

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 $C(\tau)$ data. Technically, this is a highly nontrivial task[1]. To see this, we use the relation between $C(\tau)$ and $A(\omega)$ [1, 2]:

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

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:

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

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

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

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 $C(\tau)$ 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 $\{\gamma_0, \gamma_1, \dots, \gamma_j, \dots\} \subset \mathcal{D}$, 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)

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

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 $\{\mathcal{Y}_0, \mathcal{Y}_1, \dots, \mathcal{Y}_{N-1}\} \subset \mathcal{D}$ and target data $\{\mathcal{C}_0, \mathcal{C}_1, \dots, \mathcal{C}_{N-1}\} \subset \mathcal{D}$, we can find a holomorphic function $s(z) : \mathcal{D} \rightarrow \bar{\mathcal{D}}$ such that $s(\mathcal{Y}_j) = \mathcal{C}_j$ for all j by combining eq. (6), eq. (7) and the linear fractional transform:

$$\xi(z, \mathcal{Y}_j) = \frac{z - \mathcal{Y}_j}{1 - z\mathcal{Y}_j^*} \quad (8)$$

and $s(z)$ has the following recursion relation:

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

where $\gamma_j = s_j(\mathcal{Y}_j)$.

Proof. eq. (8) builds a one to one correspondence of a Schur function $s(z)$ with another Schur function $\tilde{s}(z)$.

$$\tilde{s}(\xi^{-1}(z, \mathcal{Y})) = s(z), \text{ or } s(\xi(z, \mathcal{Y})) = \tilde{s}(z) \quad (10)$$

From eq. (10), we have:

$$\gamma_j = s_j(0) = \tilde{s}_j(\xi^{-1}(0, \mathcal{Y})) = \tilde{s}_j(\mathcal{Y}_j) \quad (11)$$

inserting eq. (10) and eq. (11) to eq. (5), we have:

$$\tilde{s}_j(\xi^{-1}(z, \mathcal{Y}_j)) = \frac{\gamma_j + z\tilde{s}_{j+1}(\xi^{-1}(z, \mathcal{Y}_j))}{1 + \gamma_j^* z \tilde{s}_{j+1}(\xi^{-1}(z, \mathcal{Y}_j))} \quad (12)$$

replace $\xi^{-1}(z, \mathcal{Y}_j) \in \mathcal{D}$ by $\tilde{z} \in D$, we have:

$$\tilde{s}_j(\tilde{z}) = \frac{\gamma_j + \xi(\tilde{z}, \mathcal{Y}_j)\tilde{s}_{j+1}(\tilde{z})}{1 + \gamma_j^* \xi(\tilde{z}, \mathcal{Y}_j)\tilde{s}_{j+1}(\tilde{z})} \quad (13)$$

□

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

$$s(z)[z, s_{N+1}(z)] = \frac{a_N(z)s_{N+1}(z) + b_N(z)}{c_N(z)s_{N+1}(z) + d_N(z)} \quad (14)$$

where

$$\begin{pmatrix} a_N(z) & b_N(z) \\ c_N(z) & d_N(z) \end{pmatrix} = \prod_{j=1}^N \begin{pmatrix} \xi(z, \mathcal{Y}_j) & \gamma_j \\ \gamma_j^* \xi(z, \mathcal{Y}_j) & 1 \end{pmatrix} \quad (15)$$

with j increasing from left to right. There is a freedom to choose $s_{N+1}(z)$. The inverse relation of is

$$s_N(z) = \frac{c_N(z)s_1(z) - a_N(z)}{-d_N(z)s_1(z) + b_N(z)} \quad (16)$$

where we define $s(z) \equiv s_1(z)$.

