Notes: Nevanlinna analytical Continuation Method

Shuang Liang[*]

Institute of Physics, Chinese Academy of Sciences

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Abstract

This is the abstract.

CONTENTS

[*] sliang@iphy.ac.cn

I. THE ANALYTIC CONTINUATION PROBLEM

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

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

where $K(\tau,\omega) = \frac{e^{-\tau\omega}}{1-\lambda e^{-\beta\omega}}$ is the kernel, $\lambda = \pm 1$ for bosons/fermions respectively. One may consider to solve the problem by firstly discretize τ and ω and get:

$$G(\tau_i) = \sum_{j=1}^{N_\omega} K_{ij} A(\omega_j) \tag{2}$$

Then do SVD decomposition of rectangular matrix K, write $K_i j = U_{il}\lambda_l V_{lj}$. Finally the spectral function reads

$$A(\omega_j) = \sum_{l=1}^{N_\tau} \frac{1}{\lambda_l} V_{ij} \sum_{i=1}^{N_\omega} G(\tau_i) U_{il} \tag{3}$$

It seems fine at the first glanse. However, if we consider the properties of $K(\tau,\omega)$, we would notice that it is highly sigular since it is exponentially small for large $|\omega|$, so small errors $G(\tau)$ would be amplified by exponentially small λ_l. This problem is well-known ill-posed[3, 4] and enormous efforts have been made[].

II. HOW TO SOLVE?

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Here we introduce the recently developed Nevanlinna analytic continuation method[5].

III. NEVANLINNA ANALYTIC CONTINUATION METHOD

The Nevanlinna analytic continuation method[5] is an interpolation method. The key step is to build the conformal mappings from the open upper half of the complex plane $\mathcal{C}^+$ to a closed unit disk $\bar{\mathcal{D}}$ in the complex plane and make use of the Schur algorithm[6] to do the interpolate.

A. Schur function

Wikipedia: Schur class

A Schur class($\mathcal{S}$) consists of the Schur functions, which are the holomorphic functions from the open unit disk $\mathcal{D}$ to the closed unit disk $\bar{\mathcal{D}}$. Schur[6] studied these functions and found that Schur function $g_0(z)$ can be written as a continued fraction expansion from:

$$g_0(z) = \gamma_0 + \frac{1 - |\gamma_0|^2}{\gamma_0^* + \frac{1}{z\gamma_1 + \frac{z(1-|\gamma_1|^2)}{\gamma_1^* + \frac{1}{z\gamma_2 + \cdots}}}} \tag{4}$$

using the recurrence relation:

$$zg_{j+1}(z) = \frac{g_j(z) - \gamma_j}{1 - \gamma_j^* g_j(z)} \tag{5}$$

where $g_j \in \mathcal{S}$ and $\gamma_j = g_j(0)$ are called Schur parameters and $|\gamma_j| \leq 1$.

B. The Nevanlinna–Pick theorem

Wikipedia: The Nevanlinna–Pick theorem

The Nevanlinna–Pick theorem states the following. Given the initial data consisting of n points $\{\gamma_0, \ldots, \gamma_{n-1}\} \in \mathcal{D}$ and target data $\{z_0, \ldots, z_{n-1}\} \in \mathcal{D}$, there exists a holomorphic function $g(z) : \mathcal{D} \to \bar{\mathcal{D}}$ such that $g(\lambda_j) = z_j$ for all j, if and only if the Pick matrix

$$P_{jk} = \frac{1 - z_k^* z_j}{1 - \lambda_j^* \lambda_k} \tag{6}$$

is positive semi-definite. Furthermore, the function $g(z)$ is unique if and only if the Pick matrix has zero determinant.

C. Interpolation of Green's functions

The retared Green's function $G^R(\omega + i\eta)$ and the Masubara Green's function $G(i\omega_n)$ can be expressed consistently by replacing the variables $i\omega_n$ and $\omega + i\eta$ with a single complex variable z. $G(z)$ is analytic in the upper half plane. Our problem is that once we have Masubara frequencies $\{i\omega_n\} \in \mathcal{C}^+$ and target data $\{G(i\omega_n)\} \in \mathcal{C}$, where $\mathcal{C}$ is the complex plane, how can we get interpolate them and get the holomorphic function $G(z)$?

