Notes: Nevanlinna analytical Continuation Method

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(Dated: November 22, 2021)

Abstract

This is the abstract.

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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, $\lambda = \pm 1$ 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 [6–8] to do the interpolate.

A. Schur Algorithm

Schur Algorithm was introduced by I. Schur[9] in Section 1 of Ref.[6]. Here we list the main results we need while for a detailed introduction, see Ref.[8].

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 $\bar{\mathcal{D}}$. For a given Schur function $s_0(z)$, the Schur algorithm defines a set of $\{s_j(z) \in \mathcal{S}\}_{0\leq j<\infty}$ starting from $s_0(z)$ by the recurrence relation:

$$zs_{j+1}(z) = \frac{s_j(z) - \gamma_j}{1 - \gamma_j^* s_j(z)} \tag{4}$$

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

On the other hand, given an arbitrary strictly contractive sequence of Schur parameters $\{\gamma_0, \gamma_1, \ldots, \gamma_j, \ldots\} \in \mathcal{D}$, one can construct a unique Schur function $s_0(z)$ by means of a continued fraction algorithm. In which we use the inverse relation of eq. (4)

$$s_j(z) = \frac{\gamma_j + zs_{j+1(z)}}{1 + \gamma_j^* z s_j(z)} \tag{5}$$

to construct the n-th Schur approximant, which we will denote by $s_0(z; \gamma_0, \gamma_1, \ldots, \gamma_n)$. Namely, we write:

$$\begin{aligned} &s_n(z;\gamma_n) = \gamma_n \\ &s_j(z;\gamma_j,\gamma_{j+1},\ldots\gamma_n) = \frac{\gamma_j + zs_{j+1}(z;\gamma_{j+1},\ldots\gamma_n)}{1+\gamma_j^* z s_{j+1}(z;\gamma_{k+1},\ldots\gamma_n)} \end{aligned} \tag{6}$$

where $j = n-1, n-2, \ldots, 1, 0$.

The Schur algorithm can used to solve the interpolation problem in $\mathcal{D}$. For given $\{\mathcal{Y}_0, \mathcal{Y}_1, \ldots, \mathcal{Y}_N\} \in \mathcal{D}$ and $\{\gamma_0, \gamma_1, \ldots, \gamma_N\} \in \mathcal{D}$, the Schur function $s: \mathcal{D} \to \mathcal{D}$ and $s(\mathcal{Y}_j) = \gamma_j$ for $j = 0, 1, \ldots, N$ can be easily constructed by combining eq. (6) and the linear fractional transform $f(z, \mathcal{Y}_j) = \frac{z - \mathcal{Y}_j}{1 - z\mathcal{Y}_j^*}$:

$$\begin{aligned} &s_N(z;\gamma_N) = \gamma_N \\ &s_j(z;\gamma_j,\gamma_{j+1},\ldots\gamma_N) = \frac{\gamma_j + f(z,\mathcal{Y}_j)s_{j+1}(z;\gamma_{j+1},\ldots\gamma_N)}{1+\gamma_j^* f(z,\mathcal{Y}_j)s_{j+1}(z;\gamma_{k+1},\ldots\gamma_N)} \end{aligned} \tag{7}$$

where $j = N-1, N-2, \ldots, 1, 0$.

B. Generalized Schur Algorithm

C. The Nevanlinna–Pick theorem

Wikipedia: The Nevanlinna–Pick theorem

The Nevanlinna–Pick theorem states the following. Given the initial data consisting of n points $\{\lambda_0, \ldots, \lambda_{n-1}\} \in \mathcal{D}$ 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

$$P_{jk} = \frac{1 - z_k^* z_j}{1 - \lambda_j^* \lambda_k} \tag{8}$$

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

D. 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[10]. 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 $\bar{\mathcal{D}}$.

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[7]. Then one can apply the Nevanlinna iterative algorithm to interpolate the Schur functions[11]. 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

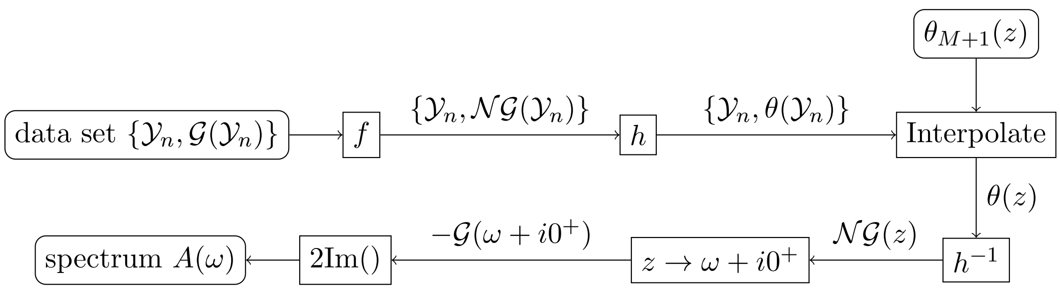

FIG. 2. Calculation flow chart

For fermionic Green's functions, the mapping from $\mathcal{C}^+$ to $\bar{\mathcal{C}}^+$ is simple. Since 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.

Appendix A: Conformal transforms

1. The linear fractional transform

The linear fractional transform is:

$$f(z,\mathcal{Y})=\frac{z-\mathcal{Y}}{1-z\mathcal{Y}^*} \tag{A1}$$

It is a one to one mapping of the open unit disk $\mathcal{D}$ onto itself and a one to one mapping of the unit circle $\mathcal{T}$. It maps point $\mathcal{Y}$ to the center of $\mathcal{D}$.

2. The Mobius transform

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

$$h(z,\mathcal{Y})=\frac{z-\mathcal{Y}}{z-\mathcal{Y}^*} \tag{A2}$$

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:

$$h^{-1}(\tilde{z},\mathcal{Y})=\frac{\mathcal{Y}-\tilde{z}\mathcal{Y}^*}{1-\tilde{z}} \tag{A3}$$

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

Proof of $|h(z,\mathcal{Y})|\leq 1$ for $z\in\bar{\mathcal{C}}^+$ and $|h(z,\mathcal{Y})|=1$ if z is real. We already know that $\mathrm{Im}z\geq 0,\mathrm{Im}\mathcal{Y}>0$.

$$\begin{aligned}|h(z,\mathcal{Y})|^2&=\frac{z-\mathcal{Y}}{z-\mathcal{Y}^*}\frac{z^*-\mathcal{Y}^*}{z^*-\mathcal{Y}}=\frac{|z|^2+|\mathcal{Y}|^2-z\mathcal{Y}^*-z^*\mathcal{Y}}{|z|^2+|\mathcal{Y}|^2-z\mathcal{Y}-z^*\mathcal{Y}^*}\\&=\frac{|z|^2+|\mathcal{Y}|^2-2(\mathrm{Re}z\mathrm{Re}\mathcal{Y}+\mathrm{Im}z\mathrm{Im}\mathcal{Y})}{|z|^2+|\mathcal{Y}|^2-2(\mathrm{Re}z\mathrm{Re}\mathcal{Y}-\mathrm{Im}z\mathrm{Im}\mathcal{Y})}\end{aligned} \tag{A4}$$

If Im$z = 0$, $|h(z, \mathcal{Y})|^2 = 1$. If Im$z > 0$, $|h(z, \mathcal{Y})|^2 < 1$. And we notice that if Im$\mathcal{Y} = 0$, we map all points in $\bar{\mathcal{C}}$ to point 1 except for point $\mathcal{Y}$ itself.

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