ΩMaxEnt user guide

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Contents

1 Introduction

1.1 Overview

This is the user guide for the program Ω*MaxEnt*, a tool to perform the analytic continuation of Matsubara data using a maximum entropy aproach. It can treat fermionic or bosonic data, given as a function of Matsubara frequency or imaginary time, with either a diagonal or general covariance matrix. For the fermionic case, the output is a positive spectral function $A(\omega)$ and, for the bosonic case, it is the function $\sigma(\omega) = A(\omega)/\omega$, also positive.

A specific feature of Ω*MaxEnt* is the method it uses to find the optimal value of the entropy weight parameter α. It does not use either the *classic* approach or Bryan's, but instead locates the range of α where only information is fitted and the range where noise is also fitted. The optimal value is then chosen in the crossover between the two regimes. The program also offers useful graphical diagnostic tools for assessing the quality of the results.

In addition, the program uses a cubic spline to model the spectral function and uses the Matsubara frequency spectral representation of the Green function instead of the imaginary time version. Those two choices allow to compute the Green function corresponding to a given spectral function with high accuracy by a piecewise analytical integral. The use of a non-uniform grid for the spectral function and contraints on moments instead of a high Matsubara frequency cutoff also allows to improve calculation efficiency without losing accuracy. Basically, the code is optimized to ensure that the errors in the results comes from the errors in the data and not from numerical approximations.

You can obtain results by providing only a data file name to the program. It is however highly recommended to provide also errors (standard deviation or covariance

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matrix) if reliable estimates are available. You can also further improve the results by providing more information, like some known moments of the spectral function, a default model, or by providing a frequency grid adapted to the expected structures of the spectral function.

The next two subsection of this introduction present the basic theoretical aspects necessary to understand what you are doing when using this program. Then section 2 describes how to use Ω*MaxEnt* step-by-step. You can execute the program already at the end of subsection 2.2 to get some preliminary results. The following subsections give you the possibility to use more information you might possess to improve the result. Some explanations on how the program works and advices on how to interpret and improve the results are given at the end of the section. Lists of the output figures and the output files are given in subsections 2.8 and 2.12, respectively. Finally, section 3 presents a list of all the input parameters with a short description of each one.

For simplicity, throughout this guide, the Matsubara data is referred to as the "Green function" G, but the data can be a correlation function, a self-energy or any Matsubara function satisfying the conditions given in the next section. The result obtained with the program is also referred to as the spectral function A, although for bosonic data, it is actually $\sigma(\omega) = A(\omega)/\omega$.

1.2 Type of data accepted

The program can treat data that can be expressed as

$$G(i\omega_n) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{A(\omega)}{i\omega_n - \omega} \tag{1.1}$$

or

$$G(\tau) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{e^{-\omega\tau} A(\omega)}{1 \pm e^{-\beta\omega}}, \tag{1.2}$$

where $A(\omega) > 0$ for fermions or $\sigma(\omega) = A(\omega)/\omega > 0$ for bosons, and the $+$ and $-$ signs in the denominator of (1.2) are for fermions and bosons, respectively. The overall sign on the right-hand side of those expressions can also be different, the program will detect which convention you are using.

Those expressions are spectral representations which apply very generally to Green and correlation functions. They imply that $G(-i\omega_n) = G^*(i\omega_n)$ and that $\text{Re}[G(i\omega_n)]$ and $\text{Im}[G(i\omega_n)]$ behave asymptotically as $1/\omega_n^2$ and $1/(i\omega_n)$, respectively, as $\omega_n \to \infty$.

The positivity of $A(\omega)$ or $\sigma(\omega)$ is an additional constraint necessary for the maximum entropy method to be applicable. Assuming the same sign convention as in (1.1), it implies that $sign(\text{Im}[G(i\omega_n)]) = -sign(\omega_n)$ in the case of fermions and that $\text{Re}[G(i\omega_n)] < 0$ for bosons.

ΩMaxEnt can treat directly any data satisfying those conditions. This includes a wide variety of Green or correlation functions, but also the dynamical part of a self-energy $\Sigma(i\omega_n)$. In the latter case, it is better to know in advance the value of the static part if it is not already subtracted from the data.

ΩMaxEnt takes column-wise data files with only spaces between the columns.

1.3   What the program does

Finding the spectrum $A(\omega)$ corresponding to a given $G(i\omega_n)$ by numerically inverting expression (1.1) or (1.2) does not work. The errors on $A(\omega)$ resulting from the ones on $G(i\omega_n)$ would be greatly amplified and the result would not make sense. This is what is called an *ill-conditioned* problem. Instead, the program uses the *maximum entropy* approach, which consists in minimizing

$$Q = \chi^2 - \alpha S \,, \tag{1.3}$$

where

$$\chi^2 = \sum_{mn} (G_m - K_m A)^T C_{mn}^{-1} (G_n - K_n A) \,, \tag{1.4}$$

where A is the vector obtained after discretizing ω, K_n is a row vector such that $K_n A$ is an approximation to (1.1), and C is the covariance matrix. S is a differential entropy, defined as

$$S = - \int \frac{d\omega}{2\pi} A(\omega) \ln \frac{A(\omega)}{D(\omega)} \,, \tag{1.5}$$

where $D(\omega)$ is called the *default model*, and α is a parameter to be determined. The solution that minimize (1.3) if χ^2 is negligible, namely that maximizes the entropy S, is $e^{-1} D(\omega)$, hence the name *default model*. $D(\omega)$ is defined in a way to include what is known *a priori* about the spectrum.

The *maximum entropy* approach is based on Bayesian inference, which consists basically in using the information you know in advanced about the spectrum to deduce it from incomplete or noisy data, which alone is not sufficient to obtain acceptable results. In the present case, the entropy term αS is used to include that information.

To find the optimal value for α, the program first computes the solution to $\min(\chi^2 - \alpha S)$ for a large range of α. The location of the optimal α can then be found by a simple analysis of the shape of the function $\log(\chi^2)$ as a function of $\log(\alpha)$. The procedure is described in subsection 2.9.

Note that if we diagonalize the covariance matrix C, defining

$$\tilde{\mathbf{C}} = \mathbf{U}^\dagger \mathbf{C} \mathbf{U} \,, \tag{1.6}$$

χ^2 can be written

$$\chi^2 = (\tilde{G} - \tilde{\mathbf{K}} A)^T (\tilde{G} - \tilde{\mathbf{K}} A) \,, \tag{1.7}$$

where

$$\tilde{G} = \sqrt{\tilde{\mathbf{C}}^{-1}}\mathbf{U}^\dagger G \,,$$

$$\tilde{\mathbf{K}} = \sqrt{\tilde{\mathbf{C}}^{-1}}\mathbf{U}^\dagger \mathbf{K} \,. \tag{1.8}$$

This form is more useful for practical calculations and analysis of the results.

2 Step-by-step guide to Ω*MaxEnt*

2.1 The parameter files

The program uses two parameter files: *OmegaMaxEnt_input_params.dat* and *Omega-MaxEnt_other_params.dat*. The main parameter file used to control the calculation is *OmegaMaxEnt_input_params.dat*. The other parameter file should be modified by experienced users only, or according to instructions in this guide. The only mandatory parameter in *OmegaMaxEnt_input_params.dat* is the data file name on the first line. Although not recommended, you can obtain results even if all the other fields are left blank. When a parameter can have the values "yes" or "no", leaving the field blank or putting anything else than "yes" corresponds to the default value "no". The parameters other than the data file name are divided in two sections. The parameters defined in the section OPTIONAL PREPROCESSING TIME PARAMETERS are used to set all the variables in the optimization problem. The parameters defined in the section OPTIONAL MINIMIZATION TIME PARAMETERS control what happens during the search for the optimal solution to the problem. They can be modified without triggering the preprocessing. Some of them can be modified during the optimization itself, as explained in subsection 2.7.

Before doing your first analytic continuation with Ω*MaxEnt*, create the two parameter files by executing the file *OmegaMaxEnt*. The file *OmegaMaxEnt_input_params.dat* will be created with all the fields blank and *OmegaMaxEnt_other_params.dat* will be created

with the default values of its parameters. When you define a parameter in *OmegaMax-Ent_input_params.dat*, that parameter is printed on the terminal as the program reads the file. As for the parameters in *OmegaMaxEnt_other_params.dat*, they are printed out only if you modify the default value. It is important not to modify any parameter's name, namely, any caracter up to ':' on a line. If you define a parameter or modify one's default value in one of the two parameter files and this parameter is not printed on screen when the program reads the file, it means you inadvertently modified its name in the parameter file and the program cannot find it anymore. If that happens, destroy the file and execute Ω*MaxEnt* to create the default version of the missing parameter file.