Based on the knowledge of Schur function, if we can find maps to map the initial data set $\{G(i\omega_n)\}$ from $\mathcal{C}^+$ to $\mathcal{D}^+$ and the target target data $\{G(i\omega_n)\}$ from $\mathcal{C}$ to $\bar{\mathcal{D}^+}$, then we can apply the Schur function. To accomplish this task, we can to make use of the generalized Schur algorithm[7]. It generalize the method from $g(z) \in \mathcal{S}$ to all contractive functions $\theta(z) \in \mathcal{B}$, which are holomorphic functions mapping from $\mathcal{C}^+$ to $\bar{\mathcal{D}}$.

The mapping from $\mathcal{C}^+/\bar{\mathcal{C}}^+$ to $\mathcal{D}^+/\bar{\mathcal{D}}^+$ is called Mobius transform. It has the form:

$$h(z, \mathcal{Y}) = \frac{z - \mathcal{Y}}{z - \mathcal{Y}^*} \tag{7}$$

where $\mathcal{Y} \in \bar{\mathcal{C}}^+$ and $\mathcal{Y} \neq 0$. We can easily prove that $|h(z, \mathcal{Y})| \leq 1$ for $z \in \bar{\mathcal{C}}^+$ and $|h(z, \mathcal{Y})| = 1$ if z is real. $h(z, \mathcal{Y})$ maps $\mathcal{Y} \in \bar{\mathcal{C}}^+$ to the center of the unit disk $\mathcal{D}$ and the real axis as the edge of $\bar{\mathcal{D}}$, the rest part of upper half complex plane is wrapped inside the unit disk. If $\tilde{z} \in \mathcal{D}$, the inverse transform is:

$$h^{-1}(\tilde{z}, \mathcal{Y}) = \frac{\mathcal{Y} - \tilde{z}\mathcal{Y}^*}{1 - \tilde{z}} \tag{8}$$

Angin one can prove $\mathrm{Im}h^{-1}(\tilde{z}, \mathcal{Y}) = (\mathrm{Im}\mathcal{Y})(1 - |\tilde{z}|^2) > 0$.

IV. OLD

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[8]. 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.

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

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

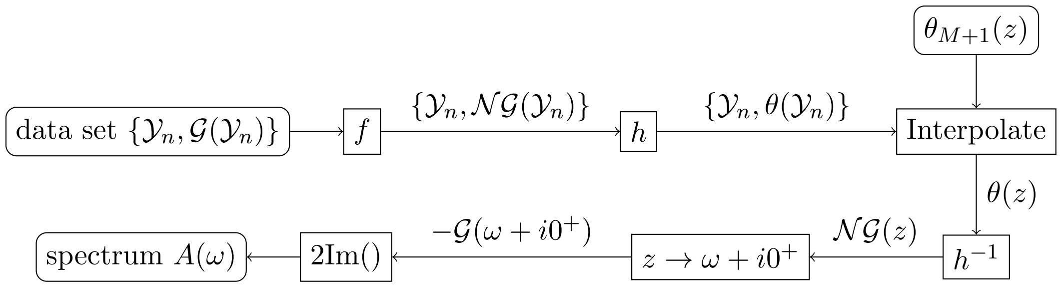

FIG. 2. Calculation flow chart

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 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

$$h(z) = \frac{z - i}{z + i} \tag{9}$$

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:

$$\theta(z)[z; \theta_{M+1}(z)] = \frac{a(z)\theta_{M+1}(z) + b(z)}{c(z)\theta_{M+1}(z) + d(z)} \tag{10}$$

where

$$\begin{pmatrix} a(z) & b(z) \\ c(z) & d(z) \end{pmatrix} = \prod_{n=1}^{M} \begin{pmatrix} h_1(z, \mathcal{Y}_j) & \phi_j \\ \phi_j^* h_1(z, \mathcal{Y}_j) & 1 \end{pmatrix} \tag{11}$$

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.

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