

Notes: Nevanlinna analytical Continuation Method

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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 nontrivial task[1]. To see this, we use the relation between $G(\tau)$ and $A(\omega)$ [1, 2]:

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

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:

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

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

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

It seems fine at the first glance. However, if we consider the properties of $K(\tau, \omega)$, we would notice that it is highly singular 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:

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

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 $\{\gamma_0, \gamma_1, \dots, \gamma_j, \dots\} \in \mathcal{D}$, 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)

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

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

$$s_n(z; \gamma_n) = \gamma_n \quad (6)$$

$$s_j(z; \gamma_j, \gamma_{j+1}, \dots, \gamma_n) = \frac{\gamma_j + zs_{j+1}(z; \gamma_{j+1}, \dots, \gamma_n)}{1 + \gamma_j^* zs_{j+1}(z; \gamma_{j+1}, \dots, \gamma_n)} \quad (7)$$

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

Given the initial data consisting of N points $\{\mathcal{Y}_0, \mathcal{Y}_1, \dots, \mathcal{Y}_{N-1}\} \in \mathcal{D}$ and target data $\{\gamma_0, \gamma_1, \dots, \gamma_{N-1}\} \in \mathcal{D}$, we can find a holomorphic function $s(z) : \mathcal{D} \rightarrow \bar{\mathcal{D}}$ such that $s(\mathcal{Y}_j) = \gamma_j$ for all j by combining eq. (6), eq. (7) and the linear fractional transform $\xi(z, \mathcal{Y}_j) = \frac{z - \mathcal{Y}_j}{1 - z\mathcal{Y}_j^*}$:

$$s_{N-1}(z; \gamma_{N-1}) = \frac{\gamma_{N-1} + \xi(z, \mathcal{Y}_{N-1})s_N(z)}{1 + \gamma_{N-1}^* \xi(z, \mathcal{Y}_{N-1})s_N(z)} \quad (8)$$

$$s_j(z; \gamma_j, \gamma_{j+1}, \dots, \gamma_N) = \frac{\gamma_j + \xi(z, \mathcal{Y}_j)s_{j+1}(z; \gamma_{j+1}, \dots, \gamma_N)}{1 + \gamma_j^* \xi(z, \mathcal{Y}_j)s_{j+1}(z; \gamma_{j+1}, \dots, \gamma_N)} \quad (9)$$

where $j = N-2, N-3, \dots, 1, 0$ and $s_0(z) \equiv s(z)$. In eq. (8), we notice that there is an degrees of freedom to choose an arbitrary $s_N(z) \in \mathcal{S}$, eq. (6) correponds the special case $s_{n+1}(z) = 0$.

G. Pick and R. Nevanlinna studied the interpolation problem independently in 1917[10] and 1919[11] respectively, showing that an interpolating function exists if and only if the Pick matrix

$$P_{jk} = \frac{1 - \gamma_k^* \gamma_j}{1 - \mathcal{Y}_j^* \mathcal{Y}_k} \quad (10)$$

is positive semi-definite. Furthermore, the function $s(z)$ is unique if and only if the Pick matrix has zero determinant. It is called the [the Nevanlinna–Pick theorem](#).

B. Generalized Schur Algorithm

Schur algorithm can be modified to expand all contractive functions($\in \mathcal{B}$)[12], which are holomorphic functions mapping from the upper half plane \mathcal{C}^+ to $\bar{\mathcal{D}}$.

Given the initial data consisting of N points $\{\mathcal{Y}_0, \mathcal{Y}_1, \dots, \mathcal{Y}_{N-1}\} \in \mathcal{C}^+$ and target data $\{\gamma_0, \gamma_1, \dots, \gamma_{N-1}\} \in \bar{\mathcal{D}}$, in order to find a holomorphic function $\theta(z) \in \mathcal{B}$ such that $\theta(\mathcal{Y}_j) = \gamma_j$ for all j , we should make use of the Mobius transform $h(z, \mathcal{Y}) = \frac{z - \mathcal{Y}}{z - \mathcal{Y}^*}$ which maps $\mathcal{C}^+/\bar{\mathcal{C}}^+$ to $\mathcal{D}/\bar{\mathcal{D}}$, which means it establishes a one-to-one correspondence of $\theta(z)$ to a schur function $s(z)$ with:

$$\theta(h^{-1}(z, \mathcal{Y})) = s(z), \text{ or } s(h(z, \mathcal{Y})) = \theta(z) \quad (11)$$

We denote $h(z, \mathcal{Y}_j)$ as $h_j(z)$ form now on.

The recursion relation between $\theta_j(z)$ and the next contractive function $\theta_{j+1}(z)$ can be easily build as follows. From eq. (11), we have:

$$s_j(0) = \theta_j(h_j^{-1}(0)) = \theta_j(\mathcal{Y}_j) = \gamma_j \quad (12)$$

Let $\theta_{j+1}(z) = s_{j+1}(h_j(z))$, then use the recursion relation eq. (4), we have:

$$z\theta_{j+1}(h_j^{-1}(z)) = \frac{\theta_j(h_j^{-1}(z)) - \gamma_j}{1 - \gamma_j^* \theta_j(h_j^{-1}(z))} \stackrel{\text{def}}{=} \phi_j(h_j^{-1}(z)) \quad (13)$$

Form the first and the third terms of eq. (13) we have:

$$\phi_j(h_j^{-1}(z)) = z\theta_{j+1}(h_j^{-1}(z)) = h(h_j^{-1}(z), \mathcal{Y}_j)\theta_{j+1}(h_j^{-1}(z)) \quad (14)$$

replace $h_j^{-1}(z)$ with $z \in \mathcal{D}$ by $z \in \mathcal{C}^+$, we have

$$\phi_j(z) = h_j(z)\theta_{j+1}(z) \quad (15)$$

We can read from eq. (15) that $\phi(z) \in \mathcal{B}$ and $\phi_j(\mathcal{Y}_j) = 0$.

