

Summary : Quantum dynamics for a fractal spectrum : Thouless coefficient - Thouless formula - quantum dynamics for a Fibonacci potential and for a Cantor spectrum in the tight-binding model

We note K the triadic Cantor set, embedded in $[0, 1]$, and $d\mu$ the associated measure. $d\mu$ verifies :

$$\int_k f(x) d\mu(x) = \frac{1}{2} \int_k f\left(\frac{x}{3}\right) d\mu(x) + \frac{1}{2} \int_k f\left(\frac{x+2}{3}\right) d\mu(x) \quad (1)$$

Return probability

cf. correlation-fun-cantor.pdf

Thouless coefficient

Thouless formula

Fibonacci potential in the tight-binding model

Quantum dynamics for a triadic Cantor set spectrum in the tight-binding model

We consider an infinite 1D lattice, with sites k labelled from 0 to ∞ . We define a potential V on this system such that the discrete Schrodinger operator : $H = -\Delta + V$, which acts on $l_2(\mathbb{Z})$, has a triadic Cantor set spectrum. As in the previous paragraph, the eigenfunctions $\{\phi_\epsilon\}_{\epsilon \in K}$, evaluated on the sites k , can be seen as polynomials in ϵ :

$$\phi_\epsilon(k) = p_k(\epsilon) \quad (2)$$

We are interested of the evolution of a wave packet, described by the normalized wave function $\psi(t)$, evolving according to Schrodinger's equation :

$$i \frac{d\psi(t)}{dt} = H\psi(t)$$

The wave function is initially localized at the site 1 : $\langle k | \psi(t=0) \rangle = \delta(k-1)$. At time t , the system is in the state : $|\psi(t)\rangle = e^{-iHt} |\psi(0)\rangle$, and the value of the wave function at site k is given by :

$$|\psi(k, t)| = \int_K \phi_\epsilon(1)^* \phi_\epsilon(k) e^{-i\epsilon t} d\mu$$

Using (2), we obtain :

$$\psi(k, t) = \int_K \phi_\epsilon(1)^* \phi_\epsilon(k) e^{-i\epsilon t} d\mu \quad (3)$$

$$= \int_K p_1(\epsilon) p_k(\epsilon) e^{-i\epsilon t} d\mu \quad (4)$$

$$= \sum_{j_k \leq k} c_{j_k} \int_K e^{j_k} e^{-i\epsilon t} d\mu \quad (5)$$

with $p_k(x) = \sum_{0 \leq j_k \leq k} c_{j_k} x^{j_k}$. Thus, the dynamical behaviour of the system depends essentially on the functions :

$$h_k(t) = \int_K e^{-i\epsilon t} \epsilon^k d\mu(\epsilon)$$

aka the Fourier transforms on K of the moments x^k .

Study of $h_k(t)$

Using the Mellin transform (see annexe), we may express $h_k(t)$ as a series :

$$h_k(t) = \sum_{n \neq 0} \frac{(-it)^n}{n!} \mu_{n+k}$$

with $\mu_n = \int_K x^n d\mu$. (Note that we obtain the same expression by writing $e^{-i\epsilon t} = \sum_{n \leq 0} \frac{(-i\epsilon t)^n}{n!}$ and reversing the signs sum and integral).

It is not clear, from this expression, whether or not $h_k(t)$ has a log-periodic feature, which is expected as a fingerprint of the scaling symmetry of the spectrum expressed in (1). We shall now show that there is, however, such a behaviour. We will do so by calculating the zeroes of $h_k(t)$ and the maxima of $|h_k(t)|$.

First note that $h_0(t)$ verifies the following functional equation, derived by direct application of (1) :

$$\begin{aligned} h_0(t) &= \int_K e^{-i\epsilon t} d\mu \\ &= \frac{1}{2} \int_K e^{-i\epsilon t/3} d\mu + \frac{e^{-i2t/3}}{2} \int_K e^{-i\epsilon t/3} d\mu \\ &= \frac{1 + e^{-i2t/3}}{2} h_0(t/3) \end{aligned}$$

By repeating this process, and using $h_0(0) = \int_K 1 d\mu = 1$, we find the exact expression of $h_0(t)$:

$$h_0(t) = \prod_{k \geq 1} \frac{1 + e^{-i2t/3^k}}{2} \quad (6)$$

This is consistent with the expression derived in [1]. Furthermore, there is a perfect fit between the graph of the theoretical expression (2) and the one obtained from the direct calculation of $h_0(t)$ using :

$$h_0(t) = \lim_{n \rightarrow \infty} \left(\frac{3}{2}\right)^n \sum_{a_{j_n} \in K_n} \int_{a_{j_n}}^{a_{j_n} + 3^{-n}} e^{-ixt} dx$$

with K_n the set of the left edges of the remaining segments after n iterations in the construction of the Cantor set from the segment $[0, 1]$.

