion are defined similar to (51) via

$$m_{a\text{phys}}^2 = m_{a0}^2 + m_a^{2(4)0} + m_a^{2(6)0}. \quad (62)$$

The masses are for the off-diagonal or charged meson with two different valence quarks but the masses can be equal or different.

$$m_a^{2(4)0} = m_{aL}^{2(4)0} + m_{aR}^{2(4)0}, \quad m_a^{2(6)0} = m_{aL}^{2(6)0} + m_{aK}^{2(6)0} + m_{aR}^{2(6)0}. \quad (63)$$

One valence mass, one sea mass::

`mass=quarkmassnf({Bm1,Bm4},f0,mu,2)`

`double mv1s1nf3p4(quarkmassnf mass, Linf Liin)` returns  $m_a^{2(4)0}$

`double mv1s1nf3p4L(quarkmassnf mass, Linf Liin)` returns  $m_{aL}^{2(4)0}$

```

double mv1s1nf3p4R(quarkmassnf mass) returns  $m_{aR}^{2(4)0}$ 
double mv1s1nf3p6(quarkmassnf mass, Linf Liin, Ki Kiin) returns  $m_a^{2(6)0}$ 
double mv1s1nf3p6L(quarkmassnf mass, Linf Liin) returns  $m_{aL}^{2(6)0}$ 
double mv1s1nf3p6K(quarkmassnf mass, Ki Kiin) returns  $m_{aK}^{2(6)0}$ 
double mv1s1nf3p6R(quarkmassnf mass) returns  $m_{aR}^{2(6)0}$ 

```

Two valence mass, one sea mass::

```

mass=quarkmassnf({Bm1,Bm3,Bm4},f0,mu,3)
double mv2s1nf3p4(quarkmassnf mass, Linf Liin) returns  $m_a^{2(4)0}$ 
double mv2s1nf3p4L(quarkmassnf mass, Linf Liin) returns  $m_{aL}^{2(4)0}$ 
double mv2s1nf3p4R(quarkmassnf mass) returns  $m_{aR}^{2(4)0}$ 
double mv2s1nf3p6(quarkmassnf mass, Linf Liin, Ki Kiin) returns  $m_a^{2(6)0}$ 
double mv2s1nf3p6L(quarkmassnf mass, Linf Liin) returns  $m_{aL}^{2(6)0}$ 
double mv2s1nf3p6K(quarkmassnf mass, Ki Kiin) returns  $m_{aK}^{2(6)0}$ 
double mv2s1nf3p6R(quarkmassnf mass) returns  $m_{aR}^{2(6)0}$ 

```

One valence mass, two sea mass::

```

mass=quarkmassnf({Bm1,Bm4,Bm6},f0,mu,3)
double mv1s1nf3p4(quarkmassnf mass, Linf Liin) returns  $m_a^{2(4)0}$ 
double mv1s1nf3p4L(quarkmassnf mass, Linf Liin) returns  $m_{aL}^{2(4)0}$ 
double mv1s1nf3p4R(quarkmassnf mass) returns  $m_{aR}^{2(4)0}$ 
double mv1s1nf3p6(quarkmassnf mass, Linf Liin, Ki Kiin) returns  $m_a^{2(6)0}$ 
double mv1s1nf3p6L(quarkmassnf mass, Linf Liin) returns  $m_{aL}^{2(6)0}$ 
double mv1s1nf3p6K(quarkmassnf mass, Ki Kiin) returns  $m_{aK}^{2(6)0}$ 
double mv1s1nf3p6R(quarkmassnf mass) returns  $m_{aR}^{2(6)0}$ 

```

Two valence mass, two sea mass::

```

mass=quarkmassnf({Bm1,Bm3,Bm4,Bm6},f0,mu,4)
double mv2s2nf3p4(quarkmassnf mass, Linf Liin) returns  $m_a^{2(4)0}$ 
double mv2s2nf3p4L(quarkmassnf mass, Linf Liin) returns  $m_{aL}^{2(4)0}$ 
double mv2s2nf3p4R(quarkmassnf mass) returns  $m_{aR}^{2(4)0}$ 
double mv2s2nf3p6(quarkmassnf mass, Linf Liin, Ki Kiin) returns  $m_a^{2(6)0}$ 
double mv2s2nf3p6L(quarkmassnf mass, Linf Liin) returns  $m_{aL}^{2(6)0}$ 
double mv2s2nf3p6K(quarkmassnf mass, Ki Kiin) returns  $m_{aK}^{2(6)0}$ 
double mv2s2nf3p6R(quarkmassnf mass) returns  $m_{aR}^{2(6)0}$ 

