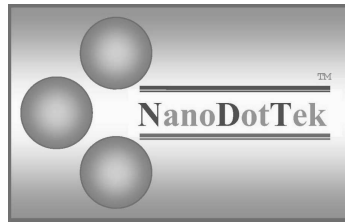


The Atomic Function $up(t)$: Nucleus, Shell and Parity

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1. Introduction

This report considers a particular example of a class of functions called *atomic functions* which are solutions to *differential-dilation equations* originally considered by Hilberg [1], and independently by Rvachev and Rvachev [2]. More recent generalizations of this earlier work can be found for example in Rvachev [3]. The class of atomic functions is perhaps best seen by viewing the scientific and engineering literature of Eastern Europe, but is largely unknown in the literature of the West. However, a few important exceptions to this statement are Cooklev, Berbecel and Venetsanopoulos [4], Derfel, Dyn and Levin [5], and also Shen [6].¹ The goal of this report is therefore to introduce the simplest, and best studied example of an atomic function most commonly denoted by $up(t)$, but also denoted by $\phi(t)$ [4]. We shall mainly stick with the notation $\phi(t)$ in this report.

This report also introduces what may be a novel series approximation to the Laplace transform of $up(t)$. In the process this transform is “picked apart” into two factors here called the *nucleus*, and the *shell*. This language seems in keeping with the terminology “atomic function.” Aside from the nucleus, and the shell the concept of the *parity* of a non-negative integer is also important. This concept is defined in Section 4, but here we simply note that the parity of integers determines the series coefficients for the nucleus of the atomic function.

The notions of nucleus, shell and parity do not seem to appear in the existing literature on atomic functions, or differential-dilation equations. As these notions are applied here only to $up(t)$, and not to other atomic functions it is not immediately obvious to what extent such ideas will have an impact (if any) on the larger theory of atomic functions, or of differential-dilation equations.

2. A Differential-Dilation Equation

Following [4] we consider the differential-dilation equation in the atomic function $\phi(t)$ (i.e., $up(t)$) which is

$$\frac{1}{2} \frac{d\phi(t)}{dt} = \phi(2t + 1) - \phi(2t - 1) \quad (2.1)$$

A closed-form solution to (2.1) is not possible. We must work with various products, and series. In fact, the Fourier transform of this equation yields

$$j\omega \Phi(\omega) = (e^{j\omega/2} - e^{-j\omega/2}) \Phi(\omega/2) \quad (j = \sqrt{-1}) \quad (2.2)$$

where $\Phi(\omega) = \int_{-\infty}^{\infty} \phi(t) e^{-j\omega t} dt$ is the Fourier transform of $\phi(t)$. With the normalization $\Phi(0) = 1$ Equation (2.2) yields

$$\Phi(\omega) = \prod_{k=1}^{\infty} \frac{\sin(\omega/2^k)}{\omega/2^k} \quad (2.3)$$

¹This report does not claim to be a complete survey of all available literature on atomic functions, or of differential-dilation equations.

It can be shown that $\phi(t)$ is nonzero only for $t \in [-1, 1]$ (i.e., has support only on a finite interval). An expression for this atomic function is

$$\phi(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \left\{ \prod_{k=1}^{\infty} \text{sinc}(\omega/2^k) \right\} e^{j\omega t} d\omega \quad (2.4)$$

(inverse Fourier transform (IFT) of $\Phi(\omega)$), where $\text{sinc } x = \sin x/x$. Of course, this is really not a practical means to “compute” the atomic function. A more practical scheme suggested in Kravchenko and Basarab [7] is the following. It derives from the elementary application of complex Fourier series expansions such as are introduced in Zarowski [8].