From (2), we easily deduce the zeroes of $h_0(t)$: it is the set :

$$Z_0 = \left\{ t_m = \frac{3\pi}{2}(2m + 1), m \in \mathbb{Z} \right\}$$

We also get the local maxima of $|h_0(t)|$:

$$M_0 = \{v_{n,m} = \pi m 3^n, m \in \mathbb{Z}, n \in \mathbb{N}^*\}$$

with the property :

$$h_0(v_{n,m}) = \prod_{k \geq n+1} \frac{1 + e^{-i2t/3} \overbrace{k}^{k'} - n}{2} = \prod_{k' \geq 1} \frac{1 + e^{-i2t/3^{k'}}}{2} = h_0(v_{0,m})$$

Furthermore, the product $\prod_{k' \geq 1} \frac{1 + e^{-i2t/3^{k'}}}{2}$ is convergent and consists of nonzero terms, therefore it is nonzero. Taking $n \rightarrow \infty$, we can therefore deduce that $h_0(t)$ does not converge to zero when $t \rightarrow \infty$ (as also found in [1]).

Now, using (1) again, we derive the following recurrence formula for $h_k(t)$:

$$\begin{aligned} h_k(t) &= \int_K e^{-ict} \epsilon^k d\mu \\ &= \frac{3^{-k}}{2} \int_K e^{-ict/3} \epsilon^k d\mu + \frac{3^{-k} e^{-i2t/3}}{2} \int_K e^{-ict/3} (\epsilon + 2)^k d\mu \\ &= \frac{3^{-k}}{2} h_k(t/3) + \frac{3^{-k}}{2} e^{-i2t/3} \sum_{j=0}^k \binom{k}{j} h_j(t/3) 2^{k-j} \end{aligned}$$

We will use this relation to show, by recurrence, that the set Z_k of zeroes of h_k , $k \neq 0$ contains the set :

$$\{t_{m,n} = \frac{\pi}{2}(2m+1)3^{k+1}, m \in \mathbb{Z}\}$$

First, we deduce that, if $t_{n,m} = \frac{\pi}{2}(2m+1)3^2$, $m \in \mathbb{Z}$, then :

$$h_1(t_{n,m}) = \frac{3^{-1}}{2} h_1(t_{n,m}/3) - \frac{3^{-1}}{2} (h_1(t_{n,m}/3) + \underbrace{h_0(t_{n,m}/3)}_0)$$

since $t_{n,m}/3 \in Z_0$. Thus : $\{t_{m,n} = \frac{\pi}{2}(2m+1)3^2, m \in \mathbb{Z}\} \subset Z_1$. The generalization to higher k is trivially derived using the recurrence relation above.

It seems that there are no other zeroes for $h_k(t)$, e.g. that

$$Z_k = \{t_{m,n} = \frac{\pi}{2}(2m+1)3^{k+1}, m \in \mathbb{Z}\}$$

but it is not rigorously proven ; the numerics however seem to support this hypothesis (see fig. 1).

We therefore deduce that $h_k(t)$ has the same zeroes than $h_{k-1}(t/3)$.

Using a similar reasoning, we can study the points at which the module $|h_k(t)|$ has a local maximum. The maxima of $|h_0(t)|$ are reached at the points : $t_{m,n} = 3^n m \pi$. Using the recurrence relation between the h_k , one can see that