Form the second and the third terms of eq. (13) we can read:

$$\phi_j(z) = \frac{\theta_j(z) - \gamma_j}{1 - \gamma_j^* \theta_j(z)} \quad (16)$$

Together with eq. (15) we get the recursion relation between $\theta_j(z)$ and $\theta_{j+1}(z)$:

$$\theta_j(z) = \frac{\phi_j(z) + \gamma_j}{1 + \gamma_j^* \phi_j(z)} = \frac{h_j(z)\theta_{j+1}(z) + \gamma_j}{1 + \gamma_j^* h_j(z)\theta_{j+1}(z)} \quad (17)$$

The recursive final $\theta(z)$ can conveniently be written in a matrix form:

$$\theta(z)[z; \theta_N(z)] = \frac{a(z)\theta_N(z) + b(z)}{c(z)\theta_N(z) + d(z)} \quad (18)$$

where

$$\begin{pmatrix} a(z) & b(z) \\ c(z) & d(z) \end{pmatrix} = \prod_{j=1}^{N-1} \begin{pmatrix} h_j(z) & \gamma_j \\ \gamma_j^* h_j(z) & 1 \end{pmatrix} \quad (19)$$

Like in eq. (6), there is a also freedom to choose $\theta_N(z)$. One can use this freedom to select the “best” of all consistent functions.

C. Interpolation of Green’s functions

The retarded 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[12]. 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 recursively 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 $z \rightarrow \omega + i0^+$. The calculation process is shown in fig. 2.

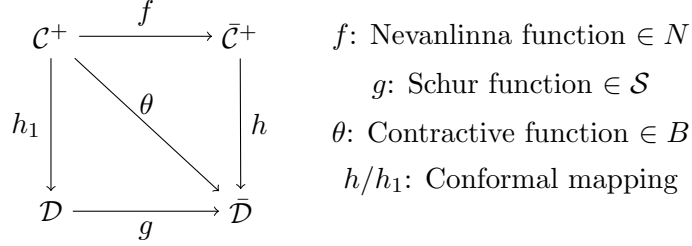


FIG. 1. Conformal mappings

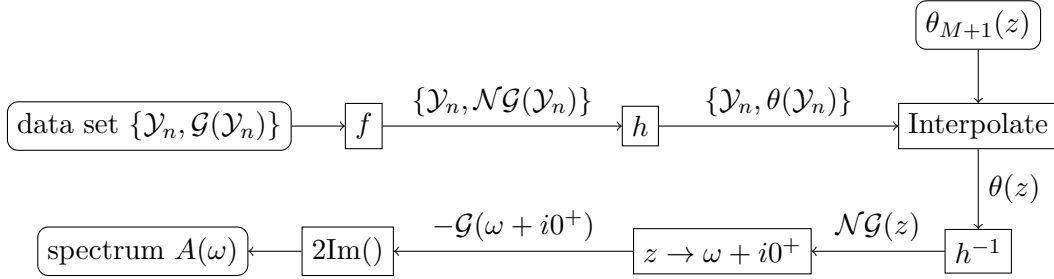


FIG. 2. Calculation flow chart

For fermionic Green's functions, the mapping from \mathcal{C}^+ to $\bar{\mathcal{C}}^+$ is simple. Since $\text{Im}\mathcal{G}(z) \leq 0$ if $z \in \mathcal{C}^+$, the mapping is just to take $\mathcal{G} \rightarrow -\mathcal{G} = \mathcal{N}\mathcal{G}$ 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 $\mathcal{C}_n = \mathcal{N}\mathcal{G}(i\omega_n) = -\mathcal{G}(i\omega_n)$.

Appendix A: Conformal transforms

1. The linear fractional transform

The linear fractional transform is:

$$\xi(z, \mathcal{Y}) = \frac{z - \mathcal{Y}}{1 - z\mathcal{Y}^*} \quad (\text{A1})$$

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:

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

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:

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

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

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 $\text{Im}z \geq 0, \text{Im}\mathcal{Y} > 0$.

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

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

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

- [4] Ingo Peschel, Xiaoqun Wang, Matthias Kaulke, and Karen Hallberg. *Density-Matrix Renormalization-a New Numerical Method in Physics: Lectures of a Seminar and Workshop Held at the max-planck-institut für physik komplexer systeme, Dresden, Germany, August 24th to September 18th, 1998*. Springer, 1999.
- [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*, 1917(147):205–232, 1917.
- [7] 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.
- [8] Harry Dym and Victor Katsnelson. Contributions of issai schur to analysis. *PROGRESS IN MATHEMATICS-BOSTON-*, 210:xci–xcj, 2003.
- [9] Schur published under the name of both I. Schur, and J. Schur, the latter especially in *Journal für die reine und angewandte Mathematik*. This has led to some confusion. See:[Issai Schur](#).
- [10] Georg Pick. Über die beschränkungen analytischer funktionen durch vorgegebene funktionenwerte. *Mathematische Annalen*, 78(1):270–275, 1917.
- [11] Rolf Nevanlinna. Über beschränkte funktionen, die in gegebenen punkten vorgeschriebene werte annehmen. *Ann. Acad. Sci. Fenn. Ser. A 1 Mat. Dissertationes*, 1919.
- [12] Vadym M Adamyan, J Alcober, and IM Tkachenko. Reconstruction of distributions by their moments and local constraints. *Applied Mathematics Research eXpress*, 2003(2):33–70, 2003.