If $f(t)$ is T -periodic then it has the complex Fourier series expansion

$$f(t) = \sum_{n=-\infty}^{\infty} f_n \exp\left(j\frac{2\pi}{T}nt\right), \quad \text{where } f_n = \frac{1}{T} \int_{-T/2}^{T/2} f(t) e^{-j\frac{2\pi}{T}nt} dt \quad (2.5)$$

Since $\phi(t)$ is supported only on $[-1, 1]$ we may periodically extend this function over the entire time-axis t . In this case we may use (2.5) to write that ($T = 2$ here)

$$\begin{aligned} \phi(t) &= \sum_{n=-\infty}^{\infty} \phi_n e^{j\pi n t}, \quad \text{where } \phi_n = \frac{1}{2} \int_{-1}^{+1} \phi(t) e^{-j\pi n t} dt \\ &= \frac{1}{2} \int_{-\infty}^{\infty} \phi(t) e^{-j\omega t} dt \Big|_{\omega = \pi n} = \frac{1}{2} \Phi(\pi n) \end{aligned} \quad (2.6)$$

To work with this series we need the Fourier transform (2.3). Fortunately, not too many factors need to be kept to obtain good approximations to $\Phi(\pi n)$. As it is apparent (from (2.3)) that $\Phi(-\omega) = \Phi(\omega)$, and recalling that $\Phi(0) = 1$ we see that

$$\phi(t) = \frac{1}{2} \sum_{n=-\infty}^{\infty} \Phi(\pi n) e^{j\pi n t} = \frac{1}{2} + \sum_{k=1}^{\infty} \Phi(\pi k) \cos(\pi k t) \quad (2.7)$$

To obtain this we have made use of identity $\cos \theta = \frac{1}{2}(e^{j\theta} + e^{-j\theta})$. A computable approximation to the atomic function merely involves truncating (2.7)

$$\phi(t) \approx \frac{1}{2} + \sum_{k=1}^N \Phi(\pi k) \cos(\pi k t) \quad (2.8)$$

In practice N need not be large (e.g., $N = 10$). A plot of $up(t) = \phi(t)$ appears in Fig. 1.

Using Equation (2.8) to plot $\phi(t)$ is not the only method. Another possible approach will be noted in Section 4.

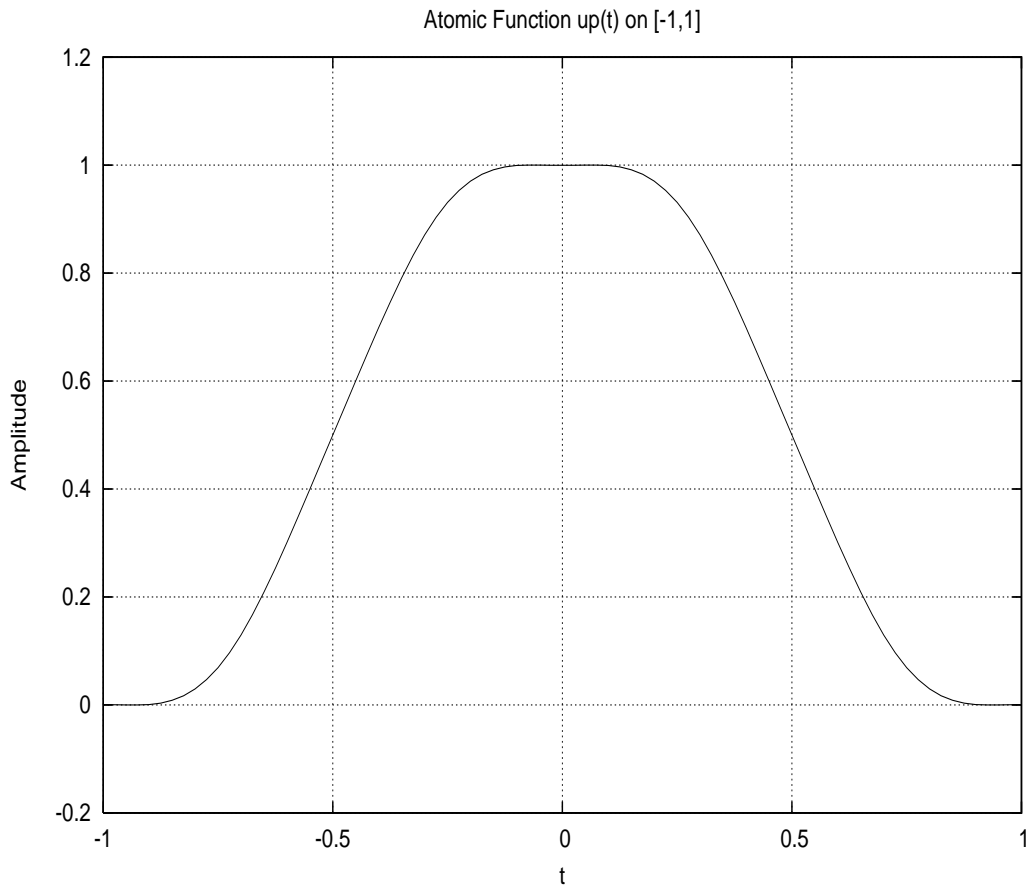


Figure 1: Plot of atomic function $up(t)$ (that is, $\phi(t)$) using the rapidly converging Fourier series method (2.8).