$$h_k(t_{m,n}) \approx 3^{-k} h_0(t_{m,n-1})$$

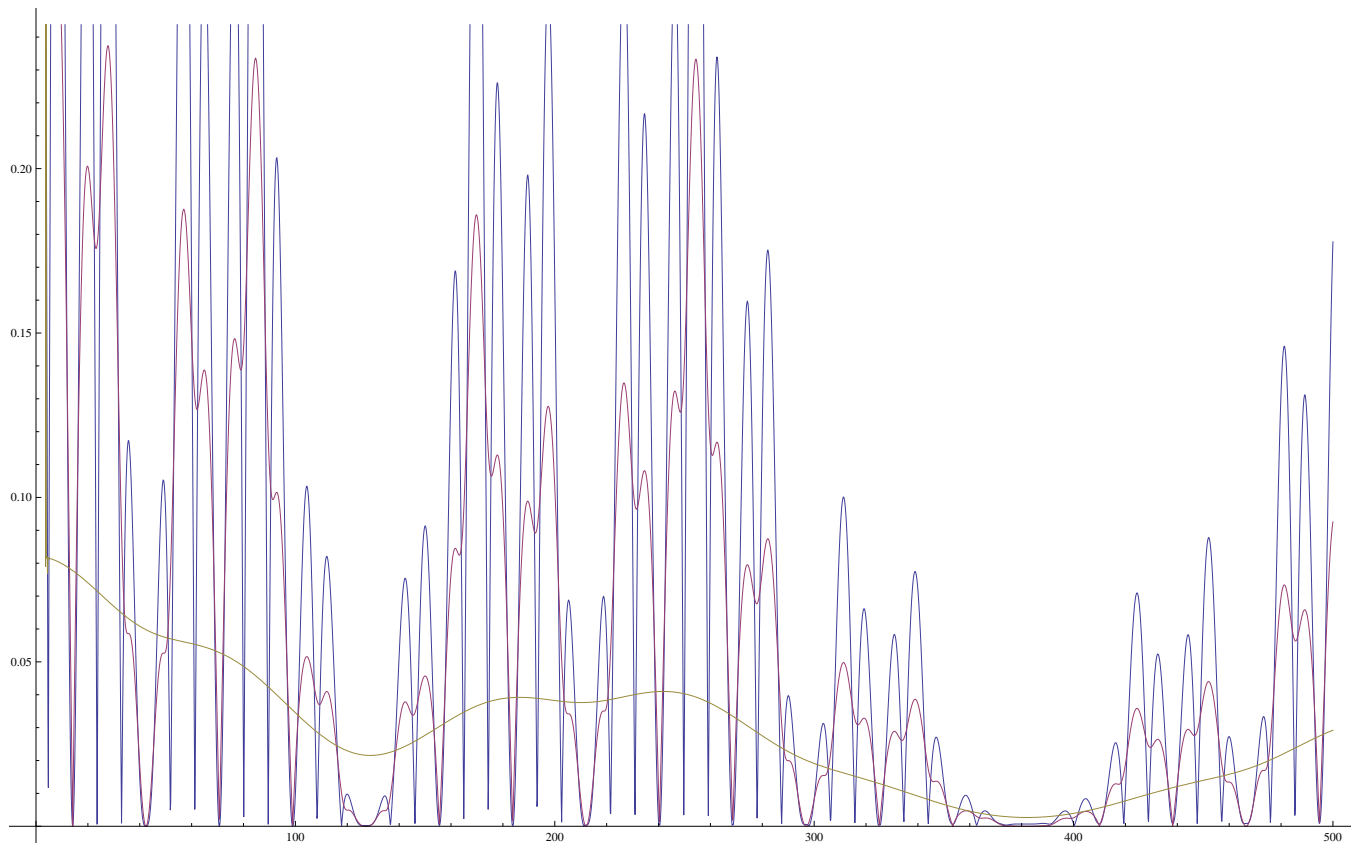


FIGURE 1 – Numerical curves of $|h_0(t)|$ (blue), $|h_1(t)|$ (red) and $|h_{31}(t)|$ (yellow).