Unless mentioned otherwise, all the input parameters referred below are defined in the file *OmegaMaxEnt_input_params.dat*.

2.2   Set the input data

Put the input file name on the line "data file", the first line in *OmegaMaxEnt_input_params.dat*. If your data file is not in the same directory as the code, you can set "input directory" in subsection INPUT FILES PARAMETERS which tells the program where to look first for your files. If a file is not found in that directory, the program then looks for it in the current directory.

2.2.1 $G(i\omega_n)$ as input

The data is always assumed to be given by columns in the data file, with the first column being the Matsubara frequency ω_n when the input data is $G(i\omega_n)$. By default the next two columns are assumed to be the real and imaginary parts of G, respectively:

$$\omega_n \qquad \text{Re}[G] \qquad \text{Im}[G] \tag{2.1}$$

If G is not on the 2nd and 3rd columns, write the correct column numbers on the lines "Re(G) column in data file" and "Im(G) column in data file" in the subsection INPUT FILES PARAMETERS.

2.2.2   Temperature

If the Matsubara frequencies do not have high precision in your data file or if the first column gives only the frequency indices, set the parameter "temperature" in the subsection DATA PARAMETERS.

2.2.3 $G(\tau)$ as input

For a Green function given in imaginary time $G(\tau)$, first set the parameter "imaginary time data" to "yes" in the subsection DATA PARAMETERS. By default, the columns in the data file are assumed to be

$$\tau \qquad G \tag{2.2}$$

If G is not on the 2nd column, put the correct column number on the line "column of G(tau) in data file" in subsection INPUT FILES PARAMETERS. Note that the imaginary time grid must be *uniform* and go from 0 to $1/T$, where T is the temperature. If the temperature is specified in the subsection DATA PARAMETERS, the imaginary time grid will be redefined using the provided temperature. Otherwise, T is assumed to be $1/\tau_{max}$, where τ_{max} is the last value of τ in the input file.

To get good results if your data is $G(\tau)$, the step $\Delta\tau$ must be small enough. See subsection 2.4.4 for more details.

2.2.4 Bosonic data

If G is bosonic, set the parameter "bosonic data" to "yes" in subsection DATA PARAM-
ETERS.

If $G(i\omega_n)$ is also real (or $G(\tau)$ is symmetric with respect to $\tau = \beta/2$), set "Im(G)
column in data file" to a value ≤ 0. The code will then assume an odd spectral function
($\sigma(\omega)$ even). This is the case of a correlation function of observables having the same
signature under time reversal.

2.2.5 Self-energy

If your data is a self-energy and the static part (the Hartree-Fock value) has been sub-
tracted, it can be treated the same way as a Green function. Otherwise, if you know the
value of the static part, set parameter "static part of data" in subsection DATA PARAM-
ETERS. If you do not know it, an estimate is the value of $\mathrm{Re}[\Sigma(i\omega_n)]$ at high frequency.
If you have enough frequencies, the latter function should become constant. If you have
put the correct value, when the moments are evaluated (see section 2.4.1), there should
be a plateau in the value of M_1 that is plotted as a function of the fit starting frequency.
If it is not the case, then the provided value is incorrect. However, if there are not many
frequencies in the asymptotic part of the data, it is possible that only the beginning of a
saturation can be seen. Note that "display preprocessing figures" must be set to "yes"
in section PREPROCESSING EXECUTION OPTIONS to see the figures when the mo-
ments are evaluated.

2.2.6 Most basic execution

If you do not have more information than the Green function itself, you can execute
Ω*MaxEnt* now. See section 2.7 for more details on the execution. If you have more
information or want to learn about other functionalities, follow the next steps or see

section 3.

2.3 Set errors

As mentioned in section 1.3, the data's covariance matrix C is used during the calculation. For a given set of data $G(i\omega_n)$, the accuracy of C actually controls how well the information contained in G can be transferred into the resulting spectrum $A(\omega)$. For the remaining of the guide, unless mentioned otherwise, the term "error" is used in a broad sense, sometimes meaning the standard deviation of data points or, more generally, referring to the covariance matrix.

The program can treat the case of a general, non-diagonal, covariance matrix, but you can simply provide the standard deviation in the case of diagonal covariance.

2.3.1 Uncorrelated errors

If the errors on the elements of G are uncorrelated, define the parameter "error file" in the subsection INPUT FILES PARAMETERS and the correct column numbers on the lines "Re(G) column in error file" and "Im(G) column in error file" if the input is $G(i\omega_n)$, or on the line "column of $G(\tau)$ error in error file" if the input is $G(\tau)$, unless the column number(s) correspond to the default value(s).

2.3.2 Correlated errors

If the errors are correlated between elements of G and you have the covariance matrix

$$C_{ij} = \frac{1}{N-1} \sum_{l=1}^{N} \left(G_i^l - \langle G_i \rangle \right) \left(G_j^l - \langle G_j \rangle \right) \tag{2.3}$$

where N is the number of sample values for each element G_i, G_i^l is the lth sample of G_i, and

$$\langle G_i \rangle = \frac{1}{N} \sum_{l=1}^{N} G_i^l, \tag{2.4}$$

then, in subsection INPUT FILES PARAMETERS, provide that matrix using the parameters "re-re covariance file", "im-im covariance file" and "re-im covariance file", if the input is $G(i\omega_n)$, or "imaginary time covariance file", if the input is $G(\tau)$. Those files must contain an equal number of lines and columns.

2.3.3   Basic execution

If you do not have more information, you can execute $\Omega MaxEnt$ now. See section 2.7 for more details on the execution. If you have more information or want to learn about other functionalities, follow the next steps or see section 3.

2.4   Control how moments are used

The part of the Green function at frequencies $\omega_n > W$, where $A(|\omega| > W) = 0$, can be expressed as a high frequency expansion, of which the coefficients are the moments of the spectral function $A(\omega)$. However, because of finite precision and noise, the information on high order moments is not present in the data. Therefore, the high frequencies of $G(i\omega_n)$ contain the information about a few moments only. It is thus numerically equivalent, but computationally more efficient to replace the large number of constraints corresponding to those high frequencies in the calculation by the few contraints corresponding to those moments.

The moments are also used during the definition of the real frequency grid and the default model, since they tell us about global properties of the spectrum, among which the center and the width of the spectrum.

2.4.1 Use ΩMaxEnt to extract moments

If the Matsubara frequency cutoff $\omega_{n_{max}}$ of your data is in the asymptotic part of $G(i\omega_n)$, namely that the condition $\omega_{n_{max}} > W$ is satisfied, the program can extract moments from your data by fitting a high frequency expansion to the asymptotic part, and determine the onset of the asymptotic regime at the same time. Unless you provide enough moments or real frequency grid parameters, ΩMaxEnt will try to extract them and use them in the calculation instead of the high frequencies they are extracted from. When it performs that procedure, if you set the parameter "display preprocessing figures" to "yes" in subsection PREPROCESSING EXECUTION OPTIONS, you can check for convergence in the computation of the moments from the figures of the norm M_0 and the first moment M_1 plotted as a function of the starting frequency of the fit. If there is a plateau in those curves above a certain frequency, then the values are converged.

In any case, you can force the program to extract the moments by setting "evaluate moments" to "yes" in subsection COMPUTATION OPTIONS. You can also control how many moments are used during the computation of the spectrum with the parameter "maximum moment" in the same subsection. By default, ΩMaxEnt imposes the first 4 moments (including the norm M_0) to the spectrum for fermions, and the first 3 moments for bosons. For example, if you want the program to impose only the norm and the first moment, set "maximum moment" to 1.

You can also control the maximum frequency to be used in the calculation with the parameter "Matsubara frequency cutoff" in subsection FREQUENCY GRID PARAME-TERS. For example, if you do not have enough frequencies in the asymptotic frequency range, it is probably better to use all the frequencies instead of the moments by setting "maximum moment" to 0 (if the norm is known exactly) and "Matsubara frequency cutoff" to a value larger than the last frequency in your data.

2.4.2 Special case of the norm of the spectrum

If your spectrum is normalized to 1, namely, if the leading high frequency term of the Green function is $1/(i\omega_n)$, you do not have to provide the norm. Also, if you have real bosonic Matsubara data and have set "Im(G) column in data file" to 0 or less, the norm is automatically assumed to be 0.

