Maxent Example - Non-interacting Case

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Abstract

This document is part of a tutorial on the use of Maxent, a program for doing analytical continuation using the maximum entropy method. It will explain how to provide the program with the proper parameter file, data format for bosonic frequency data, and understand the output. This program uses the ALPSCore libraries[1, 2]

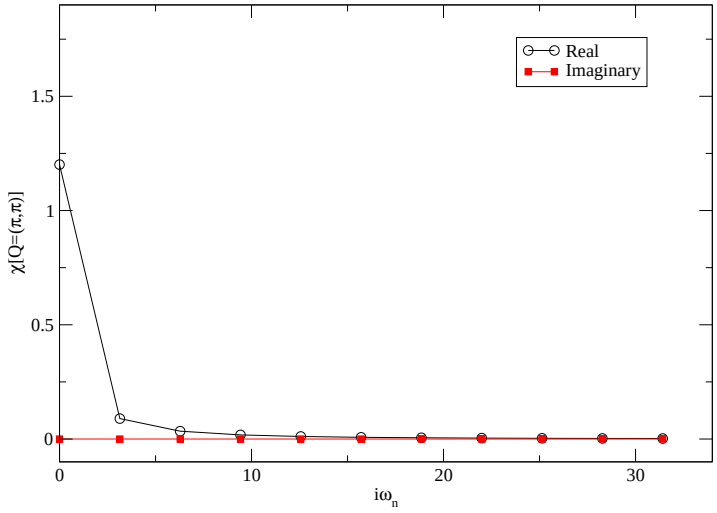
Contents

1 Introduction

Using DMFT and DCA with $U = 6$ and $\mu = -1.25$ ($n = 0.9$), we can generate the magnetic susceptibility χ of a 8-site Hubbard model

$$H = -\sum_{<ij>\sigma} t_{ij}\left(c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$

In particular, we will continue the magnetic susceptibility at $Q = (\pi, \pi)$, which is shown below



2 File Structure

We'e included several files that will be used to generate the remainder of this document:

Filenames and Descriptions

- *G_ im* = Im$[G(i\omega_n)]$, also input format for maxent
  - column format: $i\omega_n$ Im$[G(i\omega_n)]$ $\sigma_{I,n}$

Input file - G_im

```
0 1.20109669923 0.0001
3.14159265359 0.0894052697042 0.0001
6.28318530718 0.0342718849381 0.0001
```

- *G_ re* = Re$[G(i\omega_n)]$
  - column format: $i\omega_n$ Re$[G(i\omega_n)]$ $\sigma_{R,n}$

Input file - G_re

```
0 -1.27890161453e-15 1.27890161453e-16
3.14159265359 4.895943813e-06 4.895943813e-07
6.28318530718 7.44279002171e-06 7.44279002171e-07
```

- *dat_ in* = $\chi(i\omega_n)$ input format for Maxent
  - column format: $i\omega_n$ $Im[\chi(i\omega_n)]\sigma_{R,n}$ $Im[\chi(i\omega_n)]$ $\sigma_{I,n}$

Input file - dat_in

```
0 1.20109669923 0.0001 -1.27890161453e-15 1.27890161453e-16
3.14159265359 0.0894052697042 0.0001 4.895943813e-06 4.895943813e-07
6.28318530718 0.0342718849381 0.0001 7.44279002171e-06 7.44279002171e-07
```

3 Using Maxent

These files are easily used with Maxent. Here is the parameter file for this input

Param File in.param

```
NORM = 1.20109669923          #the particular normalization for this data
OMEGA_MAX = 40                #Spectral function is larger than default bounds
KERNEL = bosonic              #Using bosonic data
BETA = 2.0                    #inverse temperature
NFREQ = 1000                  #number of output frequencies
NDAT = 22                     #number of input data points*2 due to non-PH symmetry
DATASPACE = frequency         #frequency data
PARTICLE_HOLE_SYMMETRY = 0    #non PH symmetric data
DATA=dat_in                   #name of data file
```

3.1 Internal Kernel

While the expression for the spectral function of bosonic data is

$$\mathrm{Im}[\chi(i\omega_n)] = \int d\omega \frac{A(\omega)}{i\omega_n + \omega},$$

when trying to determine $\omega = 0$ at $i\omega_n = 0$ we run into a problem. To fix this, we simply try to find $A(\omega)/\omega$ so that expression now reads:

$$\mathrm{Im}[\chi(i\omega_n)] = \int d\omega \frac{\omega}{i\omega_n + \omega} \cdot (A(\omega)/\omega)$$

The fitting routine then finds the normalized $A(\omega)/\omega$ and produces that and the proper output (see below).

