Supplemental material to the article Complex singularities of fluid velocity autocorrelation function

Methods.

A. Pade-approximation: numerical multipont continued fraction algorithm. Here we discuss the construction of the Padé-approximants that interpolate a function given N knot points. Pade-approximants are the rational functions (ratio of two polinomials). A rational function can be represented by a continued fraction. Typically the continued fraction expansion for a given function approximates the function better than its series expansion.

Algorithm: for a function $f(x_i) = u_i$ with values u_i at N knots x_i , $i = 1, 2, 3, \ldots, N$, the Pade-approximant is

$$C_N(x) = \frac{a_1}{\frac{a_2(x-x_1)}{\frac{a_3(x-x_2)}{\frac{a_4(x-x_3)}{\dots a_N(x-x_{N-1})+1}+1} + 1}},$$
(1)

where a_i we determine using the condition, $C_N(x_i) = u_i$, which is fulfilled if a_i satisfy the recursion relation

$$a_i = g_i(x_i), \quad g_1(x_i) = u_i, \quad i = 1, 2, 3, \dots, N.$$
 (2)

$$g_p(x) = \frac{g_{p-1}(x_{p-1}) - g_{p-1}(x)}{(x - x_{p-1}) g_{p-1}(x)}, \quad p \ge 2.$$
(3)

B. Pade-approximation: illustrating test-examples. 1. Oscillator power spectrum amplitude: approximation of the analytical function with 4 poles. As the first test example we take the function

$$f_{\rm OSC}(\omega) = \frac{1}{(\omega^2 - \omega_0^2)^2 + (\omega\gamma)^2}.$$
 (4)

This function is proportional to the oscillator power spectrum. We take $\omega = 3$ and $\gamma = 2$ and build the Pade-approximant using 300 uniformly distributed knots at $\omega \in (-10, 10)$. The result of the analytical continuation is show in Fig. 1. We

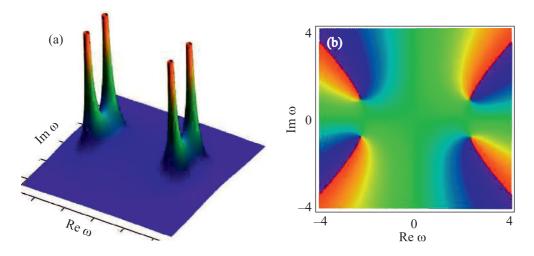


Figure 1: Analytical continuation of oscillator power spectrum from the real axis to the complex plain by multipoint Pade-approximant: panel a shows the absolute value while and panel b is the argument

worked with double precision. The relative error of the analytical approximation was less than 10^{-10} even in the pole-regions.

2. Stability of the Pade-approximation. We add gaussian noise with zero mean and $\sigma = 5 \cdot 10^{-4}$ to the oscillator power spectrum considered above, see Fig. 2. Analytical continuation is shown in panels b and c. The "main" poles are still clearly seen. So analytical continuation by Pade-approximation is quite resistive to noise if the noise correlation length is short enough.

3. Analytical continuation of *ln*-function by the Pade Approximant. Now we illustrate how behaves singular function in the complex plain when we do its Pade analytical continuation. We take

$$f_{\ln}(\omega) = \ln(1+\omega). \tag{5}$$

We build the Pade-approximant using 300 uniformly distributed knots at real $\omega \in (0, 50)$. The result of the analytical continuation is shown in Fig. 3. There is cut $(-\infty, -1)$ in the complex ω -plain. Analytical continuation based on the Pade-approximant reproduces the cut by the array of poles and knots (where $f_{\ln} = 0$), see Fig. 3. Away from the cut the accuracy of the analytical continuation is satisfactory as in the upper illustrating example while $|\omega| < 50$.