Otherwise if the norm is not 1, use "norm of spectral function" in subsection DATA PARAMETERS to provide it. If you do not know it, you can let the program extract it first and use the value printed in the terminal. To do so, set "evaluate moments" to "yes" in subsection COMPUTATION OPTIONS and "preprocess only" to "yes" in PREPRO-CESSING EXECUTION OPTIONS to prevent the actual calculation from starting after the preprocessing. It is also better to set "display preprocessing figures" to "yes" to verify convergence on the figure of M_0. Once "norm of spectral function" is set, you can disable "preprocess only" and continue the execution.

If you do not know the norm and there is not enough frequencies in your data to allow the program to extract it, namely there is no plateau in the figure of M_0, just tell the program not to use moments at all by setting "maximum moment" to -1 or less.

2.4.3 Providing moments

If you know some moments of the spectral function with good precision, you can provide them with their respective errors in subsection DATA PARAMETERS.

If you provide enough moments (first and second for fermions, first for bosons), the program will not try to extract them from your data. In that case however, it is recommended to set "evaluate moments" and "display preprocessing figures" to "yes" in subsection COMPUTATION OPTIONS when running $\Omega MaxEnt$ for the first time with a given set of data. This way, provided that your data has some frequencies in the asymptotic part of G (if so, there will be a plateau in the figures of M_0 and M_1),

you can verify if the moments you provided have values close to the ones extracted, which will be printed in the terminal. In addition, the program will also print where the asymptotic regime sets in. This verification step is important to make sure you do not impose wrong moments to the spectrum, which is worse than not imposing any. When making that verification, set "preprocess only" to "yes" to prevent the actual calculation from starting.

Once you provided moments, if your Matsubara frequency cutoff is far in the asymptotic part of G (there are long plateaus in the figures of M_0 and M_1 when "evaluate moments"), set "Matsubara frequency cutoff" in subsection FREQUENCY GRID PARAMETERS to the onset value given by the program. Note that this is done automatically if "evaluate moments" is enabled. If the asymptotic regime is not reached at the cutoff, you can make sure that all the frequencies are used, whatever the value of "evaluate moments" is, by setting "Matsubara frequency cutoff" to a value larger than the cutoff.

2.4.4 $G(\tau)$ as input data

If you have imaginary time data, the first two finite moments M_1 and M_2 are necessary to Fourier transform $G(\tau)$ before computing the spectrum from the resulting $G(i\omega_n)$ (with which Ω*MaxEnt* works internally). Thus in that case either you provide those moments, or the program extracts them from $G(\tau)$. In the latter case, it does so using a polynomial fit to $G(\tau)$ around the boundaries $\tau = 0$ and β. The condition for that fit to give the correct moments is that $\Delta\tau < 1/W$ (see introduction of section 2.4 for the definition of W), where $\Delta\tau$ is the imaginary time step. This condition is equivalent to $\omega_{n_{max}} > W$. Ideally, $\Delta\tau$ should be at least a few times smaller than $1/W$. Thus, if you provide $G(\tau)$ as the input data and do not know M_1 and M_2, make sure the imaginary time step is small enough so that this condition is satisfied. If you do know M_1 and M_2 with good accuracy, note however that, even though the Fourier transform of $G(\tau)$ will be accurate,

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the Fourier transform of the error will not be if $\Delta\tau$ is not small enough, which may degrade the quality of the result. It is thus preferable that the condition $\Delta\tau < 1/W$ be well satisfied in any case.

2.4.5 Basic execution

You can execute Ω*MaxEnt* here. See section 2.7 for more details on the execution. Otherwise, follow the next steps or see section 3 to learn about other functionalities.

2.5 Provide a user-defined grid

The real frequency grid used by Ω*MaxEnt* is separated in two different types of grid: a central dense part, let us call it the *main spectral range*, where most of the spectral weight should be found, and two non-uniform high frequency parts, where the step size increases approximately quadratically with the module of the frequency. Let us address how to control the grid in the main spectral range first.

By default, in that range, the program uses a uniform grid of width $SW = 2\Delta\omega_{std}$, where $\Delta\omega_{std} = \sqrt{M_2 - M_1^2}$ (fermionic case) is the standard deviation of the spectrum, and centered on $SC = M_1$ (the M_is are the moments of the spectrum). The number of frequencies in that region is defined in two possible ways: if there is a sharp and well isolated peak at low frequency, the program can estimate its width directly from the Matsubara data (see appendix A) and use a step appropriate to resolve that peak, otherwise, the step is defined as $SW/$*Rmin_SW_dw*, where *Rmin_SW_dw* is defined in file *Omega-MaxEnt_other_params.dat*. This grid is of course not optimal in many cases, especially for spectra possessing very broad and very sharp features at the same time. Fortunately, Ω*MaxEnt* offers a few ways to define a better adapted grid with the parameters of subsection FREQUENCY GRID PARAMETERS:

1. The simplest way is by setting one or more of the parameters "spectral function width", "spectral function center" and "real frequency step". The first two of those parameters are used for SW and SC, instead of the default ones defined from the moments, to define the main spectral range as $[SC - SW/2, SC + SW/2]$ with a uniform step given by "real frequency step". The default values, given in the previous paragraph, are used for those of these parameters that are left blank. You can also make sure that a specific frequency is included in the grid with the parameter "real frequency grid origin". This is useful, for example if the position of a peak is known precisely, to make sure that there is a grid point at the maximum. If "real frequency grid origin" is not defined, but "spectral function center" is, the two values will coincide.

2. One can also define a non-uniform grid in the central range by setting the parameter "use parameterized real frequency grid" to "yes" and by defining intervals and their respective steps on the line "grid parameters". The format of that line is "ω_0 $\Delta\omega_0$ ω_1 $\Delta\omega_1$ $\ldots \omega_{N-1}$ $\Delta\omega_{N-1}$ ω_N", where the ω_i's are the frequencies delimiting the intervals and the $\Delta\omega_i$'s are the steps in those intervals. The program then generates a grid with a step varying smoothly (with a hyperbolic tangent shape) between intervals. This grid is then used in the main spectral range. Note that it is important not to change the step too quickly between contiguous intervals. There should not be more than a factor of three from one interval to it neighbors, otherwise spurious structures may appear in the spectrum at the boundaries between intervals. Each interval should also contain at least 10 points, to ensure that $\Delta\omega$ vary smoothly with ω, a necessary condition to obtain high quality results. Another parameter, *RW_grid*, defined in *OmegaMaxEnt_other_params.dat*, controls how that non-uniform grid is generated. It defines the ratio of an interval width to the transition region between its step and the neighboring intervals' steps.

3. Finally, you can provide your own grid with the parameter "real frequency grid

file". The grid must be on the first column of the file. Note however that, unless it is a grid that was previously generated by $\Omega MaxEnt$, it will be used only in the main spectral range, which is defined either by the default values of SW and SC or by "spectral function width" and "spectral function center". On the other hand, if the file you provide is a spectrum obtained by the program in a previous calculation, the whole grid, including the high frequency parts, will be identical to the provided one.

As for the grid in the regions outside the central region, it is always defined in the same way by the program. Instead of having a uniform step $\Delta\omega$, the grid in those regions is such that $\Delta u = u_{i+1} - u_i$ is constant, where $u_i = 1/(\omega_i - \omega_{0l})$ on the left side and $u_i = 1/(\omega_i - \omega_{0r})$ on the right side. Here, ω_{0l} and ω_{0r} are frequencies determined by the extrema of the grid, which can be controlled by the parameter *f_w_range* defined in file *OmegaMaxEnt_other_params.dat*. More precisely, *f_w_range* is the ratio of the total size of the grid $\omega_{max} - \omega_{min}$ to the width of the main spectral range SW.

2.6 Provide a user-defined default model

By default, the default model is a gaussian of width equal to the standard deviation $\Delta\omega_{std} = \sqrt{M_2 - M_1^2}$ (fermionic case), if M_1 and M_2 are defined (provided by you or extracted from the data), or equal to parameter "spectral function width" (subsection FREQUENCY GRID PARAMETERS), and centered on M_1 (fermionic case), or "spectral function center" (subsection FREQUENCY GRID PARAMETERS) if M_1 is not defined.