```

One valence mass, three sea mass::

```

mass=quarkmassnf({Bm1,Bm4,Bm5,Bm6},f0,mu,4)
double mv1s3nf3p4(quarkmassnf mass, Linf Liin) returns  $m_a^{2(4)0}$ 

```

```

double mv1s3nf3p4L(quarkmassnf mass, Linf Liin) returns  $m_{aL}^{2(4)0}$ 
double mv1s3nf3p4R(quarkmassnf mass) returns  $m_{aR}^{2(4)0}$ 
double mv1s3nf3p6(quarkmassnf mass, Linf Liin, Ki Kiin) returns  $m_a^{2(6)0}$ 
double mv1s3nf3p6L(quarkmassnf mass, Linf Liin) returns  $m_{aL}^{2(6)0}$ 
double mv1s3nf3p6K(quarkmassnf mass, Ki Kiin) returns  $m_{aK}^{2(6)0}$ 
double mv1s3nf3p6R(quarkmassnf mass) returns  $m_{aR}^{2(6)0}$ 

```

Two valence mass, three sea mass::

```

mass=quarkmassnf({Bm1,Bm3,Bm4,Bm5,Bm6},f0,mu,5)
double mv2s3nf3p4(quarkmassnf mass, Linf Liin) returns  $m_a^{2(4)0}$ 
double mv2s3nf3p4L(quarkmassnf mass, Linf Liin) returns  $m_{aL}^{2(4)0}$ 
double mv2s3nf3p4R(quarkmassnf mass) returns  $m_{aR}^{2(4)0}$ 
double mv2s3nf3p6(quarkmassnf mass, Linf Liin, Ki Kiin) returns  $m_a^{2(6)0}$ 
double mv2s3nf3p6L(quarkmassnf mass, Linf Liin) returns  $m_{aL}^{2(6)0}$ 
double mv2s3nf3p6K(quarkmassnf mass, Ki Kiin) returns  $m_{aK}^{2(6)0}$ 
double mv2s3nf3p6R(quarkmassnf mass) returns  $m_{aR}^{2(6)0}$ 

```

Defined in `massdecayvevPQ.h`, implemented in `massdecayvevPQ.cc` and examples of use in `testmassdecayvevPQ.cc`.

## 9.2 Decay constants

The expansion are defined similar to (55) via

$$F_{a\text{phys}} = F_0 \left( 1 + F_a^{(4)0} + F_a^{(6)0} \right). \quad (64)$$

The decay constants are for the off-diagonal or charged meson with two different valence quarks but the masses can be equal or different. The normalization corresponds to the pion decay constant  $F_\pi \approx 92$  MeV.

$$F_a^{(4)0} = F_{aL}^{(4)0} + F_{aR}^{(4)0}, \quad F_a^{(6)0} = F_{aL}^{(6)0} + F_{aK}^{(6)0} + F_{aR}^{(6)0}. \quad (65)$$

One valence mass, one sea mass::

```

mass=quarkmassnf({Bm1,Bm4},f0,mu,2)
double fv1s1nf3p4(quarkmassnf mass, Linf Liin) returns  $F_a^{(4)0}$ 
double fv1s1nf3p4L(quarkmassnf mass, Linf Liin) returns  $F_{aL}^{(4)0}$ 
double fv1s1nf3p4R(quarkmassnf mass) returns  $F_{aR}^{(4)0}$ 
double fv1s1nf3p6(quarkmassnf mass, Linf Liin, Ki Kiin) returns  $F_a^{(6)0}$ 
double fv1s1nf3p6L(quarkmassnf mass, Linf Liin) returns  $F_{aL}^{(6)0}$ 
double fv1s1nf3p6K(quarkmassnf mass, Ki Kiin) returns  $F_{aK}^{(6)0}$ 
double fv1s1nf3p6R(quarkmassnf mass) returns  $F_{aR}^{(6)0}$ 