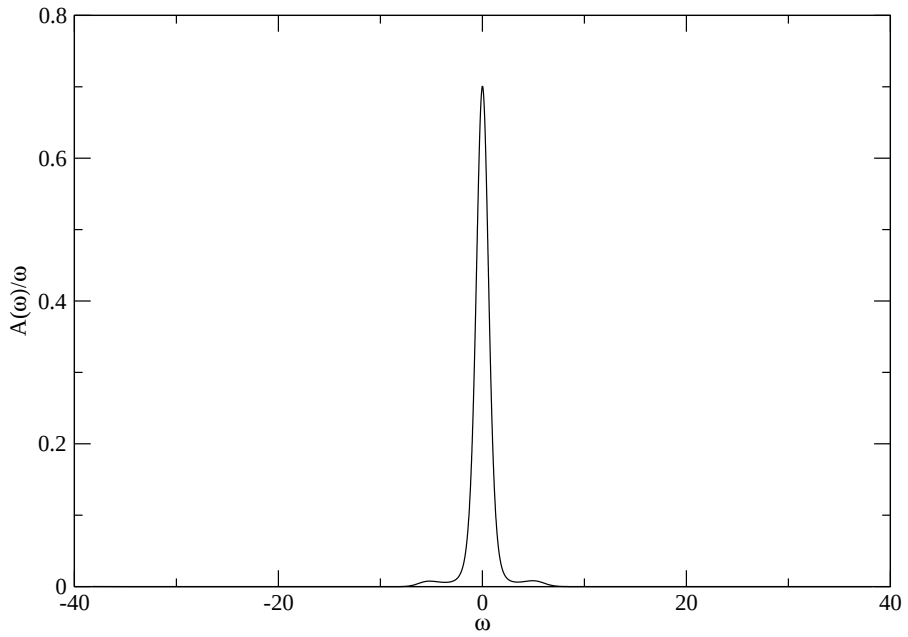
3.2 Output Guide

For the particular output of Maxent, please see the other example PDF files.

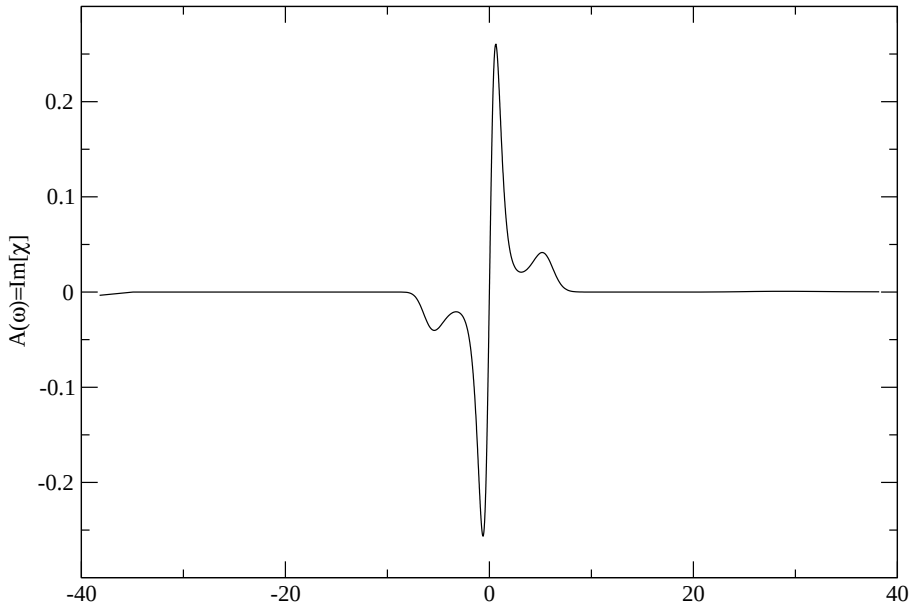
If text output is on, Maxent produces 10 files:

name.out.avspec.dat	Fitted spectral function (Imχ/ω) using Bayesian - **Bryan's method**
name.out.avspec_bose.dat	$A(\omega) = \mathrm{Im}[\chi]$ with the proper sign and normalization; using **Bryan's method**
name.out.chi2.dat	Estimated χ^2 for each α value solution
name.out.chispec.dat	Spectral function satisfying the best χ^2 - **classic Maxent**
name.out.fits.dat	Fits of each α value, see comments in file
name.out.maxspec.dat	Fitted spectral function (Imχ/ω) with the highest probability - **historic Maxent**
name.out.maxspec_bose.dat	$A(\omega) = \mathrm{Im}[\chi]$ with the proper sign and normalization; using **historic Maxent**
name.out.out.h5	All output data in the hdf5 format
name.out.prob.dat	The posterior probability of each α value
name.out.spex.dat	All spectral functions produced; one for each α

In our example here is the ''spectral'' output $A(\omega/\omega)$ from avspec:



while here is the proper spectral function $A(\omega)$ is found to be



It is important to note the kernel of the output, so that the proper back continuation can be performed. It is easiest to work with the xxspec.dat file so a frequency at $i\omega_n = 0$ can be generated as the true kernel (discussed in (3.1)) is singular.

References

[1] Alexander Gaenko, Emanuel Gull, Andrey E. Antipov, Lukas Gamper, and Gabriele Carcassi. ALPSCore: Version 0.4.5. May 2015. doi:10.5281/zenodo.17398.

[2] B Bauer et al. The ALPS project release 2.0: open source software for strongly correlated systems. *Journal of Statistical Mechanics: Theory and Experiment*, 2011(05):P05001, 2011. doi:10.1088/1742-5468/2011/05/P05001.