If you want to use a different default model, there are two options:

1. You can use the parameters "default model center" (DC), "default model half width" (DW) and "default model shape parameter" (DS) in subsection COMPU-TATION OPTIONS to use a default model that has a *generalized normal distribu-*

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tion form. As special cases, if $DS = 1$, this corresponds to a Laplace distribution, if $DS = 2$, it is a gaussian, and as $DS \to \infty$, the distribution becomes uniform in the range $[DC - DW, DC + DW]$. It is recommended to set "default model shape parameter" to a value larger than 1, since for $DS \leq 1$, there is a discontinuity in the derivative at DC, which is not physical in general, except in the presence of a Van Hove singularity.

2. You can also use your own default model by setting the parameter "default model file" (subsection COMPUTATION OPTIONS). It is assumed that the first column is the grid and the second column is the function value. The grid on which your function is defined can be arbitrary, the program uses cubic splines to interpolate your function on the active grid, namely the one set previously during preprocessing. If your grid does not extend over the whole active grid, the program will extend your function with gaussians matching it as smoothly as possible at the extrema of your grid.

The default model is always normalized to the same value as the spectrum, namely M_0 in the fermionic case, or $G(i\omega_n = 0)$ in the bosonic case.

2.7 Execution

Ω*MaxEnt* runs in an interactive loop. There are a few ways, given below, to pause the execution to see the result at a given stage and with a given set of input parameters. At the pause, the program always asks if you want to continue execution. To do so, simply press ENTER, or enter anything else than 'y' to stop. During a pause, you can make changes to the parameter files. Depending on the type of changes you made, execution can resume either from the point it halted, or at an earlier stage. If you modify a parameter in section OPTIONAL PREPROCESSING TIME PARAMETERS during a pause, the preprocessing starts over. On the other hand, the parameters in section OPTIONAL

MINIMIZATION TIME PARAMETERS, with the exception of "initialize preprocessing", can be modified during a pause without triggering the preprocessing when execution continues. Some parameters in that subsection will however cause the minimization stage to restart at the initial (highest) α if they are modified, namely "output directory", "spectral function sample frequencies", "initial value of alpha" and "initialize maxent".

To pause execution, you can use one of the following parameters:

- "preprocess only" (subsection PREPROCESSING EXECUTION OPTIONS),

- "minimum value of alpha" (α_{min}) (subsection COMPUTATION PARAMETERS),

- "number of values of alpha computed in one execution" ($N_{\alpha_{max}}$) (subsection MINIMIZATION EXECUTION OPTIONS).

The parameter "preprocess only" can be used to do some verifications with input parameters, and try different values, before starting the actual calculation. For example, you can verify the values of moments with the ones extracted from the data, or check that your grid has a reasonable number of frequencies. If "display preprocessing figures" is enabled (subsection PREPROCESSING EXECUTION OPTIONS), the preprocessing stops when a group of figures is displayed, and you have to close them to resume it. This pause is not the right time to modify the parameter files however, since they will not be read when execution resumes once the figures are closed. Once you are satisfied with the input parameters, you can disable "preprocess only" to start computing the spectrum.

The parameters "minimum value of alpha" and "number of values of alpha computed in one execution" can be used to look at the results at intermediate stages during minimization time, where the spectrum is computed as a function of α. By default, at each pause during that part of the calculation, the program displays figures showing the results at the optimal α, if it has been found, and at the last (lowest) value of α computed. A list of the output figures is given in section 2.8. Once you have closed all the figures, the program asks you if you want to continue execution. You can also choose which groups of

figures are displayed with parameters "show optimal alpha figures", "show lowest alpha figures" and "show alpha dependant curves" in subsection DISPLAY OPTIONS.

If you have set "minimum value of alpha" and α_{min} is reached before the condition for the calculation to be over is satisfied (see section 2.13), the program will tell you that α_{min} is not small enough and will reduce it by the factor *f_alpha_min*, defined in file *OmegaMaxEnt_other_params.dat*, before asking if you want to continue execution. If you have set "number of values of alpha computed in one execution", the spectrum will be computed for $N_{\alpha_{max}}$ values of α each time the calculation is resumed, unless that parameter is emptied during a pause.

2.8 Output figures

The following functions are plotted when the execution stops during the minimization stage:

- $\log(\chi^2)$ versus $\log(\alpha)$,

- Curvature of $\log(\chi^2)$ vs $\log(\alpha)$,

- Spectral function at the *lowest* α (α_{low}): A vs ω,

- Spectral function at the *optimal* α (α_{opt}): A_{opt} vs ω (if $\alpha_{low} < \alpha_{opt}$),

- Spectral function at sample frequencies: $A(\omega_{samp})$ versus α,

- Normalized error $\Delta\tilde{G} = \tilde{G}_{in} - \tilde{G}_{out}$ versus frequency index n (diagonal covariance) or covariance eigenvector index i_c (general covariance), at the *lowest* α,

- Normalized error $\Delta\tilde{G}_{opt}$ versus frequency index n (diagonal covariance) or covariance eigenvector index i_c (general covariance), at the *optimal* α (if $\alpha_{low} < \alpha_{opt}$),

- Autocorrelation of $\Delta\tilde{G}$ vs Δn (diagonal covariance) or Δi_c (general covariance) at the *lowest* α,

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- Autocorrelation of $\Delta\tilde{G}_{opt}$ vs Δn (diagonal covariance) or Δi_c (general covariance) at the *optimal* α (if $\alpha_{low} < \alpha_{opt}$).

In the figure showing the spectrum at α_{opt}, a spectrum at a value of α slightly below α_{opt} and one at a value slightly above are also plotted. Those two other values of α, say α_{opt-} and α_{opt+}, delimit the range of the crossover region between the *information-* and the *noise-fitting* regimes. Along with the optimal spectrum, the spectra at α_{opt-} and α_{opt+} tell how stable the spectrum is around α_{opt}, and thus how accurate the results are (see also section 2.11).

2.9   How the optimal α is chosen

If you look at $\log\left(\chi^2\right)$ as a function of $\log\left(\alpha\right)$ for a large enough range of α, you will notice that there are three regimes in that function. At high α, the entropy term αS dominates in the quantity $Q = \chi^2 - \alpha S$ that is minimized with respect to the spectrum A (see section 1.3). Thus, χ^2 decreases very slowly with α and the spectrum stays close to default model. We may call this the *default model regime*. At intermediate values of α, χ^2 decreases rapidly as α decreases. This is the regime where the information in input data G_{in} is gradually integrated in the spectrum $A(\omega)$ (or $G_{out} = \mathbf{K}A$) as α decreases. It is thus an *information-fitting regime*. Finally, when most of the information in G_{in} is already present in $A(\omega)$, the noise in G_{in} starts to be integrated into $A(\omega)$, as $\Delta G = G_{in} - G_{out}$ becomes smaller than the error on G_{out}. At that point, the rate of change of χ^2 with α decreases rapidly, and becomes very small, in what we may call the *noise-fitting regime*. The optimal alpha should clearly be chosen where most of the information in G_{in} is contained in $A(\omega)$ (or G_{out}), but not its noise. It should therefore be somewhere in the crossover region between the *information-* and the *noise-fitting regime*.

The change of decreasing rate of χ^2 with α can be identified by a peak in the curvature of $\log\left(\chi^2\right)$ vs $\log\left(\alpha\right)$. The optimal α, say α_{opt}, can simply be chosen at the highest peak

maximum. However, in some cases, peaks other than the one marking the onset of the *noise-fitting regime* may be present in the curvature at values of α larger than α_{opt}. To avoid choosing those peaks by accident instead of the correct one, one can choose the optimal α at the highest peak maximum in the curvature of $\log\left(\chi^2\right)$ vs $\gamma\log\left(\alpha\right)$, where γ is typically between 0.1 and 0.5, instead. The factor γ increases the ratio of the amplitudes of the correct peak and the other peaks located at higher α, which reduces the probability of choosing the wrong peak. It displaces the position of the crossover peak maximum toward the *noise-fitting* region however, but only very slightly if γ is not too small, so that it barely affects the result.

As will be mentioned in section 2.12, the spectra are saved for a certain range of α around the optimal one. Therefore, you can also choose yourself the value of α that you find the most reasonable from the output figures and use the spectrum saved in the corresponding file instead of the one saved in "optimal_spectral_function_tem#_alpha#.dat" (see section 2.12).

If, for some reason, the value of α chosen by the program is not the one you think is optimal, for example if there are more than one peak in the curvature $\log\left(\chi^2\right)$ vs $\log\left(\alpha\right)$ in the region where the optimal alpha should be located, you can also choose the region where the program will search for the optimal α with the parameters "maximum optimal alpha" and "minimum optimal alpha" in subsection COMPUTATION PARAMETERS.