4. Analytical continuation by the Pade-approximant of the function with the

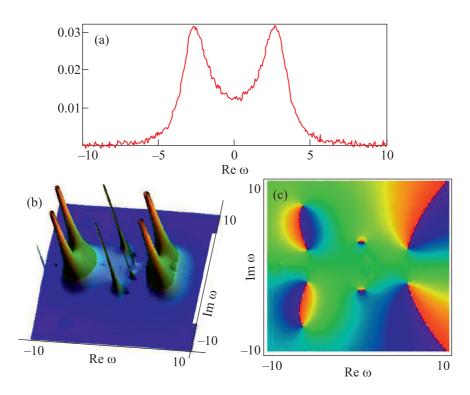


Figure 2: (a) – We add gaussian noise with zero mean and $\sigma = 5 \cdot 10^{-4}$ to the oscillator power spectrum. Analytical continuation is shown in panel b and c. The "main" poles show high degree of resistivity to noise

square root singularity. Finally we take the function with the square root singularity to test the Pade-approximation:

$$f_{\rm sqr}(\omega) = \sqrt{\omega - i}.$$
 (6)

We build the Pade-approximant using 300 uniformly distributed knots at real $\omega \in (-10, 10)$. Then we analytically continue the Pade polinomial (it is in fact complex even at real ω) to the complex ω -plain as shown in Figs. 4a and b. Array of peaks and dips in Fig. 4a represent the branch cut: this is typical for Pade-approximation. Graphs c and d show "exact" absolute value and argument of the function. The branch cut parallel to the real axis is typical choice for "computer" build in functions (we have used Mathcad). Pade-approximation have chosen different direction for the branch cut, parallel to the imaginary axis, see panels a and b. Fig. 4e is the density plot of the absolute value of the difference between the exact and Pade-approximation $|f_{\rm ln} - f_{\rm ln}^{({\rm pade})}|/(|f_{\rm ln}| - |f_{\rm ln}^{({\rm pade})}|)$. The coincidence

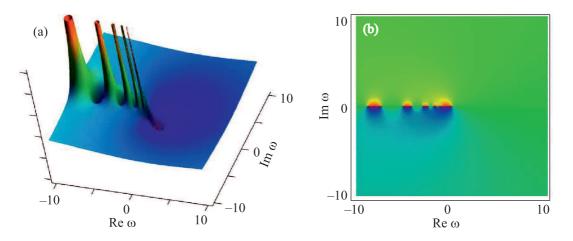


Figure 3: Analytical continuation of the logarithm: panel a shows the absolute value while and panel b is the argument

is perfect everywhere except the white zone where the functions differ because the branch cuts of the Pade-approximation and the "exact function" are different.

C. Limits of applicability of Pade-approximation. As follows from the examples, if we approximate a function by the Pade-polinomial at certain domain at the real axis then the analytical continuation is more or less perfect at the circle in the complex plain (around that domain) with the radius about the length of the domain.

The branch cuts are represented by an array of poles. There is a problem with the branch cuts: we can draw them differently in the complex plain, only edges are fixed. Different choice of the branch cut curve corresponds different analytical continuation. But the Pade-polynomial chooses the cut curve somehow "automatically": we do not well control that. So the Pade-approximation is a useful tool if one needs to identify the position and types of the singularities of the function in the complex plain like poles and the branch cut edges. For functions without branches analytical continuation in unique and the Pade-approximation well produces it.

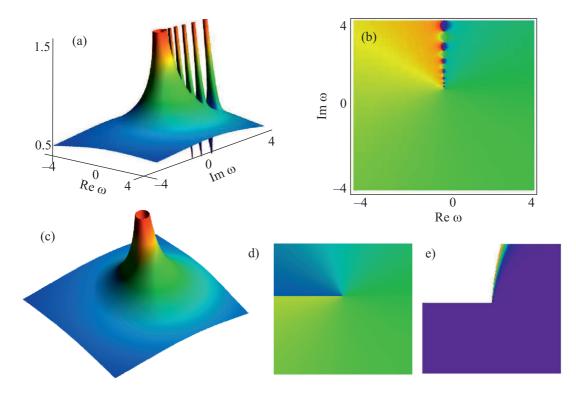


Figure 4: Analytical continuation of the square root function: panel a shows the absolute value while and panel b is the argument. Array of peaks and dips in panel a represent the branch cut. Graphs panels c and d show "exact" absolute value and argument of the function. Fig.e is the density plot of the relative difference between the exact and Pade-approximation. The coincidence is perfect everywhere except the white zone where the functions differ because the branch cuts of the approximation and the "exact function" have been chosen differently