Now we discuss a little more about the calculation of γ_j . The first step of the recursion gives:

$$s(z) \equiv s_1(z) = \frac{\xi(z, \mathcal{Y}_1)s_2(z) + \gamma_1}{\gamma_1^* \xi(z, \mathcal{Y}_1)s_2(z) + 1} \quad (17)$$

$\therefore \gamma_1 = s_1(\mathcal{Y}_1) = \mathcal{C}_1$. and

$$s_2(z) = \frac{\gamma_1^* \xi(z, \mathcal{Y}_1)s_1(z) - \xi(z, \mathcal{Y}_1)}{-s_1(z) + \gamma_1} \quad (18)$$

$$\therefore \gamma_2 = s_2(\mathcal{Y}_2) = \frac{\gamma_1^* \xi(\mathcal{Y}_2, \mathcal{Y}_1)s_1(\mathcal{Y}_2) - \xi(\mathcal{Y}_2, \mathcal{Y}_1)}{-s_1(\mathcal{Y}_2) + \gamma_1} = \frac{\mathcal{C}_1^* \xi(\mathcal{Y}_2, \mathcal{Y}_1)\mathcal{C}_2 - \xi(\mathcal{Y}_2, \mathcal{Y}_1)}{-\mathcal{C}_2 + \mathcal{C}_1}.$$

For the j -th ($j \geq 3$) step of the recursion:

$$s_1(z) = \frac{a_j(z)s_{j+1}(z) + b_j(z)}{c_j(z)s_{j+1}(z) + d_j(z)} \quad (19)$$

where

$$\begin{pmatrix} a_j(z) & b_j(z) \\ c_j(z) & d_j(z) \end{pmatrix} = \prod_{k=1}^j \begin{pmatrix} \xi(z, \mathcal{Y}_k) & \gamma_k \\ \gamma_k^* \xi(z, \mathcal{Y}_k) & 1 \end{pmatrix} \quad (20)$$

and γ_k as well as $\begin{pmatrix} a_j(z) & b_j(z) \\ c_j(z) & d_j(z) \end{pmatrix}$ are calculated in previous steps. Then γ_{j+1} reads:

$$\begin{aligned} \gamma_{j+1} = s_{j+1}(\mathcal{Y}_{j+1}) &= \frac{c_j(\mathcal{Y}_{j+1})s_1(\mathcal{Y}_{j+1}) - a_N(\mathcal{Y}_{j+1})}{-d_j(\mathcal{Y}_{j+1})s_1(\mathcal{Y}_{j+1}) + b_j(\mathcal{Y}_{j+1})} \\ &= \frac{c_j(\mathcal{Y}_{j+1})\mathcal{C}_{j+1} - a_N(\mathcal{Y}_{j+1})}{-d_j(\mathcal{Y}_{j+1})\mathcal{C}_{j+1} + b_j(\mathcal{Y}_{j+1})} \end{aligned} \quad (21)$$

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

$$P_{jk} = \frac{1 - \mathcal{C}_k^* \mathcal{C}_j}{1 - \mathcal{Y}_j^* \mathcal{Y}_k} \quad (22)$$

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 $\{\mathcal{Y}_0, \mathcal{Y}_1, \dots, \mathcal{Y}_{N-1}\} \subset \mathcal{C}^+$ and target data $\{\mathcal{C}_0, \mathcal{C}_1, \dots, \mathcal{C}_{N-1}\} \subset \bar{\mathcal{D}}$, in order to find a holomorphic function $\theta(z) \in \mathcal{B}$ such that $\theta(\mathcal{Y}_j) = \mathcal{C}_j$ 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:

$$\theta(h^{-1}(z, \mathcal{Y})) = s(z), \text{ or } s(h(z, \mathcal{Y})) = \theta(z) \quad (23)$$

We denote $h(z, \mathcal{Y}_j)$ as $h_j(z)$ from 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. (23), we have:

$$\gamma_j = s_j(0) = \theta_j(h_j^{-1}(0)) = \theta_j(\mathcal{Y}_j) = \gamma_j \quad (24)$$

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

$$z\theta_{j+1}(h_j^{-1}(z)) = \frac{\theta_j(h_j^{-1}(z)) - \gamma_j}{1 - \gamma_j^* \theta_j(h_j^{-1}(z))} \stackrel{\text{def}}{=} \phi_j(h_j^{-1}(z)) \quad (25)$$

Form the first and the third terms of eq. (25) we have:

$$\phi_j(h_j^{-1}(z)) = z\theta_{j+1}(h_j^{-1}(z)) = h_j(h_j^{-1}(z))\theta_{j+1}(h_j^{-1}(z)) \quad (26)$$

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

$$\phi_j(z) = h_j(z)\theta_{j+1}(z) \quad (27)$$

We can read from eq. (27) that $\phi_j(z) \in \mathcal{B}$ and $\phi_j(\mathcal{Y}_j) = 0$.