When the error (standard deviation or covariance) is known precisely, the crossover region is narrow, and it is clear what is the optimal value. This is because, in that ideal case, the ratio of ΔG and the error tends to stay comparable at different ω_n (or covariance eigenvector index i_c) as α decreases, and thus the noise in G_{in} starts to be fitted around the same value of α at *all* frequencies ω_n (i_c). On the other hand, if the error is not well estimated, the crossover region, where both noise and information are fitted at the same time, becomes wider. The choice of optimal α is then more arbitrary. In that case, the best solution is of course to improve the error, if that is possible. If not, you

can also use the other output figures to help you choose the α that corresponds to the best compromise according to your judgement. In particular, in addition to the spectrum itself, the figures described in subsections 2.10 and 2.11 can help you diagnose more precisely the problems with the errors, in order to improve it, or help you find the best compromise in the choice of the optimal α.

2.10   Properties of $\Delta\tilde{G} = \tilde{G}_{in} - \tilde{G}_{out}$ at the optimal α

The analytic continuation operation consists essentially in fitting the function $\tilde{G}_{out} = \check{\mathbf{K}}A$ to the input data $\tilde{G}_{in}$, where $\tilde{G}$ is a Green function vector expressed in the eigenbasis of the covariance matrix, and normalized by the standard deviation in that basis. The function $\Delta\tilde{G} = \tilde{G}_{in} - \tilde{G}_{out}$ as a function of ω_n (or covariance eigenvector index i_c) is very useful to assess the quality of the fit. To have a good fit, that function must satisfy the two following conditions:

1) $\Delta\tilde{G}$ is essentially noise at the optimal α:

When most of the information contained in G_{in} is also in G_{out}, but not the noise, $\Delta\tilde{G}$ is essentially the noise in G_{in} at the optimal α. In addition, because $\Delta\tilde{G}$ is normalized, it has a standard deviation of 1. This is what we obtain when the covariance matrix of the data is accurate. If the error is simply multiplied by an global factor f_{err}, α_{opt} will simply be reduced by f_{err}^2 and the standard deviation of $\Delta\tilde{G}$ reduced by f_{err}, but no effect will be seen on the spectrum at the (new) optimal α. However, if the ratio of the errors in different frequency ranges is not well estimated, G_{out} will eventually contain some of the noise of G_{in} in a given frequency range, namely $\Delta\tilde{G}$ will be smaller than the error in that range, while not yet containing all the information in another range. $\Delta\tilde{G}$ will then have both noisy regions and structured ones. If that problem is too serious, distorsions appear in some parts of the spectrum $A(\omega)$, although some of the information in G_{in} does not yet appear in it. That problem can be reduced by rescaling the errors in one frequency

range with respect to the other. This can be done by multiplying the errors by a smooth function of frequency.

2) There is no correlations between neighboring frequencies (or i_c) of $\Delta\tilde{G}$:

Look at the autocorrelation of $\Delta\tilde{G}$ as a function of Matsubara index differences Δn (or Δi_c) to see if the noise in $\Delta\tilde{G}$ is correlated or not between neighboring frequencies. At the optimal α, the autocorrelation should look like a noisy Kronecker delta function. The value at the origin is equal to χ^2/N_{χ^2}, where N_{χ^2} is the number of terms in χ^2, which should be close to 1 at α_{opt} if the magnitude of the error is correct. In most cases, the actual error is not very precise, therefore, only the structure of the autocorrelation really matters.

If you have assumed that the covariance is diagonal, and observe, even though $\Delta\tilde{G}$ seems to contain only noise, that the autocorrelation does not have a noisy Kronecker delta shape for $\alpha \leq \alpha_{opt}$, you should use a non-diagonal covariance matrix instead of a diagonal one.

2.11 Spectrum at sample frequencies vs α

When the execution stops during minimization, the program also plots the spectrum at a number of sample frequencies as a function of $\log\alpha$. By default, the program uses *Nwsamp* uniformly distributed frequencies in the main spectral region, where *Nwsamp* is defined in file *OmegaMaxEnt_other_params.dat*. To choose the sample frequencies yourself, use parameter "spectral function sample frequencies" in subsection OUTPUT FILES PARAMETERS in file *OmegaMaxEnt_input_params.dat*.

In an ideal case, where the error (standard deviation or covariance) is known precisely, the curves corresponding to different frequencies have stable, or "quasi-stable", point at the *same* α, which happens to be located in the crossover between the *information*- and the *noise-fitting* regions, where the optimal α (α_{opt}) is chosen using the $\log\left(\chi^2\right)$ vs

$\log(\alpha)$ curve (see subsection 2.9). If the error is small enough, the curves are actually stable around α_{opt}, and eventually have plateaus that overlap around α_{opt} as the error gets even smaller, which indicates quantitatively accurate results. Otherwise, the curves are "quasi-stable" at α_{opt}, namely they have either extrema, or inflexion points with a non-vanishing derivative. Below α_{opt}, in the *noise-fitting* region, the results eventually become unstable and the curves can increase or decrease very quickly.

On the other hand, if the error is not well known, there is necessarily some imbalance between different Matsubara frequency ranges. The result of that imbalance will be that the (quasi-)stable points in different real frequency regions of the spectrum will not be aligned. Those regions will have different "optimal" values of α, and thus there will be no well defined single optimal α. In that case, if possible, it is preferable to modify the error to improve balance between frequency ranges. Otherwise, if the value determined automatically by the program does not appear to be the best, the spectrum sample frequencies curves, combined with the figures of $\Delta \tilde{G}$ and its autocorrelation, can help you choose a better compromise.

To summarize, the *spectrum sample frequencies vs* α curves tell you

1. what the optimal α is in a given real frequency range,

2. if the errors are well balanced between different Matsubara frequency regions,

3. if your data is precise enough to have quantitatively accurate results.

2.12   Output files

You can control how and where the output files are saved with the parameters in subsection OUTPUT FILES PARAMETERS of section OPTIONAL MINIMIZATION TIME PARAMETERS of *OmegaMaxEnt_input_params.dat*. When the minimization stage starts, the program creates two directories for the output files: *OmegaMaxEnt_output_files*

and *OmegaMaxEnt_final_result*, which are located in "output directory", if this parameter is defined, else in "input directory" (subsection DATA PARAMETERS), if defined, or in the current directory otherwise.

Typically, the solutions to $\min(\chi^2 - \alpha S)$ are computed for hundreds of values of α before the optimal spectral function is obtained. The results in a certain range above and below the optimal α may be useful but the rest of the results are not. By default, in directory *OmegaMaxEnt_output_files*, the program saves the results in a range $[10^{-r}\alpha_{opt}, 10^r \alpha_{opt}]$, where r is equal to parameter *save_alpha_range* defined in file *OmegaMaxEnt_other_params.dat*. To define differently the range of α within which the results are saved, you can use parameters "maximum alpha for which results are saved" and "minimum alpha for which results are saved" in subsection OUTPUT FILES PARAMETERS.

The following files, with their respective formats, are saved in directory *OmegaMaxEnt_final_result*:

optimal_spectral_function_tem#_alpha#.dat   spectral function at α_{opt},

$\omega \qquad A_{opt}(\omega) \qquad$ (fermions),

$\omega \qquad A_{opt}(\omega)/\omega \qquad$ (bosons),

optimal_spectral_functions_tem#_alpha#_#_#.dat   spectral functions around α_{opt},

$\omega \qquad A_{opt-}(\omega) \quad A_{opt}(\omega) \quad A_{opt+}(\omega)$,

$\omega \qquad \sigma_{opt-}(\omega) \quad \sigma_{opt}(\omega) \quad \sigma_{opt+}(\omega)$,

G_opt_tem#_alpha#.dat   output Green function at α_{opt},

$\omega_n \qquad \mathrm{Re}[G] \quad \mathrm{Im}[G]$,

error_G_opt_tem#_alpha#.dat   Normalized output error at α_{opt},

$\mathrm{Re}[\Delta\tilde{G}] \qquad \mathrm{Im}[\Delta\tilde{G}]$,

moments_optimal_spectrum_tem#_alpha#.dat   moments of the spectral function at α_{opt},

$M_i^{in} \qquad M_i^{out}$,

auto_corr_error_G_opt_tem#_alpha#.dat   autocorrelation of $\Delta\tilde{G}$ at α_{opt},

$\Delta n \quad AC_{Re}(\Delta n) \quad AC_{Im}(\Delta n)$ (diagonal covariance)

$\Delta i \quad AC_1(\Delta i_c) \quad AC_2(\Delta i_c)$ (general covariance)

and the following files are saved in directory *OmegaMaxEnt_output_files* :

spectral_function_tem#_alpha#.dat	spectral function at a given α,
	$\omega \quad A(\omega) \quad$ (fermions),
	$\omega \quad A(\omega)/\omega \quad$ (bosons),
G_out_tem#_alpha#.dat	output Green function,
	$\omega_n \quad \mathrm{Re}[G] \quad \mathrm{Im}[G]$,
error_G_out_tem#_alpha#.dat	Normalized output error,
	$\mathrm{Re}[\Delta\tilde{G}] \quad \mathrm{Im}[\Delta\tilde{G}]$,
moments_G_out_tem#_alpha#.dat	moments of the spectral function,
	$M_i^{in} \quad M_i^{out}$,
chi2_vs_alpha_tem#.dat	χ^2 versus α,
	$\alpha \quad \chi^2$,
Asamp_vs_alpha_tem#.dat	$A(\omega)$ at sample frequencies versus α,
	$\alpha \quad A(\omega_1) \quad A(\omega_2) \quad \ldots \quad A(\omega_N)$.

