Pade approximation

We represent the Green's function with the following continuous fraction expansion

$$G(z) = \cfrac{a_1}{1 + \cfrac{a_2(z-z_1)}{1+\cfrac{a_3(z-z_2)}{1+\cdots \cfrac{a_{n-1}(z-z_{n-2})}{1+a_n(z-z_{n-1})}}}} \tag{1}$$

For large n, this representation becomes exact.

To build this continuous fraction, we first write $G(z)$ in the rational form

$$G(z) = \frac{A_n(z)}{B_n(z)} \tag{2}$$

and we compute polynomials A_n and B_n with the following recursion relation

$$A_{i+1}(z) = A_i(z) + (z - z_i)a_{i+1}A_{i-1}(z) \tag{3}$$

$$B_{i+1}(z) = B_i(z) + (z - z_i)a_{i+1}B_{i-1}(z) \tag{4}$$

and starting conditions

$$A_0 = 0 \tag{5}$$

$$A_1 = a_1 \tag{6}$$

$$B_0 = 1 \tag{7}$$

$$B_1 = 1 \tag{8}$$

We will check the few lowest orders of this continuous fraction/recursion. At the lowest order, we have

$$\frac{A_1}{B_1} = a_1 \tag{9}$$

We use the recursion relation to get A_2 and B_2:

$$A_2 = a_1 \tag{10}$$

$$B_2 = 1 + (z - z_1)a_2 \tag{11}$$

which gives

$$\frac{A_2}{B_2} = \frac{a_1}{1 + a_2(z - z_1)} \tag{12}$$

In the next order, we get

$$A_3 = a_1 + (z - z_2)a_3a_1 \tag{13}$$

$$B_3 = 1 + (z - z_1)a_2 + (z - z_2)a_3 \tag{14}$$

which gives

$$\frac{A_3}{B_3} = \frac{a_1(1 + (z - z_2)a_3)}{1 + (z - z_2)a_3 + (z - z_1)a_2} = \frac{a_1}{1 + \frac{a_2(z-z_1)}{1+a_3(z-z_2)}} \tag{15}$$

In the next order, we have

$$A_4 = a_1(1 + a_3(z - z_2)) + (z - z_3)a_4a_1 = a_1(1 + a_3(z - z_2) + a_4(z - z_3))$$

$$B_4 = 1 + (z - z_1)a_2 + (z - z_2)a_3 + (z - z_3)a_4(1 + (z - z_1)a_2) = 1 + a_3(z - z_2) + a_4(z - z_3) + a_2(z - z_1)(1 + a_4(z - z_3))$$

which gives

$$\frac{A_4}{B_4} = \frac{a_1(1 + a_3(z - z_2) + a_4(z - z_3))}{1 + a_3(z - z_2) + a_4(z - z_3) + a_2(z - z_1)(1 + a_4(z - z_3))} = \tag{16}$$

$$\frac{a_1}{1 + \frac{a_2(z-z_1)(1+a_4(z-z_3))}{1+a_3(z-z_2)+a_4(z-z_3)}} = \frac{a_1}{1 + \frac{a_2(z-z_1)}{1+\frac{a_3(z-z_2)}{1+a_4(z-z_3)}}} \tag{17}$$

Clearly, the recursion relation can be used to get A_n and B_n for an arbitrary order n.

To represent G with the continuous fraction expansion, we need to compute coefficients a_i from the value of G at some set of points z_i in the complex plane (such as the Matsubara points).

We first notice that

$$G(z_1) = a_1 \tag{18}$$

$$G(z_2) = \frac{a_1}{1 + a_2(z_2 - z_1)} \tag{19}$$

$$G(z_3) = \frac{a_1}{1 + \frac{a_2(z_3-z_1)}{1+a_3(z_3-z_2)}} \tag{20}$$

and in general $G(z_m) = \frac{A_m(z_m)}{B_m(z_m)}$

We can use the first equation to compute a_1, the second to compute a_2, etc. At order m we can get all a_m. There exists a recursion relation to compute all coefficients very efficiently. We define a matrix $P(i,j)$, which has the following properties

$$P(1,i) \equiv G(z_i) \tag{21}$$

$$P(i,j) = \frac{P(i-1,i-1) - P(i-1,j)}{(z_j - z_{i-1})P(i-1,j)} \tag{22}$$

We will next show that $P(i,i)$ is

$$P(i,i) = a_i \tag{23}$$

We start with the first order $P(1,1) = a_1$. In the second order we have

$$P(1,2) = G(z_2) = \frac{a_1}{1 + a_2(z_2 - z_1)} \tag{24}$$

hence

$$a_2 = \frac{a_1 - G(z_2)}{(z_2 - z_1)G(z_2)} = \frac{P(1,1) - P(1,2)}{(z_2 - z_1)P(1,2)} \tag{25}$$

which is clearly compatible with the above recursion relation.

Next, we compute $P(2,3)$ and $P(3,3)$ with the recursion relation, and we will check that $P(3,3) = a_3$. We have

$$P(2,3) = \frac{P(1,1) - P(1,3)}{(z_3 - z_1)P(1,3)} = \frac{a_1 - G(z_3)}{(z_3 - z_1)G(z_3)} \tag{26}$$

Next we express $P(3,3)$ with recursion relation

$$a_3 = P(3,3) = \frac{P(2,2) - P(2,3)}{(z_3 - z_2)P(2,3)} = \frac{a_2 - \frac{a_1-G(z_3)}{(z_3-z_1)G(z_3)}}{(z_3 - z_2)\frac{a_1-G(z_3)}{(z_3-z_1)G(z_3)}} \tag{27}$$

which is equivalent to

$$1 + a_3(z_3 - z_2) = \frac{a_2}{\frac{a_1-G(z_3)}{(z_3-z_1)G(z_3)}} \tag{28}$$

or

$$\frac{a_2(z_3 - z_1)}{1 + a_3(z_3 - z_2)} = \frac{a_1}{G(z_3)} - 1 \tag{29}$$

or

$$\frac{a_1}{1 + \frac{a_2(z_3 - z_1)}{1 + a_3(z_3 - z_2)}} = G(z_3) \tag{30}$$

hence $P(3,3)$ is indeed a_3.