```

Two valence mass, one sea mass::

```

mass=quarkmassnf({Bm1,Bm3,Bm4},f0,mu,3)
double fv2s1nf3p4(quarkmassnf mass, Linf Liin) returns  $F_a^{(4)0}$ 
double fv2s1nf3p4L(quarkmassnf mass, Linf Liin) returns  $F_{aL}^{(4)0}$ 
double fv2s1nf3p4R(quarkmassnf mass) returns  $F_{aR}^{(4)0}$ 
double fv2s1nf3p6(quarkmassnf mass, Linf Liin, Ki Kiin) returns  $F_a^{(6)0}$ 
double fv2s1nf3p6L(quarkmassnf mass, Linf Liin) returns  $F_{aL}^{(6)0}$ 
double fv2s1nf3p6K(quarkmassnf mass, Ki Kiin) returns  $F_{aK}^{(6)0}$ 
double fv2s1nf3p6R(quarkmassnf mass) returns  $F_{aR}^{(6)0}$ 

```

One valence mass, two sea mass::

```

mass=quarkmassnf({Bm1,Bm4,Bm6},f0,mu,3)
double fv1s1nf3p4(quarkmassnf mass, Linf Liin) returns  $F_a^{(4)0}$ 
double fv1s1nf3p4L(quarkmassnf mass, Linf Liin) returns  $F_{aL}^{(4)0}$ 
double fv1s1nf3p4R(quarkmassnf mass) returns  $F_{aR}^{(4)0}$ 
double fv1s1nf3p6(quarkmassnf mass, Linf Liin, Ki Kiin) returns  $F_a^{(6)0}$ 
double fv1s1nf3p6L(quarkmassnf mass, Linf Liin) returns  $F_{aL}^{(6)0}$ 
double fv1s1nf3p6K(quarkmassnf mass, Ki Kiin) returns  $F_{aK}^{(6)0}$ 
double fv1s1nf3p6R(quarkmassnf mass) returns  $F_{aR}^{(6)0}$ 

```

Two valence mass, two sea mass::

```

mass=quarkmassnf({Bm1,Bm3,Bm4,Bm6},f0,mu,4)
double fv2s2nf3p4(quarkmassnf mass, Linf Liin) returns  $F_a^{(4)0}$ 
double fv2s2nf3p4L(quarkmassnf mass, Linf Liin) returns  $F_{aL}^{(4)0}$ 
double fv2s2nf3p4R(quarkmassnf mass) returns  $F_{aR}^{(4)0}$ 
double fv2s2nf3p6(quarkmassnf mass, Linf Liin, Ki Kiin) returns  $F_a^{(6)0}$ 
double fv2s2nf3p6L(quarkmassnf mass, Linf Liin) returns  $F_{aL}^{(6)0}$ 
double fv2s2nf3p6K(quarkmassnf mass, Ki Kiin) returns  $F_{aK}^{(6)0}$ 
double fv2s2nf3p6R(quarkmassnf mass) returns  $F_{aR}^{(6)0}$ 

```

One valence mass, three sea mass::

```

mass=quarkmassnf({Bm1,Bm4,Bm5,Bm6},f0,mu,4)
double fv1s3nf3p4(quarkmassnf mass, Linf Liin) returns  $F_a^{(4)0}$ 
double fv1s3nf3p4L(quarkmassnf mass, Linf Liin) returns  $F_{aL}^{(4)0}$ 
double fv1s3nf3p4R(quarkmassnf mass) returns  $F_{aR}^{(4)0}$ 
double fv1s3nf3p6(quarkmassnf mass, Linf Liin, Ki Kiin) returns  $F_a^{(6)0}$ 
double fv1s3nf3p6L(quarkmassnf mass, Linf Liin) returns  $F_{aL}^{(6)0}$ 
double fv1s3nf3p6K(quarkmassnf mass, Ki Kiin) returns  $F_{aK}^{(6)0}$ 
double fv1s3nf3p6R(quarkmassnf mass) returns  $F_{aR}^{(6)0}$ 