The $opt+$ and $opt-$ subscripts for the data in file **optimal_spectral_functions_tem#_alpha#_#_#.dat** refer to values of α slightly above and below α_{opt}. Those values delimit the crossover region between *information-* and *noise-fitting* regimes (see also section 2.8).

2.13 When is the calculation over

The program assumes that the calculation is over when 1) the optimal α has been found, and 2) the following condition is satisfied:

$$\min\left(\frac{d\log(\chi^2)}{d\gamma\log(\alpha)}\right) < RMAX\_dlchi2\_lalpha * \max\left(\frac{d\log(\chi^2)}{d\gamma\log(\alpha)}\right), \qquad (2.5)$$

where *RMAX_dlchi2_lalpha* and $\gamma = $ *f_scale_lalpha_lchi2* are defined in *OmegaMaxEnt_other_params.dat*.

You can also stop the calculation before those condition are satisfied with parameters "minimum value of alpha" (subsection COMPUTATION PARAMETERS) or "number

of values of alpha computed in one execution" (subsection MINIMIZATION EXECU-
TION OPTIONS). In those cases, the calculation is only paused however, as discussed
in section 2.7, unless the two conditions above are satisfied.

In any case, the calculation is not over until the lowest α is deep in the *noise-fitting*
regime. This can be determined easily from the figure of $\log \chi^2$ versus $\log \alpha$, on which
you should see a plateau at high α, an intermediate region of large slope, and a quasi-
plateau (a region of very small slope) at low α. The latter quasi-plateau should be wide
enough to be sure that it is not just a smaller slope region in the *information-fitting*
regime. To verify that the lowest α is indeed in the *noise-fitting* region, see that the
function $\Delta \tilde{G}$ versus ω_n (or covariance eigenvector index) contains only noise.

2.14   How to improve the results

Typically, the first results you obtain with a given set of data are not the best you can
obtain. This can be because the default grid is not optimal for the spectrum, or the default
model needs some adjustments, or because the errors used are not accurate. The first step
to improve the results is to define a grid more adapted to the spectrum using subsection
FREQUENCY GRID PARAMETERS. For example, if some peaks are defined by only
a few points, you can either increase the step everywhere in the main spectral region, or
use a non-uniform grid, to improve the resolution of those peaks. It may also happen
that the main spectral region is too narrow and not optimally aligned with the spectrum.
You should adjust it so that it covers all the frequency region where the spectral weight
is located. The rest of the grid should cover only the tails of the spectrum. See section
2.5 for more details on how to define the grid.

The default model may also be too wide, too narrow, or misaligned with the spec-
trum. If so, you can modify its parameters in subsection COMPUTATION OPTIONS.
Note however that the default model should stay mostly featureless. The structure in the

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spectrum should come from the data and not from the default model.

Finally, if $\Delta\tilde{G}$ and its autocorrelation do not have the properties given in section 2.10, or the spectrum sample frequencies curves as a function of $\log(\alpha)$ do not have the same (quasi-)stable points (see section 2.11), then you should improve your errors if it is possible. Advices on how to improve the error are given in section section 2.10.

3   List of input parameters

The following is a complete list of the parameters defined in file *OmegaMaxEnt_input_params.dat*.

3.1   OPTIONAL PREPROCESSING TIME PARAMETERS

3.1.1   DATA PARAMETERS

- *bosonic data*

  Set this parameter to "yes" if your data is bosonic.

- *imaginary time data*

  Set this parameter to "yes" for imaginary time data.

- *temperature*

  If only the Matsubara frequency indices are given in your data file, or if the frequencies are not very precise, you can use this parameter to provide the temperature. It must be given in energy units ($k_B = 1$).

- *norm of spectral function*

  If the Green function is not normalized to 1 and you know the norm, you can use this parameter to provide it. The norm corresponds to the coefficient of $1/(i\omega_n)$

in the high frequency expansion of Matsubara functions having the spectral representation (1.1). It is recommended to set "evaluate moments" to "yes" (subsection COMPUTATION OPTIONS) to verify that the provided value is close to the norm extracted from your data and printed in the terminal.

If the Green function is not normalized to 1 and you *do not* know the norm, see subsection 2.4.2 for instructions.

The program assumes that the norm is known with relative precision *err_norm* (default value 10^{-6}), a parameter in file *OmegaMaxEnt_other_params.dat*.

For real bosonic Matsubara data, the norm is 0. However, in that case, set "Im(G) column in data file" (subsection INPUT FILES PARAMETERS) to a value ≤ 0 instead, and do not put anything for the norm.

- 1st *moment*

  If you know the first moment of the spectral function, use that parameter to provide it. The first moment corresponds to the coefficient of $1/(i\omega_n)^2$ in the high frequency expansion of of Matsubara functions having the spectral representation (1.1). It is recommended to set "evaluate moments" to "yes" (subsection COMPUTATION OPTIONS) to verify that your value is close to the one extracted from your data and printed in the terminal.

- 1st *moment error*

  If you provided the first moment, use that parameter to provide its (absolute) error. Otherwise, the value *default_error_M* $*\Delta\omega_{std}$ will be used, where *default_error_M* is a parameter in file *OmegaMaxEnt_other_params.dat* and $\Delta\omega_{std}$ is the standard deviation of the spectrum.

- 2nd *moment*

  If you know the second moment of the spectral function, use that parameter to provide it. The second moment corresponds to the coefficient of $1/(i\omega_n)^3$ in the high

frequency expansion of of Matsubara functions having the spectral representation (1.1). It is recommended to set "evaluate moments" to "yes" (subsection COMPUTATION OPTIONS) to verify that your value is close to the one extracted from your data and printed in the terminal.

- 2nd *moment error*

  If you provided the second moment, use that parameter to provide its (absolute) error. Otherwise, the value *default_error_M*, defined in *OmegaMaxEnt_other_params.dat*, will be used as the relative error.

- 3rd *moment*

  If you know the third moment of the spectral function, use that parameter to provide it. The third moment corresponds to the coefficient of $1/(i\omega_n)^4$ in the high frequency expansion of of Matsubara functions having the spectral representation (1.1). It is recommended to set "evaluate moments" to "yes" (subsection COMPUTATION OPTIONS) to verify that your value is close to the one extracted from your data and printed in the terminal.

- 3rd *moment error*

  If you provided the third moment, use that parameter to provide its (absolute) error. Otherwise, the value *default_error_M* $*\Delta\omega_{std}^3$ will be used, where *default_error_M* is defined in file *OmegaMaxEnt_other_params.dat* and $\Delta\omega_{std}$ is the standard deviation of the spectrum.

- *static part of data*

  If your data is a self-energy that contains a static part, use that parameter to provide its value. If you do not know that value, see section 2.2.5 for instructions.

3.1.2 INPUT FILES PARAMETERS

- *input directory*

  If your data is not in the same directory as the program, use that parameter to set the input directory. This way, the paths are not required for parameters that are file names. The directory can be relative to the program's directory. Note that if the program does not find a file in the provided directory, it will also look for it in the current directory. This allows you to use both the current and another directory at the same time. Just remember that, if files with the same name exist in the current and the provided directory, the ones in the latter will be used.

- *Re(G) column in data file*

  For Matsubara frequency data, use that parameter if the real part is not on the second column of your data file.

