Notes: Nevanlinna analytical Continuation Method

Shuang Liang*

Institute of Physics, Chinese Academy of Sciences

(Dated: October 27, 2021)

Abstract

This is the abstract.

CONTENTS

* sliang@iphy.ac.cn

I. THE ANALYTIC CONTINUATION PROBLEM

Another way is to extract real frequency dynamical information from imaginary-time correlation functions $G(\tau)$ by analytic continuation. Technically, this is a highly nontirvial task[1]. To see this, we use the relation between $G(\tau)$ and $A(\omega)$ [1, 2]:

$$G(\tau) = \int_{-\infty}^{\infty} d\omega \frac{e^{-\tau\omega}}{1-\lambda e^{-\beta\omega}} A(\omega) \tag{1}$$

For large $|\omega|$, the kernal $K(\tau, \omega) = \frac{e^{-\tau\omega}}{1-\lambda e^{-\beta\omega}}$ is exponentially small, so the large $|\omega|$ features of $A(\omega)$ depend upon subtle features in $G(\tau)$. To obtain $A(\omega)$ from $G(\tau)$ is thus akin to parameterizing a two-neuclei redioactive decay problem[3]:

$$y = Ae^{-at} + Be^{-bt} \tag{2}$$

This type of problem is well known to be ill-posed and F. S. Acton describe it as a problem "not to compute"[4].

Thankfully, we can take the advantage of the cMPO method that one can get very accurate values of $C_{AB}(\tau)$ as well as $C_{AB}(i\omega_n)$, and to use the recently developed Nevanlinna analytic continuation method[5]. The method is briefly demonstrated below.

II. NEVANLINNA ANALYTIC CONTINUATION

A. Schur algorithm

The Nevanlinna analytic continuation method[5] is basically an interpolation method. In this method, one should firstly using conformal transforms to map the Masubara Green's functions $\mathcal{G}$, which is analytic in the upper half of the complex plane $\mathcal{C}^+$ and contains singularities in the lower half plane, to a closed unit disk $\bar{\mathcal{D}}$ in the complex plane. The mappings are shown in fig. 1. It becomes a Schur class($\mathcal{S}$) function and would have a continued fraction expansion where the parameters can be rescrsively defined[6]. Then one can apply the Nevanlinna iterative algorithm to interpolate the Schur functions[7]. Finally, one can do a inverse conformal transform back to $\mathcal{C}^+$ and obtains $\mathcal{G}(z)$, it's then natural to do analytic continuation $z \to \omega + i0^+$. The calculation process is shown in fig. 2.

For fermionic Green's functions, the mapping from $\mathcal{C}^+$ to $\bar{\mathcal{C}^+}$ is simple. Since $\mathrm{Im}\mathcal{G}(z) \leq 0$ if $z \in \mathcal{C}^+$, the mapping is just to take $\mathcal{G} \to -\mathcal{G} = \mathcal{N}\mathcal{G}$ and $\mathcal{N}\mathcal{G} \subset N$. While for bosonic Green's

$$
\begin{tikzcd}
\mathcal{C}^+ \arrow[r, "f"] \arrow[d, "h_1"'] \arrow[dr, "\theta"] & \bar{\mathcal{C}}^+ \arrow[d, "h"] \\
\mathcal{D} \arrow[r, "g"'] & \bar{\mathcal{D}}
\end{tikzcd}
$$

f: Nevanlinna function $\in N$
g: Schur function $\in \mathcal{S}$
θ: Contractive function $\in B$
h/h_1: Conformal mapping

FIG. 1. Conformal mappings

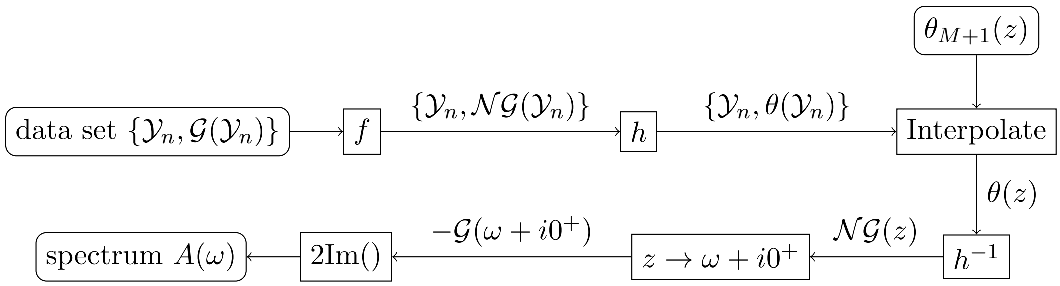

FIG. 2. Calculation flow chart

functions, this mapping is a little bit complicated and we will discuss in the next section. The data set we have is $\{i\omega_n, \mathcal{G}(i\omega_n)\}$, here we denote $\mathcal{Y}_n = i\omega_n$ and $\mathcal{C}_n = \mathcal{N}\mathcal{G}(i\omega_n) = -\mathcal{G}(i\omega_n)$.

Then we use the Möbius transform

$$h(z) = \frac{z - i}{z + i} \tag{3}$$

to map $\mathcal{C}_n \subset N$ to $\theta(\mathcal{Y}_n) = h(\mathcal{C}_n) \subset \bar{\mathcal{D}}$. The recursive final $\theta(z)$ can conveniently be written in a matrix form:

$$\theta(z)[z; \theta_{M+1}(z)] = \frac{a(z)\theta_{M+1}(z) + b(z)}{c(z)\theta_{M+1}(z) + d(z)} \tag{4}$$

where

$$\begin{pmatrix} a(z) & b(z) \\ c(z) & d(z) \end{pmatrix} = \prod_{n=1}^{M} \begin{pmatrix} h_1(z, \mathcal{Y}_j) & \phi_j \\ \phi_j^* h_1(z, \mathcal{Y}_j) & 1 \end{pmatrix} \tag{5}$$

where $h_1(z, \mathcal{Y}_n) = \frac{z - \mathcal{Y}_n}{z - \mathcal{Y}_n^*}$ is a conformal map form $\mathcal{C}^+$ to $\mathcal{D}$. $\theta_j(z)$ is the interpolation function of j-th step and $\phi_j = \theta_j(\mathcal{Y}_j)$. There is a freedom to choose $\theta_{M+1}(z)$. One can use this freedom to select the "best" of all consistent spectral functions.

[1] Mark Jarrell and James E Gubernatis. Bayesian inference and the analytical continuation of imaginary-time quantum monte carlo data. *Physics Reports*, 269(3):133–195, 1996.

[2] Ming-Wen Xiao. *Lecture notes: Linear Response Theory*. School of Physics, Nanjing University.

[3] James Gubernatis, Naoki Kawashima, and Philipp Werner. *Quantum Monte Carlo Methods: Algorithms for Lattice Models*. Cambridge University Press, 2016.

[4] Forman S. Acton. *Numerical Methods that Work (Spectrum)*. The Mathematical Association of America, 1997.

[5] Jiani Fei, Chia-Nan Yeh, and Emanuel Gull. Nevanlinna analytical continuation. *Physical Review Letters*, 126(5):056402, 2021.

[6] J Schur. Über potenzreihen, die im innern des einheitskreises beschränkt sind. *Journal für die reine und angewandte Mathematik (Crelles Journal)*, 1918(148):122–145, 1918.

[7] Rolf Nevanlinna. Uber beschrankte funktionen, die in gegeben punkten vorgeschrieben werte annehmen. *Ann. Acad. Sci. Fenn. Ser. A 1 Mat. Dissertationes*, 1919.