```

Two valence mass, three sea mass::

```

mass=quarkmassnf({Bm1,Bm3,Bm4,Bm5,Bm6},f0,mu,5)
double fv2s3nf3p4(quarkmassnf mass, Lint Liin) returns  $F_a^{(4)0}$ 
double fv2s3nf3p4L(quarkmassnf mass, Lint Liin) returns  $F_{aL}^{(4)0}$ 
double fv2s3nf3p4R(quarkmassnf mass) returns  $F_{aR}^{(4)0}$ 
double fv2s3nf3p6(quarkmassnf mass, Lint Liin, Ki Kiin) returns  $F_a^{(6)0}$ 
double fv2s3nf3p6L(quarkmassnf mass, Lint Liin) returns  $F_{aL}^{(6)0}$ 
double fv2s3nf3p6K(quarkmassnf mass, Ki Kiin) returns  $F_{aK}^{(6)0}$ 
double fv2s3nf3p6R(quarkmassnf mass) returns  $F_{aR}^{(6)0}$ 

```

Defined in `massdecayvevPQ.h`, implemented in `massdecayvevPQ.cc` and examples of use in `testmassdecayvevPQ.cc`.

### 9.3 Masses at finite volume

The expressions treated in this section have been derived in [30]. It contains the routines for the finite volume corrections for the masses of the off-diagonal or charged mesons in partially quenched ChPT with three sea quark flavours.

A general remark is that care should be taken to set the precision in the loop integrals sufficiently high. For the one-loop integrals setting it very high is usually no problem. For the sunset integrals the evaluation can become very slow. It is strongly recommended to play around with the settings and compare the outputs for the two ways to evaluate the integral. The theta and Bessel function evaluation approach the correct answer differently. For most cases it is possible to have `rsacc` set smaller than `racc`.

For many applications it is useful to calculate the very time consuming parts, those labeled `6RV`, once and store them. They only depend nontrivially on the masses and size of the finite volume. The decay constant dependence is very simple, an overall factor at each order, and there is no dependence on the NLO LECs  $L_i^r$ .

The results presented in this section are with periodic boundary conditions and an infinite extension in the time direction. They are also restricted to the case where the particle is at rest, i.e.  $\vec{p} = 0$ .

The expansion are defined similar to (60) via

$$\begin{aligned}
\Delta^V m_a^2 &= m_a^{2V} - m_a^{2V=\infty} = m_a^{2V(4)0} + m_a^{2V(6)0} . \\
m_a^{2V(6)0} &= m_{aL}^{2V(6)0} + m_{aR}^{2V(6)0} .
\end{aligned} \tag{66}$$

The masses are for the off-diagonal or charged meson with two different valence quarks but the masses can be equal or different.

`x` should be `b` or `t` depending on whether you want to use the finite volume integrals using bessel functions or theta functions.

One valence mass, one sea mass::

```
mass=quarkmassnf({Bm1,Bm4},f0,mu,2)
double mv1s1nf3p4Vx(quarkmassnf mass, double L) returns  $m_a^{2V(4)0}$ 
double mv1s1nf3p6Vx(quarkmassnf mass, Linf Liin, double L) returns  $m_a^{2V(6)0}$ 
double mv1s1nf3p6LVx(quarkmassnf mass, Linf Liin, double L) returns  $m_{aL}^{2V(6)0}$ 
double mv1s1nf3p6RVx(quarkmassnf mass, double L) returns  $m_{aR}^{2V(6)0}$ 
```

Two valence mass, one sea mass::

```
mass=quarkmassnf({Bm1,Bm3,Bm4},f0,mu,3)
double mv2s1nf3p4Vx(quarkmassnf mass, double L) returns  $m_a^{2V(4)0}$ 
double mv2s1nf3p6Vx(quarkmassnf mass, Linf Liin, double L) returns  $m_a^{2V(6)0}$ 
double mv2s1nf3p6LVx(quarkmassnf mass, Linf Liin, double L) returns  $m_{aL}^{2V(6)0}$ 
double mv2s1nf3p6RVx(quarkmassnf mass, double L) returns  $m_{aR}^{2V(6)0}$ 
```