3. Relation to B-splines

Before continuing we digress somewhat to say more about the atomic function $\phi(t)$, and its connection with B-splines [9],[10]. There is also a connection with the *central limit theorem (CLT)* [11] that is worth noting.

Suppose that $u(x)$ is the unit-step function. From [10] the first B-spline is

$$N_1(x) = u(x) - u(x - 1) \tag{3.1}$$

which is a unit-length square pulse of unit height. More generally, the *mth-order cardinal B-spline*

is denoted by $N_m(x)$, and is given by

$$N_m(x) = \underbrace{N_1(x) * \cdots * N_1(x)}_{m \text{ factors to convolve}} \quad (3.2)$$

An alternative formula is

$$N_m(x) = \frac{1}{(m-1)!} \sum_{k=0}^m (-1)^k \binom{m}{k} (x - k)_+^{m-1} \quad (3.3)$$

where $x_+ = \max(0, x)$, and $x_+^{m-1} = (x_+)^{m-1}$ for $m \geq 2$. It can be shown that $N_m(x)$ is supported only on the interval $[0, m]$.

Now suppose that U_k for all $k = 0, 1, \dots, m-1$ is a uniform random variable (RV) with probability density function (pdf) $u(x + .5) - u(x - .5)$. Thus, $E[U_k] = 0$, and $E[U_k^2] = 1/12$ (variance of RV U_k for all k). Define the sum RV

$$X_m = \sqrt{\frac{12}{m}} \sum_{k=0}^{m-1} U_k \quad (3.4)$$

At this point we will further assume that the RVs U_k are mutually statistically independent. Recall now that the central limit theorem (CLT) [11] states that

$$P[a \leq X_m \leq b] \xrightarrow{m \rightarrow \infty} \frac{1}{\sqrt{2\pi}} \int_a^b e^{-x^2/2} dx \quad (3.5)$$

where $P[A]$ denotes the probability of occurrence of the random event A . Expression (3.5) is telling us that the RV X_m is tending to that of a Gaussian RV possessing a mean value of zero, and with unity variance as m increases.

Now further recall that the pdf of the sum of independent RVs is given by convolving the pdfs of each RV in the sum. Since $N_1(x)$ is the expression for the pdf of a uniform RV on $[0, 1]$ from (3.2) we conclude that $N_m(x)$ is the pdf for the sum of m independent uniform RVs on $[0, 1]$. This implies that the pdf of RV $\sqrt{m/12} X_m$ is given by $N_m(x + m/2)$. We see that $N_m(x)$ looks increasingly like a Gaussian pulse as m increases.

The Fourier transform of $N_1(x)$ is

$$\mathcal{F}\{N_1(x)\} = e^{-j\omega/2} \frac{\sin(\omega/2)}{\omega/2} \quad (3.6)$$

Because $\mathcal{F}\{x(t) * y(t)\} = X(\omega)Y(\omega)$ (convolution theorem) from (3.2) we must have

$$\mathcal{F}\{N_m(x)\} = e^{-jm\omega/2} \prod_{k=1}^m \frac{\sin(\omega/2)}{\omega/2} \quad (3.7)$$

This reminds us of (2.3) if we allow $m \rightarrow \infty$, except that the scaling of ω is quite different in the two cases.

In summary, the construction of $\phi(t)$, and the Gaussian pulse $g(x) = \frac{1}{\sqrt{2\pi}}e^{-x^2/2}$ can both be viewed as limiting operations involving the convolution of B-splines.

4. Nucleus, Shell and Parity

Now we develop an alternative series description for the atomic function $\phi(t)$.