- *Im(G) column in data file*

  For Matsubara frequency data, use that parameter if the imaginary part is not on the third column of your data file.

  For the bosonic case, if the imaginary part vanishes exactly, set this parameter to a value ≤ 0. The "spectrum" $\sigma(\omega)$ is then assumed to be even and only the positive part of the grid is used in the calculation.

- *error file*

  Use this parameter if you have an error file where the error is given by columns. This is for the case of diagonal covariance. Otherwise, use the covariance file parameters.

- *Re(G) column in error file*

  For Matsubara frequency data, use that parameter if an error file is provided and the error on the real part is not on the second column of the file.

- *Im(G) column in error file*

  For Matsubara frequency data, use that parameter if an error file is provided and the error on the imaginary part is not on the third column of the file.

- *re-re covariance file*

  For Matsubara frequency data, if you have a covariance matrix, use that parameter to provide the $\text{Re}(G)$-$\text{Re}(G)$ part of the matrix. There must be an equal number of rows and columns in the file.

- *im-im covariance file*

  For Matsubara frequency data, if you have a covariance matrix, use that parameter to provide the $\text{Im}(G)$-$\text{Im}(G)$ part of the matrix. There must be an equal number of rows and columns in the file.

- *re-im covariance file*

  For Matsubara frequency data, if you have a covariance matrix, use that parameter to provide the $\text{Re}(G)$-$\text{Im}(G)$ part of the matrix. There must be an equal number of rows and columns in the file.

- *column of G(tau) in data file*

  For imaginary time data, use that parameter if the function value is not on the second column of your data file.

- *column of G(tau) error in error file*

  For imaginary time data, if an error file is provided, use that parameter if the error is not on the second column.

- *imaginary time covariance file*

  For imaginary time data, use that parameter if you have a covariance matrix.

3.1.3   FREQUENCY GRID PARAMETERS

- *Matsubara frequency cutoff*

  Use this parameter to set the maximum Matsubara frequency to be used during the calculation. It is however recommended to read subsections 2.4.1 and 2.4.3 to learn how to use it properly.

- *spectral function width*

  You can use this parameter to set the width of the main spectral region, namely, the dense part of the real frequency grid.

- *spectral function center*

  Use this parameter to set the center of the main spectral region.

- *real frequency grid origin*

  Use this parameter to ensure the grid contains a specific frequency.

- *real frequency step*

  If you are using a uniform grid in the main spectral region, you can use this parameter to set the step in that region.

- *real frequency grid file*

  Use that parameter to provide a user-defined frequency grid.

- *use parameterized real frequency grid*

  To use "grid parameters" on the next line, set this parameter to "yes".

- *grid parameters*

  Use this line to provide the parameters of a non-uniform grid that will be generated by the program. The left and right boundaries will define the main spectral region.

3.1.4 COMPUTATION OPTIONS

- *evaluate moments*

  If you set this parameter to "yes", the program will try to extract the spectral function's moments from your Matsubara data. Note that, depending on the other input parameters, the moments may also be extracted even if this option is disabled.

- *maximum moment*

  Use this parameter to set the maximum moment to be imposed to the spectrum. For example, to impose only the norm and the first moment, set it to 1.

- *default model center*

  Use this parameter if you want the default model to be centered on a frequency different than the (normalized) first moment.

- *default model half width*

  Use this parameter if you want the half width of the default model to be different from the standard deviation.

- *default model shape parameter*

  Use this parameter if you want the default model to be different from a gaussian (shape parameter= 2). A shape parameter of 1 corresponds to a Laplace distribution and, as the shape parameter increases, the default model becomes closer to a uniform distribution. A shape parameter > 1 is recommended, so that the derivative has no singularity.

- *default model file*

  Use this parameter to provide a user-defined default model.

- *initial spectral function file*

The program uses the default model as the initial spectral function. This is actually the solution when α is very large. However, if for some reason the program is interupted (not just paused) before the optimal result was reached, you can use this parameter and "initial value of alpha" (in subsection COMPUTATION PARAMETERS) to restart it at a value of α different from the initial one. This is useful only if the frequency grid is very large however (N_{ω_n} or $N_\omega > 1000$) and the calculation time is long. For numbers of Matsubara and real frequencies in the hundreds, the calculation is fast and you will not need that option. If you do need it, it may be useful to read section 2.12 to learn how and where the results are saved.

3.1.5 PREPROCESSING EXECUTION OPTIONS

- *preprocess only*

  Set this parameter to "yes" to pause execution at the end of preprocessing. As long as this parameter is enabled, when resuming execution, the preprocessing stage restarts if changes were made in section OPTIONAL PREPROCESSING TIME PARAMETERS during the pause, or else nothing happens. You can disable that option during the pause to start the actual calculation.

  This option, along with "display preprocessing figures", are very useful to verify the input parameters – input files, frequency grid, moments, default model, etc — and modify them if necessary, before starting the actual computation.

- *display preprocessing figures*

  Set this parameter to "yes" to display figures during the preprocessing.

- *display advanced preprocessing figures*

  Set this parameter to "yes" to display the "advanced" figures during preprocessing. Those figures show some intermediate quantities of different preprocessing operations.

- *print other parameters*

  Set this parameter to "yes" to display the parameters of file *OmegaMaxEnt_other_params.dat*.

3.2 OPTIONAL MINIMIZATION TIME PARAMETERS

3.2.1 OUTPUT FILES PARAMETERS

- *output directory*

  Use this parameter if you want to put the two output directories *OmegaMax-Ent_output_files* and *OmegaMaxEnt_final_result* in another directory than the one provided at "input directory", or the current directory otherwise.

- *output file names suffix*

  Use this parameter to add a suffix to the names of the output files (see section 2.12). For example, you can add parameter values specific to your data to archive your files more clearly. The suffix you define will be added after the default descriptive part of the file names, before "tem#".

- *maximum alpha for which results are saved*

  Use this parameter to choose the range of α for which the results are saved differently than how it is done by default, as described in section 2.12.

- *minimum alpha for which results are saved*

  Use this parameter to choose the range of α for which the results are saved differently than how it is done by default, as described in section 2.12.

- *spectral function sample frequencies*

  Use this parameter to choose which sample frequencies of the spectrum will be plotted as a function of α. See section 2.11 for a discussion about that figure.

3.2.2 COMPUTATION PARAMETERS

- *initial value of alpha*

  Use this parameter only if you do not see a plateau at high α in the figure of $\log \chi^2$ versus $\log \alpha$. Most of the time, the value determined by the program is correct. If not, set this parameter to a value a few orders of magnitudes larger than the largest value in the figure, and increase it the same way until you see the plateau.

- *minimum value of alpha*

  Use this parameter to adjust the width of the *noise-fitting* region, namely the quasi-plateau at low α in $\log \left(\chi^2 \right)$ versus $\log(\alpha)$, if necessary. This region should cover at least a few decades, to make sure that the calculation is really over, but not too many, since it is located below the optimal α, and thus useless to the results themselves. The program is designed to make sure that this region is wide enough, so this parameter might be useful mostly to reduce the width of the *noise-fitting* region.

- *maximum optimal alpha*

  Use this parameter if the program does not choose the correct peak in the curvature of $\log \chi^2$ versus $\log \alpha$, namely, the peak located in the crossover region between the *information-* and *noise-fitting* ranges of α. See subsection 2.9 for a discussion about this topic.

- *minimum optimal alpha*

  Use this parameter to ignore the peaks below a certain α in the curvature of $\log \chi^2$ versus $\log \alpha$, in case there are more than one peak in the region where the optimal α should be chosen.

3.2.3 MINIMIZATION EXECUTION OPTIONS

- *number of values of alpha computed in one execution*

  Use this parameter to force a pause once the spectrum has been computed for a certain number of values of α. The program will display figures showing the results at the current stage of the calculation. You can make some changes in section OPTIONAL MINIMIZATION TIME PARAMETERS without triggering the preprocessing, except for option "initialize preprocessing". Once you have closed the figures, the program will ask you if you want to continue the execution. If you do, computation will resume at the point it halted.

- *initialize maxent*

  Use this option to restart the minimization stage at the initial value of α after a pause. Do not forget to disable that option if the execution is paused again before the calculation is over and you modify the file *OmegaMaxEnt_input_params.dat* during the pause, unless you want the minimization stage to start over again.

  Note that if you modify either "output directory", "spectral function sample frequencies" or "initial value of alpha" during a pause, the minimization stage will also start over.