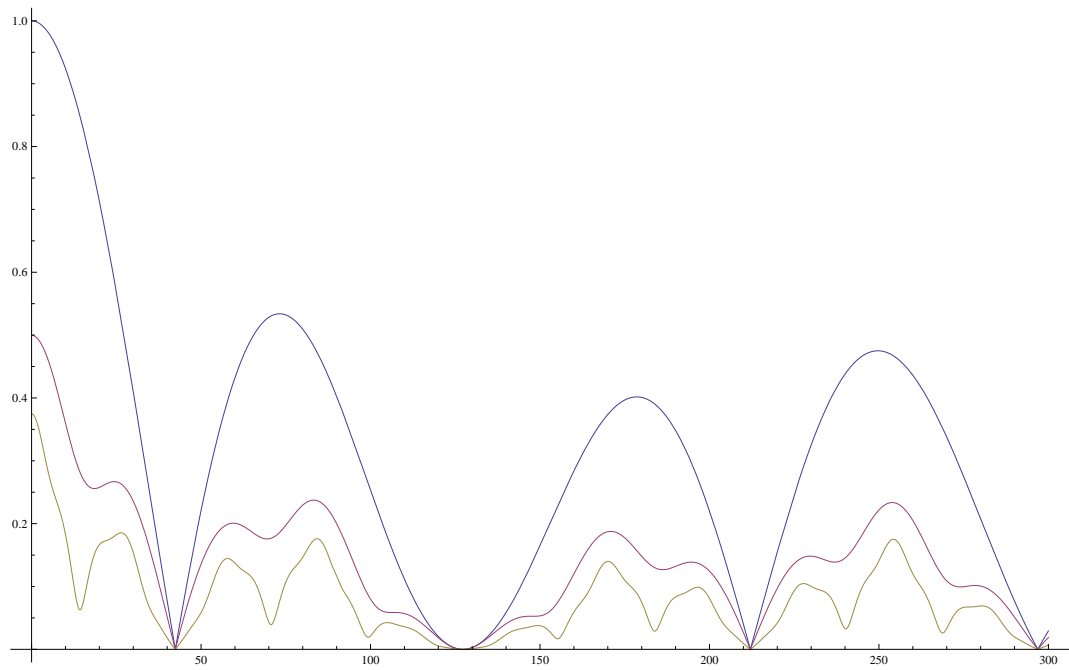


FIGURE 2 – Numerical curves of $|h_0(t/9)|$ (blue), $|h_1(t/3)|$ (red) and $|h_2(t)|$ (yellow).

Thus, we may infer, with a good approximation, that :

$$h_k(t) \propto h_{k-1}(t/3)$$

This is confirmed by the numerics (see fig. 2).

To summarize, the functions $h_k(t)$ themselves are not log-periodic, and have periodically spaced zeroes of the form $t_{m,n} = \frac{\pi}{2}(2m+1)3^n$. The fingerprint of the fractal spectrum lies in the recurrence relation :

$$h_k(t) = \frac{3^{-k}}{2} h_k(t/3) + \frac{3^{-k}}{2} e^{-i2t/3} \sum_{j=0}^k \binom{k}{j} h_j(t/3) 2^{k-j}$$

which, up to a good approximation, can be simplified into :

$$h_k(t) \propto h_{k-1}(t/3)$$

Note however that it is not a rigorous proportionality relation.

Application to the RMS and the participation ratio

In order to study how the fractal feature of the spectrum affects the dynamics of the system, we will now consider the RMS :

$$\Delta x(t)^2 = \sum_{k=1}^{\infty} k^2 |\psi(k, t)|^2$$

and the participation ratio :

$$P_\psi = \frac{1}{\int_{\text{espace}} |\langle x|\psi \rangle|^4 dx}$$

Injecting (3) in the definition of the RMS, we obtain :

$$\begin{aligned} \Delta x(t) &= \sum_{k=1}^{\infty} k^2 |\psi(k, t)|^2 \\ &= \sum_{k=1}^{\infty} k^2 \left| \sum_{j_k \leq k} c_{j_k} \int_K e^{j_k} e^{-iet} d\mu \right|^2 \\ &= \sum_{k=1}^{\infty} k^2 \left| \sum_{j_k \leq k} c_{j_k} h_{j_k}(t) \right|^2 \end{aligned}$$

Note that, even if the $h_k(t)$ have periodically spaced zeroes, this does not imply that $\Delta x(t)$ cancels for some t : in fact, since the zeroes of h_k are odd multiples of 3^{k+1} , the infinite sum in the expression of Δx insures that, for any time t , we are always before the first zero of infinitely many h_k .

Using $h_k(t) \propto h_{k-1}(t/3)$, we obtain in first approximation :

$$\Delta x(t) \propto \Delta x(t/3)$$

which leads to :

$$\Delta x(t) = t^\alpha G(\ln t)$$

with G periodic.