Form the second and the third terms of eq. (25) we can read:

$$\phi_j(z) = \frac{\theta_j(z) - \gamma_j}{1 - \gamma_j^* \theta_j(z)} \quad (28)$$

Together with eq. (27) we get the recursion relation between $\theta_j(z)$ and $\theta_{j+1}(z)$:

$$\theta_j(z) = \frac{\phi_j(z) + \gamma_j}{\gamma_j^* \phi_j(z) + 1} = \frac{h_j(z)\theta_{j+1}(z) + \gamma_j}{\gamma_j^* h_j(z)\theta_{j+1}(z) + 1} \quad (29)$$

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

$$\theta(z)[z; \theta_N(z)] = \frac{a(z)\theta_N(z) + b(z)}{c(z)\theta_N(z) + d(z)} \quad (30)$$

where

$$\begin{pmatrix} a(z) & b(z) \\ c(z) & d(z) \end{pmatrix} = \prod_{j=1}^{N-1} \begin{pmatrix} h_j(z) & \gamma_j \\ \gamma_j^* h_j(z) & 1 \end{pmatrix} \quad (31)$$

with j increasing from left to right. Like in eq. (6), there is a also freedom to choose $\theta_N(z)$.

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 \mathcal{C}^+ . Our problem is that once we have Masubara frequencies $\{i\omega_n\} \subset \mathcal{C}^+$ and target data $\{G(i\omega_n)\} \subset \mathcal{C}$, where \mathcal{C} is the complex plane, how can we get interpolate them and get the holomorphic function $G(z) : \mathcal{C}^+ \rightarrow \mathcal{C}$?

Based on the knowledge of Schur algorithm, if we can find a one-to-one correspondence of $G(z)$ and a contractive function $\theta(z) \in \mathcal{B}$, then we can futher generalize the algorithm in section III B.

To do this, we firstly introduce the Nevanlinna functions $f(z) \in \mathcal{N}$. In complex analysis, a Nevanlinna function is a complex function that is analytic in the open upper half plane \mathcal{C}^+ and has non-negative imaginary part, i.e., maps into $\bar{\mathcal{C}}^+$ (the overline denotes inclusion of the boundary). The invertible Möbius transform $h(z) = \frac{z-i}{z+i}$ maps Nevanlinna functions one to one to contractive functions:

$$\theta(z) = h(f(z)), \text{ or } f(z) = h^{-1}(\theta(z)) \quad (32)$$

Given the initial data consisting of N points $\{\mathcal{Y}_0, \mathcal{Y}_1, \dots, \mathcal{Y}_{N-1}\} \subset \mathcal{C}^+$ and target data $\{C_0, C_1, \dots, C_{N-1}\} \subset \bar{\mathcal{C}}$, The only thing we needed is to let γ_j in eq. (29) be $\gamma_j \equiv h(C_j)$.

Moreover, the corresponding Pick matrix is generalized to:

$$P_{jk} = \frac{1 - h(C_k)^* h(C_j)}{1 - h(\mathcal{Y}_j)^* h(\mathcal{Y}_k)} \quad (33)$$

The aforementioned conformaling mappings are shown in fig. 1.

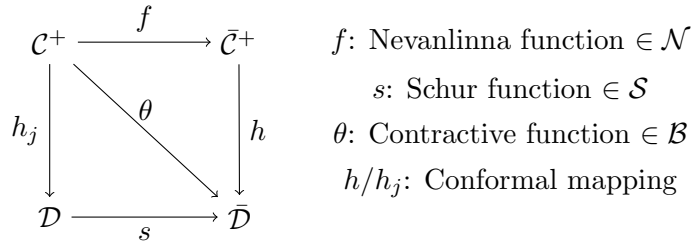


FIG. 1. Conformal mappings

Now we are ready to discuss the Green's functions. The Lehmann representation of Green's function $G(z)$ is:

$$G(z) = \frac{1}{Z} \sum_{nm} |A_{nm}|^2 \frac{e^{-\beta E_n} \pm e^{-\beta E_m}}{z - E_m + E_n} \quad (34)$$

where the "+" sign is for fermionic Green's functions and "-" sign is for bosonic Green's functions.