Begin by recalling that if $\mathcal{L}\{x(t)\} = \int_{-\infty}^{\infty} x(t) e^{-st} dt$ is the Laplace transform of $x(t)$ (s is a complex variable) then

$$\mathcal{L}\{x(at + b)\} = \frac{1}{a} e^{bs/a} X\left(\frac{s}{a}\right) \quad (a > 0) \quad (4.1)$$

Applying (4.1) to (2.1) we arrive at the Laplace transform of the atomic function

$$\Phi(s) = \left\{ \prod_{k=0}^{\infty} e^{s/2^{k+1}} \right\} \prod_{k=0}^{\infty} \frac{1 - e^{-s/2^k}}{s/2^k} \quad (4.2)$$

However, we observe that the first infinite product in (4.2) simplifies according to

$$\left\{ \prod_{k=0}^{\infty} e^{s/2^{k+1}} \right\} = \exp\left(\frac{1}{2}s \sum_{k=0}^{\infty} 2^{-k}\right) = \exp\left(\frac{1}{2}s \cdot 2\right) = e^s$$

In the time-domain this amounts to a one-unit time shift which would only affect the particular interval of support of the solution to the differential-dilation equation. Therefore, dropping this factor from (4.2) allows us to redefine the transform domain form of the atomic function to be

$$\Phi(s) = \prod_{k=0}^{\infty} \frac{1 - e^{-s/2^k}}{s/2^k} \quad (4.3)$$

In the time-domain this form of the atomic function will have support on the interval $[0, 2]$ instead of the interval $[-1, +1]$. The shape of the pulse is certainly not affected by this change.

Now define the N -factor approximation to $\Phi(s)$ according to

$$\Phi_N(s) = \prod_{k=0}^{N-1} \frac{1 - e^{-s/2^k}}{s/2^k} = \underbrace{\left\{ \prod_{k=0}^{N-1} (1 - e^{-s/2^k}) \right\}}_{= P_N(s)} \underbrace{\left\{ \prod_{k=0}^{N-1} \frac{2^k}{s} \right\}}_{= Q_N(s)} \quad (4.4)$$

We shall call the factor $P_N(s)$ the *nucleus* of $\Phi_N(s)$, and the factor $Q_N(s)$ is called the *shell* of $\Phi_N(s)$.

² Similar terminology will apply in the time-domain. At this point we note that for large enough

²If $\phi(t)$ is like an atom, then there must be a nucleus, and a (electron) shell.

N (e.g., $N = 6$) we may approximate $\phi(t)$ by applying a *numerical inverse Laplace transform (NILT)* to (4.4). One of many possible methods is the algorithm of Dubner and Abate [12]. This one is attractive as it is so easy to program it in almost any language (C/C++, Matlab/Octave, Java, etc.).

Now the product form of the nucleus in (4.4) may not always be convenient to work with. Define the *parity* of integer k to be

$$p(k) = \begin{cases} +1 & , k \text{ has an even number of ones in its binary representation} \\ -1 & , k \text{ has an odd number of ones in its binary representation} \end{cases} \quad (4.5)$$

where $k = 0, 1, \dots, 2^N - 1$, and $N \geq 1$. Define $p(0) = +1$. The following theorem specifies the desired series form for the nucleus in the Laplace domain:

Theorem: For all $N \geq 1$

$$P_N(s) = \prod_{k=0}^{N-1} (1 - e^{-s/2^k}) = \sum_{k=0}^{2^N - 1} p(k) \exp\left(-\frac{ks}{2^{N-1}}\right) \quad (4.6)$$

Proof: The proof is an elementary inductive argument. For $N = 1$ it is apparent that

$$\prod_{k=0}^0 (1 - e^{-s/2^k}) = 1 - e^{-s} = \sum_{k=0}^1 p(k) e^{-ks}$$

since $p(0) = +1$, and $p(1) = -1$. Thus, the central statement of the theorem is correct in this special case. Assume that the statement is true for $N = M$, i.e., assume that

$$\prod_{k=0}^{M-1} (1 - e^{-s/2^k}) = \sum_{k=0}^{2^M - 1} p(k) \exp\left(-\frac{ks}{2^{M-1}}\right)$$