One valence mass, two sea mass::

```
mass=quarkmassnf({Bm1,Bm4,Bm6},f0,mu,3)
double mv1s1nf3p4Vx(quarkmassnf mass, double L) returns  $m_a^{2V(4)0}$ 
double mv1s1nf3p6Vx(quarkmassnf mass, Linf Liin, double L) returns  $m_a^{2V(6)0}$ 
double mv1s1nf3p6LVx(quarkmassnf mass, Linf Liin, double L) returns  $m_{aL}^{2V(6)0}$ 
double mv1s1nf3p6RVx(quarkmassnf mass, double L) returns  $m_{aR}^{2V(6)0}$ 
```

Two valence mass, two sea mass::

```
mass=quarkmassnf({Bm1,Bm3,Bm4,Bm6},f0,mu,4)
double mv2s2nf3p4Vx(quarkmassnf mass, double L) returns  $m_a^{2V(4)0}$ 
double mv2s2nf3p6Vx(quarkmassnf mass, Linf Liin, double L) returns  $m_a^{2V(6)0}$ 
double mv2s2nf3p6LVx(quarkmassnf mass, Linf Liin, double L) returns  $m_{aL}^{2V(6)0}$ 
double mv2s2nf3p6RVx(quarkmassnf mass, double L) returns  $m_{aR}^{2V(6)0}$ 
```

One valence mass, three sea mass::

```
mass=quarkmassnf({Bm1,Bm4,Bm5,Bm6},f0,mu,4)
double mv1s3nf3p4Vx(quarkmassnf mass, double L) returns  $m_a^{2V(4)0}$ 
double mv1s3nf3p6Vx(quarkmassnf mass, Linf Liin, double L) returns  $m_a^{2V(6)0}$ 
double mv1s3nf3p6LVx(quarkmassnf mass, Linf Liin, double L) returns  $m_{aL}^{2V(6)0}$ 
double mv1s3nf3p6RVx(quarkmassnf mass, double L) returns  $m_{aR}^{2V(6)0}$ 
```

Two valence mass, three sea mass::

```
mass=quarkmassnf({Bm1,Bm3,Bm4,Bm5,Bm6},f0,mu,5)
double mv2s3nf3p4Vx(quarkmassnf mass, double L) returns  $m_a^{2V(4)0}$ 
double mv2s3nf3p6Vx(quarkmassnf mass, Linf Liin, double L) returns  $m_a^{2V(6)0}$ 
double mv2s3nf3p6LVx(quarkmassnf mass, Linf Liin, double L) returns  $m_{aL}^{2V(6)0}$ 
```

`double mv2s3nf3p6RVx(quarkmassnf mass, double L)` returns  $m_{aR}^{2V(6)0}$

Defined in `massdecayvevPQV.h`, implemented in `massdecayvevPQV.cc` and examples of use in `testmassdecayvevPQV.cc`.

## 9.4 Decay constants at finite volume

The expressions treated in this section have been derived in [30]. It contains the routines for the finite volume corrections for the decay constants of the off-diagonal or charged mesons in partially quenched ChPT with three sea quark flavours.

A general remark is that care should be taken to set the precision in the loop integrals sufficiently high. For the one-loop integrals setting it very high is usually no problem. For the sunset integrals the evaluation can become very slow. It is strongly recommended to play around with the settings and compare the outputs for the two ways to evaluate the integral. The theta and Bessel function evaluation approach the correct answer differently. For most cases it is possible to have `rsacc` set smaller than `racc`.

For many applications it is useful to calculate the very time consuming parts, those labeled `6RV`, once and store them. They only depend nontrivially on the masses and size of the finite volume. The decay constant dependence is very simple, an overall factor at each order, and there is no dependence on the NLO LECs  $L_i^r$ .

The results presented in this section are with periodic boundary conditions and an infinite extension in the time direction. They are also restricted to the case where the particle is at rest, i.e.  $\vec{p} = 0$ .

The expansion are defined similar to (61) via

$$\begin{aligned}\Delta^V F_a &= F_a^V - F_a^{V=\infty} = F_0 (F_a^{V(4)0} + F_a^{V(6)0}) . \\ F_a^{V(6)0} &= F_{aL}^{V(6)0} + F_{aR}^{V(6)0} .\end{aligned}\tag{67}$$

The decay constants are for the off-diagonal or charged meson with two different valence quarks but the masses can be equal or different.

`x` should be `b` or `t` depending on whether you want to use the finite volume integrals using bessel functions or theta functions.