We can make a more precise calculation by using directly the recurrence relation $h_k(t) = \frac{3^{-k}}{2} h_k(t/3) + \frac{3^{-k}}{2} e^{-i2t/3} \sum_{j=0}^k \binom{k}{j} h_j(t/3) 2^{k-j}$:

$$\begin{aligned} \Delta x(t) &= \sum_{k=1}^{\infty} k^2 \left| \sum_{j_k \leq k} c_{j_k} h_{j_k}(t) \right|^2 \\ &= \sum_{k=1}^{\infty} k^2 \left| \sum_{j_k \leq k} c_{j_k} \frac{3^{-j_k}}{2} h_{j_k}(t/3) + \frac{3^{-j_k}}{2} e^{-i2t/3} \sum_{l=0}^{j_k} \binom{j_k}{l} h_l(t/3) 2^{j_k-l} \right|^2 \\ &\approx \frac{1}{b} \Delta x(t/3) + R(t) \end{aligned}$$

where b can be approximated numerically (there does not seem to be a simple theoretical value for b) and $R(t)$ is a sum of terms of the form $k^2 h_j(t)^* h_{j'}(t)$.

A similar reasoning seems to indicate that the participation ratio also has a log-periodic feature, however the calculation is more complicated and I have not yet finished it.

Study of the Green function

Knowing explicitly the eigenfunctions $\phi_\epsilon(k) = p_k(\epsilon)$ allows us to study the static and time dependent Green functions of the system. In fact, the Green functions can be expressed in terms of the functions $h_k(t)$ and the moments $\mu_k = \int_K x^k d\mu$.

The time dependent Green function, defined as $G(k, k', t) = \langle k | e^{-iHt} | k' \rangle$, is a linear combination of the $h_k(t)$:

$$\begin{aligned} G(k, k', t) &= \langle k | e^{-iHt} | k' \rangle \\ &= \int_K e^{-i\epsilon t} \phi_\epsilon(k)^* \phi_\epsilon(k') d\mu(\epsilon) \\ &= \int_K e^{-i\epsilon t} p_k(\epsilon)^* p_{k'}(\epsilon) d\mu(\epsilon) \\ &= \int_K e^{-i\epsilon t} \sum_{j_k \leq k} \sum_{j'_k \leq k'} c_{j_k} c_{j'_k} e^{j_k + j'_k} d\mu(\epsilon) \\ &= \sum_{j_k \leq k} \sum_{j'_k \leq k'} h_{j_k + j'_k}(t) \end{aligned}$$

The stationary Green function, aka the Fourier transform of the propagator,

defined by $G(k, k', \epsilon) = \int_0^\infty dt G(k, k', t) e^{i\epsilon t}$, is given by :

$$\begin{aligned}
G(k, k', \epsilon) &= \int_0^\infty dt G(k, k', t) e^{i\epsilon t} \\
&= \int_K \frac{\phi_\epsilon(k)^* \phi_\epsilon(k')}{\epsilon - \epsilon'} d\mu(\epsilon') \\
&= \int_K \frac{p_k(\epsilon)^* p_{k'}(\epsilon)}{\epsilon - \epsilon'} d\mu(\epsilon') \\
&= \sum_{j_k \leq k} \sum_{j'_k \leq k'} c_{j_k} c_{j'_k} \int_K \frac{\epsilon^{j_k + j'_k}}{\epsilon - \epsilon'} d\mu(\epsilon')
\end{aligned}$$

For $\epsilon = 0$, we get :

$$\begin{aligned}
G(k, k', 0) &= \sum_{j_k \leq k} \sum_{j'_k \leq k'} c_{j_k} c_{j'_k} \int_K \frac{\epsilon^{j_k + j'_k}}{\epsilon'} d\mu(\epsilon') \\
&= \sum_{j_k \leq k} \sum_{j'_k \leq k'} c_{j_k} c_{j'_k} \mu_{j_k + j'_k}
\end{aligned}$$

It can be shown (see [2]) that :

$$\mu_n \approx n^{-\ln 2 / \ln 3} F(\ln n / \ln 3) (1 + O(\frac{1}{n}))$$

with F periodic of period one. Therefore :

$$G(k, k', 0) \approx \sum_{j_k \leq k} \sum_{j'_k \leq k'} c_{j_k} c_{j'_k} (j_k + j'_k)^{-\ln 2 / \ln 3} F(\ln(j_k + j'_k) / \ln 3)$$

Annexe

Calculation of the $h_k(t)$

We derive the expression of the functions $h_k(t) = \int_K e^{-ixt} \epsilon^k d\mu(-)$, $k \in \mathbb{N}$ using Mellin's transform.