- *initialize preprocessing*

  Use this option if you want to restart the preprocessing. Note that if you make modifications in section OPTIONAL PREPROCESSING TIME PARAMETERS, the preprocessing will also restart.

3.2.4 DISPLAY OPTIONS

- *display results at each value of alpha*

If that option is enabled, the values of $Q = \chi^2 - \alpha S$, S and χ^2 will be printed in the terminal at each value of α computed.

- *show optimal alpha figures*

  Use this parameter if you *do not* want the program to display the figures corresponding to the *optimal* α.

- *show lowest alpha figures*

  Use this parameter if you *do not* want the program to display the figures corresponding to the *lowest* α.

- *show alpha dependant curves*

  Use this parameter if you *do not* want the program to display the α-dependant curves, namely, $\log\left(\chi^2\right)$ vs $\log(\alpha)$, its curvature, and the spectrum sample frequencies vs $\log(\alpha)$.

- *reference spectral function file*

  You can use that parameter to provide a reference spectrum that will be plotted on the same figures as the spectrum.

A How the program estimates the width of a low energy peak

The presence of a peak in the spectrum at low energy produces a specific signature in the Matsubara data. For fermions, the imaginary part will seem divergent at low frequency, while for bosons, it produces a jump in the real part at low frequency. In addition, if that peak is isolated enough from the rest of the spectrum one can obtain its weight, position, and width from the coefficients of a Laurent series fitted to the low frequency part of $G(i\omega_n)$. When the signature of the presence of a well defined peak at low energy is

detected by the program, it performs that fit and print the three values in the terminal if the fit is good. The parameters *Nwn_test_metal*, *R_d2G_chi_peak*, *std_norm_peak_max* and *varM2_peak_max*, all defined in file *OmegaMaxEnt_other_params.dat*, are used to determine if the fit is performed and, if so, if it is good enough to take the result into account. The only parameter actually used by the program is the width, which provides an order of magnitude for the step that should be used in the low frequency part of the grid.

B Other parameters

The following is a complete list of the parameters defined in file *OmegaMaxEnt_other_params.dat*.

- *Nn_max*

  Maximum number of Matsubara frequencies. Once the asymptotic part has been removed, if the number of frequencies exceeds that value, a non-uniform Matsubara grid will be used.

- *Nw_min*

  Minimum number of real frequencies.

- *Nw_max*

  Maximum number of real frequencies. The execution is paused and cannot continue if the number of frequencies exceeds that number. If that happens, you can either increase that value, or use parameters of subsection FREQUENCY GRID PARAMETERS in file *OmegaMaxEnt_input_params.dat* to modify the grid. The latter option is more efficient and thus recommended.

- *Nn_fit_max*

During computation of the moments, maximum number of frequencies used in the fit of the asymptotic form of the Matsubara function when localizing the asymptotic part of the function.

- *Nn_fit_fin*

  During computation of the moments, maximum number of frequencies used in the final fit of the asymptotic form of the Matsubara function.

- *Nn_as_min*

  Minimum number of frequencies required in the asymptotic region for the computed moments to be used in the calculation.

- *Nwn_test_metal*

  Number of low frequencies used to look for the signature of a low energy peak. If the test is conclusive, the programs tries to determine the position, width and weight of the peak.

- *Niter_dA_max*

  Maximum number of iterations in the calculation of the spectrum at a given value of α using Newton's method to solve $\nabla Q = 0$.

- *Nwsamp*

  Default number of sample frequencies of the spectral function to be plotted (and saved) as a function of alpha.

- *f_w_range*

  Ratio of the total real frequency range and the main spectral range.

- *Rmin_SW_dw*

  Minimum ratio of spectral function width and frequency step.

- *tol_tem*

  Tolerance on the relative difference between the temperature extracted from the first finite Matsubara frequency and the input temperature. A warning is given if that tolerance is exceeded.

- *tol_norm*,

  Tolerance on the difference between the norm extracted from the asymptotic part of the data and the provided norm (if applicable). A warning is given if that tolerance is exceeded.

- *tol_M1*

  Tolerance on the difference between the first moment extracted from the asymptotic part of the data and the provided one (if applicable). A warning is given if that tolerance is exceeded.

- *tol_M2*

  Tolerance on the difference between the second moment extracted from the asymptotic part of the data and the provided one (if applicable). A warning is given if that tolerance is exceeded.

- *tol_M3*

  Tolerance on the difference between the third moment extracted from the asymptotic part of the data and the provided one (if applicable). A warning is given if that tolerance is exceeded.

- *default_error_G*

  Default error on the input data. When no error file is provided, a constant error of *default_error_G*$*G_{max}$ is used, where G_{max} is the maximum absolute value of the imaginary part of the data, for fermions, or the real part, for bosons.

- *err_norm*

  Relative error on norm.

- *default_error_M*

  Default error on moments.

- *tol_mean_C1*

  Tolerance used to find the onset of the asymptotic region of G from the fitted norm as a function of the starting frequency of the fit.

- *tol_std_C1*

  Tolerance used to find the onset of the asymptotic region of G from the standard deviation of the fitted norm as a function of the starting frequency of the fit.

- *tol_rdw*

  Tolerance used to decide if consecutive frequency intervals are equal. Used to detect if a frequency grid has been generated by the program.

- *Rmin_Dw_dw*

  Minimum number of steps accepted in a grid interval when using a parameterized real frequency grid ("grid parameters" in subsection FREQUENCY GRID PARAMETERS of file *OmegaMaxEnt_input_params.dat*).

- *Rdw_max*

  Maximum ratio of steps recommended in consecutive grid interval when using a parameterized real frequency grid ("grid parameters").

- *RW_grid*

  Ratio of grid interval length and the transition region between intervals in the parameterized real frequency grid.

- *RWD_grid*

  Width of the transition region of the hyperbolic tangent used to define the parameterized real frequency grid.

- *minDefM*

  Minimum value of default model.

- *f_alpha_init*

  Initial ratio of the entropy and the χ^2 contributions to the spectrum.

- *R_width_ASmin*

  Width of the minimum entropy spectrum peaks relative to the width of the default model.

- *f_Smin*

  Ratio of the minimum entropy and the optimal χ^2. Used to estimate α_{min} during the preprocessing.

- *diff_chi2_max*

  Maximum relative difference between the χ^2 of consecutive values of α. If this ratio is exceeded, the step in $\log_{10}(\alpha)$ is decreased.

- *tol_int_dA*

  Tolerance on consecutive values of the integral of $|\delta A|$, where δA is the variation in the spectrum A between iterations in the Newton's method used to compute the spectrum.

- *rc2H*

  Maximum ratio of the penalization parameter and the maximum eigenvalue of the hessian of χ^2. The penalization parameter is used to avoid negative values of the spectrum.

- *pow_alpha_step_init*

  Initial value of the step in $\log_{10}(\alpha)$.

- *pow_alpha_step_min*

  Minimal value of the step in $\log_{10}(\alpha)$.

- *chi2_alpha_smooth_range*

  Length of the part of the curve $\log_{10}(\chi^2)$ vs $\gamma \log_{10}(\alpha)$ used to compute its local curvature. γ is the parameter *f_scale_lalpha_lchi2*.

- *f_scale_lalpha_lchi2*

  γ in the calculation of the curvature of $\log_{10}(\chi^2)$ vs $\gamma \log_{10}(\alpha)$.

- *FNfitTauW*

  Factor that determines the number of values of τ used in the polynomial fit in the calculation of the moments from imaginary time data.

- *std_norm_peak_max*

  For fermions, tolerance on the standard deviation of the low frequency peak weight as a function of fitting power in the estimation of a low frequency peak width. Used to decide if there is a well defined peak or not.

- *varM2_peak_max*

  For bosons, relative tolerance on the low frequency peak variance as a function of fitting power in the estimation of a low frequency peak width. Used to decide if there is a well defined peak or not.

- *R_d2G_chi_peak*

  For bosons, ratio used to decide if the program looks for a low frequency peak.

- *RMAX_dlchi2_lalpha*

  Maximum ratio of $d \log \left(\chi^2 \right) / d \log (\alpha)$ at the lowest α, and the maximum value. Used to determine if α is deep enough in the *noise-fitting* region.

- *f_alpha_min*

  Factor by which α_{min} is reduced when estimated to be too high.

- *save_alpha_range*

  Range of α above and below the optimal value for which the results are saved, in $\log_{10}$ scale. If $r = save\_alpha\_range$, the range saved is $[10^{-r}\alpha_{opt}, 10^{r}\alpha_{opt}]$.