Now consider the case $N = M + 1$. That is,

$$\begin{aligned} \prod_{k=0}^M (1 - e^{-s/2^k}) &= \left\{ \prod_{k=0}^{M-1} (1 - e^{-s/2^k}) \right\} (1 - e^{-s/2^M}) \\ &= \left\{ \sum_{k=0}^{2^M - 1} p(k) e^{-ks/2^{M-1}} \right\} (1 - e^{-s/2^M}) \\ &= \sum_{k=0}^{2^M - 1} p(k) e^{-\frac{ks}{2^{M-1}}} - \sum_{k=0}^{2^M - 1} p(k) e^{-\left(\frac{ks}{2^{M-1}} + \frac{s}{2^M}\right)} \end{aligned}$$

$$= \sum_{k=0}^{2^M-1} p(k)e^{-2ks/2^M} - \sum_{k=0}^{2^M-1} p(k)e^{-(2k+1)s/2^M} \quad (4.7)$$

Parity possesses the following elementary properties

$$p(2k) = p(k), \text{ and } p(2k+1) = -p(k) \quad (4.8)$$

(Think of k in the form of an N -bit binary number. Multiplying k by two shifts the bits, and so does not affect the number of ones in the representation. On the other hand, if we multiply k by two, *and* add one then the parity is “flipped.”) If we now use (4.8) along with suitable changes in the summation indices of (4.7) (i.e., let $l = 2k$, and also use $l = 2k + 1$) then (4.7) reduces to

$$\prod_{k=0}^M (1 - e^{-s/2^k}) = \sum_{l=0}^{2^{M+1}-1} p(l) e^{-ls/2^M}$$

and the theorem follows by induction.

If $\delta(t)$ is the Dirac delta function, then recall that $\mathcal{L}\{\delta(t - \tau)\} = e^{-s\tau}$. Consequently,

$$p_N(t) = \mathcal{L}^{-1}\{P_N(s)\} = \sum_{k=0}^{2^N-1} p(k)\delta\left(t - \frac{k}{2^{N-1}}\right) \quad (4.9)$$

In the time-domain the nucleus is a train of Dirac impulses that get closer and closer together as N increases. These impulses have strengths that are the parities of integers $k \in [0, 2^N - 1]$. An alternative expression for $Q_N(s)$ is simply

$$Q_N(s) = \frac{2^{N(N-1)/2}}{s^N} \quad (4.10)$$

This is the Laplace transform for a polynomial of degree $N - 1$ that is multiplied by $u(t)$. In fact,

$$q_N(t) = \frac{2^{N(N-1)/2}}{(N-1)!} t^{N-1} u(t) = c_N t^{N-1} u(t) \quad (4.11)$$

From the convolution theorem again

$$\phi_N(t) = \int_{-\infty}^{\infty} p_N(\tau)q_N(t - \tau) d\tau \quad (4.12)$$

Therefore, we arrive at a third means to compute an approximation to the atomic function $\phi(t)$, namely

$$\phi_N(t) = c_N \sum_{k=0}^{2^N-1} p(k) \int_{-\infty}^{\infty} \delta\left(\tau - \frac{k}{2^{N-1}}\right) (t - \tau)^{N-1} u(t - \tau) d\tau$$

$$= c_N \sum_{k=0}^{2^N-1} p(k) \left(t - \frac{k}{2^{N-1}} \right)^{N-1} u \left(t - \frac{k}{2^{N-1}} \right) \quad (4.13)$$

This result was obtained using the sifting property of the Dirac impulse function. Equation (4.13) is analogous to (3.3).

5. Concluding Remarks

This report has introduced the atomic function $up(t)$ in a modest effort to make this function more widely known. However, this report has only considered mathematical aspects, while applications to engineering are considered elsewhere.

To be sure the notions of nucleus, shell, and parity raise interesting mathematical questions. Observe that $\{p(k)\}$ is a particular binary sequence. What would happen if we replaced this binary sequence with some other binary sequence $\{b(k)\}$? What constraints upon such sequences yield well-behaved, and compactly supported pulses as $N \rightarrow \infty$? What constraints on such sequences yield pulses that are solutions to differential-dilation equations? What about generalizations to M -ary sequences? And so on.

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