One valence mass, one sea mass::

`mass=quarkmassnf({Bm1,Bm4},f0,mu,2)`

`double fv1s1nf3p4(quarkmassnf mass, double L)` returns  $F_a^{V(4)0}$

`double fv1s1nf3p6(quarkmassnf mass, Linf Liin, double L)` returns  $F_a^{V(6)0}$

`double fv1s1nf3p6L(quarkmassnf mass, Linf Liin, double L)` returns  $F_{aL}^{V(6)0}$

`double fv1s1nf3p6R(quarkmassnf mass, double L)` returns  $F_{aR}^{V(6)0}$

Two valence mass, one sea mass::

`mass=quarkmassnf({Bm1,Bm3,Bm4},f0,mu,3)`

```

double fv2s1nf3p4(quarkmassnf mass, double L) returns  $F_a^{V(4)0}$ 
double fv2s1nf3p6(quarkmassnf mass, Linf Liin, double L) returns  $F_a^{V(6)0}$ 
double fv2s1nf3p6L(quarkmassnf mass, Linf Liin, double L) returns  $F_{aL}^{V(6)0}$ 
double fv2s1nf3p6R(quarkmassnf mass, double L) returns  $F_{aR}^{V(6)0}$ 

```

One valence mass, two sea mass::

```

mass=quarkmassnf({Bm1,Bm4,Bm6},f0,mu,3)
double fv1s1nf3p4(quarkmassnf mass, double L) returns  $F_a^{V(4)0}$ 
double fv1s1nf3p6(quarkmassnf mass, Linf Liin, double L) returns  $F_a^{V(6)0}$ 
double fv1s1nf3p6L(quarkmassnf mass, Linf Liin, double L) returns  $F_{aL}^{V(6)0}$ 
double fv1s1nf3p6R(quarkmassnf mass, double L) returns  $F_{aR}^{V(6)0}$ 

```

Two valence mass, two sea mass::

```

mass=quarkmassnf({Bm1,Bm3,Bm4,Bm6},f0,mu,4)
double fv2s2nf3p4(quarkmassnf mass, double L) returns  $F_a^{V(4)0}$ 
double fv2s2nf3p6(quarkmassnf mass, Linf Liin, double L) returns  $F_a^{V(6)0}$ 
double fv2s2nf3p6L(quarkmassnf mass, Linf Liin, double L) returns  $F_{aL}^{V(6)0}$ 
double fv2s2nf3p6R(quarkmassnf mass, double L) returns  $F_{aR}^{V(6)0}$ 

```

One valence mass, three sea mass::

```

mass=quarkmassnf({Bm1,Bm4,Bm5,Bm6},f0,mu,4)
double fv1s3nf3p4(quarkmassnf mass, double L) returns  $F_a^{V(4)0}$ 
double fv1s3nf3p6(quarkmassnf mass, Linf Liin, double L) returns  $F_a^{V(6)0}$ 
double fv1s3nf3p6L(quarkmassnf mass, Linf Liin, double L) returns  $F_{aL}^{V(6)0}$ 
double fv1s3nf3p6R(quarkmassnf mass, double L) returns  $F_{aR}^{V(6)0}$ 

```

Two valence mass, three sea mass::

```

mass=quarkmassnf({Bm1,Bm3,Bm4,Bm5,Bm6},f0,mu,5)
double fv2s3nf3p4(quarkmassnf mass, double L) returns  $F_a^{V(4)0}$ 
double fv2s3nf3p6(quarkmassnf mass, Linf Liin, double L) returns  $F_a^{V(6)0}$ 
double fv2s3nf3p6L(quarkmassnf mass, Linf Liin, double L) returns  $F_{aL}^{V(6)0}$ 
double fv2s3nf3p6R(quarkmassnf mass, double L) returns  $F_{aR}^{V(6)0}$ 

```

Defined in massdecayvevPQV.h, implemented in massdecayvevPQV.cc and examples of use in testmassdecayvevPQV.cc.

## Acknowledgements

This work is supported, in part, by the Swedish Research Council grants 621-2011-5080 and 621-2013-4287. I thank all my collaborators in the various applications for which my

version of the program made it into this collection and especially Ilaria Jemos who has tested many of the earlier versions in the course of [15].

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