The Mellin transform of h_k is :

$$\begin{aligned}
m_k(s) &= \int_0^\infty t^{s-1} h_k(t) dt \\
&= \int_K d\mu(x) x^k \int_0^\infty t^{s-1} e^{-ixt} dt \\
&= \Gamma(s) e^{-i\pi s/2} \underbrace{\int_K d\mu(x) x^{k-s}}_{l_k(s)}
\end{aligned}$$

where Γ is Euler's gamma function. The integral converges on the strip $0 < \Re(s) < 1/2$ but the final expression can be analytically extended on all \mathbb{C} , except on the countable set of poles we shall now determine. Applying (1) :

$$\begin{aligned}
l_k(s) &= \int_K d\mu(x) x^{k-s} \\
&= \frac{1}{2} \int_K d\mu(x) \frac{x^{k-s}}{3^{k-s}} + \frac{1}{2} \int_K d\mu(x) \frac{(x+2)^{k-s}}{3^{k-s}} \\
&= \frac{3^{s-k}}{2} l_k(s) + r_k(s)
\end{aligned}$$

which leads to :

$$l_k(s) = \frac{r_k(s)}{1 - 3^{s-k}/2}$$

r_k has no poles because $x+2$ is never null for $x \in K$. l_k has poles at the points : $s_{m,k} = k + \frac{\ln 2}{\ln 3} + \frac{2i\pi m}{\ln 3}$. Since $\Gamma(z)$ has poles at the negative integers $-n$, $n \in \mathbb{N}$, with residue $Res(\Gamma)_{z=-n} = \frac{(-1)^n}{n!}$, we conclude that $m_k(s)$ has poles at the points :

$$\{s_{m,k} = k + \frac{\ln 2}{\ln 3} + \frac{2i\pi m}{\ln 3}, m \in \mathbb{Z}\} \cup \mathbb{Z}^-$$

We now apply Mellin's inverse formula :

$$h_k(t) = \frac{1}{2i\pi} \int_{c-i\infty}^{c+i\infty} m_k(s) t^{-s} ds$$

with $0 < c < 1/2$ to insure the convergence of the integral. We apply the residue formula on a contour defined as the limit for $r \rightarrow \infty$ of the semicircle of figure 3. The asymptotic behaviour of the Γ function insures that the integral on the circular part goes to zero as $r \rightarrow \infty$.

Therefore, the zeroes of the Γ function alone are taken into account in the residue formula, which yields :

$$h_k(t) = \sum_{n \neq 0} \frac{(-it)^n}{n!} \mu_{n+k}$$

with $\mu_n = \int_K x^n d\mu$

References

- [1] E. HILLE and J. D. TAMARKIN, The American Mathematical Monthly, Vol. 36, No. 5 (May, 1929), pp. 255-264
- [2] P.J. Grabner , H. Prodinger, Statistics Probability Letters 26 (1996) 243-248

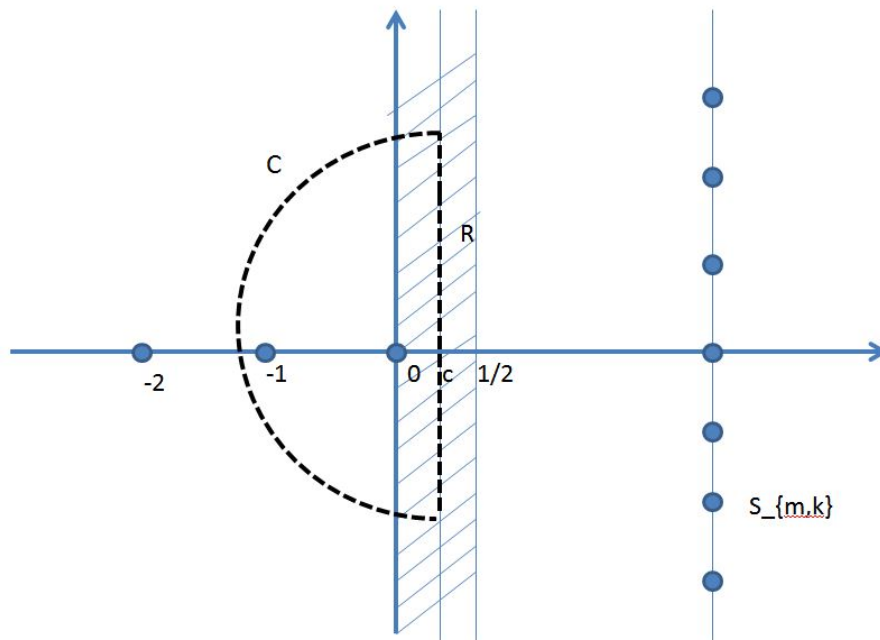


FIGURE 3 – Contour used in the residue formula.