Notes: Nevanlinna analytical Continuation Method

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Abstract

This is the abstract.

CONTENTS

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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. 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

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.

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

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

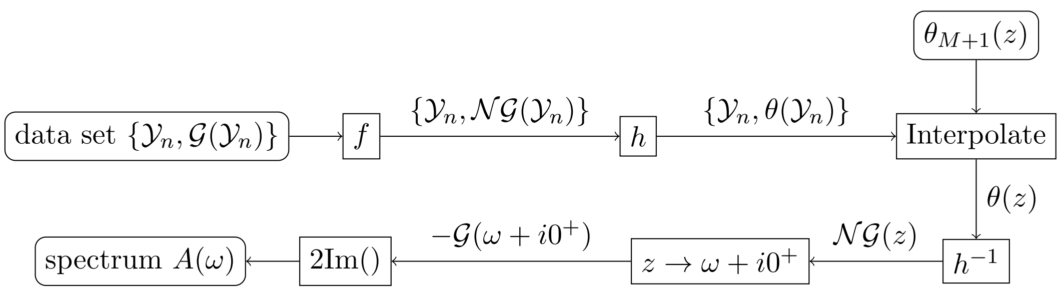

FIG. 2. Calculation flow chart

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

$$h(z) = \frac{z - i}{z + i} \tag{4}$$

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:

$$\theta(z)[z; \theta_{M+1}(z)] = \frac{a(z)\theta_{M+1}(z) + b(z)}{c(z)\theta_{M+1}(z) + d(z)} \tag{5}$$

where

$$\begin{pmatrix} a(z) & b(z) \\ c(z) & d(z) \end{pmatrix} = \prod_{n=1}^{M} \begin{pmatrix} h_1(z, \mathcal{Y}_j) & \phi_j \\ \phi_j^* h_1(z, \mathcal{Y}_j) & 1 \end{pmatrix} \tag{6}$$

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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