1. Fermionic case

In fermionic case, if we take $z = x + iy$ with $y > 0$, i.e. $z \in \mathcal{C}^+$, we can easily prove that $\text{Im}G(z) \leq 0$. Therefore $-G(z) \in \mathcal{N}$ is a Nevanlinna function.

Proof.

$$\text{Im}G(x + iy) = -\frac{1}{Z} \sum_{nm} \frac{\mathcal{Q}_{nm}^F y}{(x - E_m + E_n)^2 + y^2} \quad (35)$$

where

$$\mathcal{Q}_{nm}^F = |A_{nm}|^2 (e^{-\beta E_m} + e^{-\beta E_n}) \geq 0 \quad (36)$$

$\therefore \text{Im}G(x + iy) \leq 0$ for $y > 0$. \square

2. Bosonic case

The bosonic case is less trivial. The imaginary part of bosonic Green's function is:

$$\text{Im}G(x + iy) = -\frac{1}{Z} \sum_{nm} \frac{\mathcal{Q}_{nm}^B y}{(x - E_m + E_n)^2 + y^2} \quad (37)$$

where

$$\mathcal{Q}_{nm}^B = |A_{nm}|^2 (e^{-\beta E_m} - e^{-\beta E_n}) = \text{Sgn}(E_m - E_n) |\mathcal{Q}_{nm}^B| \quad (38)$$

$\text{Im}G(x + iy)$ doesn't have a definite sign.

However, we can prove that $\tilde{G}(z) = -zG(z)$ is a Nevanlinna function.

Proof.

$$\begin{aligned} \text{Im}\tilde{G}(x + iy) &= -\text{Im}[(x + iy)G(x + iy)] \\ &= -x\text{Im}G(x + iy) - y\text{Re}G(x + iy) \end{aligned} \quad (39)$$

where:

$$\text{Re}G(z) = \frac{1}{Z} \sum_{nm} \frac{\mathcal{Q}_{nm}^B (x - E_m + E_n)}{(x - E_m + E_n)^2 + y^2} \quad (40)$$

For given (n, m) -term:

$$\begin{aligned} \tilde{\mathcal{Q}}_{nm}^B &= xy\mathcal{Q}_{nm}^B - (x - E_m + E_n)y\mathcal{Q}_{nm}^B \\ &= y(E_m - E_n)\mathcal{Q}_{nm}^B \\ &= y|E_m - E_n||\mathcal{Q}_{nm}^B| \end{aligned} \quad (41)$$

$\therefore \tilde{Q}_{nm}^B \geq 0$ for $y > 0$.

$$\therefore \operatorname{Im} \tilde{G}(x + iy) = \frac{1}{Z} \sum_{nm} \frac{\tilde{Q}_{nm}^B}{(x - E_m + E_n)^2 + y^2} \geq 0 \quad (42)$$

and $\tilde{G}(z)$ is a Nevanlinna function. \square

Moreover, $-i\omega_n G(i\omega_n)$ is the Fourier transform of $\frac{dG(\tau)}{d\tau}$.

We can perform analytical continuation $z = \omega + i\eta$ on $\tilde{G}(z)$:

$$\begin{aligned} 2\operatorname{Im} \tilde{G}(\omega + i\eta) &= \omega[-2\operatorname{Im} G(\omega + i\eta)] - 2\eta \operatorname{Re} G(\omega + i\eta) \\ &\xrightarrow{\eta \rightarrow 0^+} \omega A(\omega) \end{aligned} \quad (43)$$

where $A(\omega)$ is the spectral function.

IV. HARDY BASIS OPTIMIZATION

Appendix A: Conformal transforms

1. The linear fractional transform

The linear fractional transform is:

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

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:

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

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:

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

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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