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DESCRIBING THE SURFACE OF MATERIALS WITH GAMMA FUNCTIONS AND ITS APPLICATION IN MICRO- AND NANO-SCALES

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ABSTRACT

The purpose of this paper is to examine the possibility of applying Gamma functions for description of the surface of materials. Here we show analytically that poles of combination of the Gamma functions describe the position of atoms appropriately in one and two dimensions. We introduce the substrate, impurity, and mixed complex functions for describing the position of atoms. It is interesting the new role is played by Gamma function, as one of the special functions, in theoretical surface and materials science. At Micro- and Nano-scales we can restrict the limit of summation and statistical software, i.e. Maple or Mathematica, may be used.

AMS Subject Classification: *33B15, 33E50.*

Key words and Phrases: *Gamma function, Special functions, Substrate function, Impurity function, Materials science, Micro- and Nano-scales.*

1. INTRODUCTION

The gamma function is one of the most important special functions and has many applications in many fields of science, for example, analytic number theory, statistics and physics. See the very useful paper of Srinivasan [1] for the historical background and basic properties of the gamma function.

In [2] Armatas and Pomonis apply Gamma functions for the description of pore size distribution (PSD) as well as for the distinction between the micro-porosity and meso-porosity in materials with ordered and/or quasi-ordered pore structure. Using the Gamma distribution for the description of the pole volume distribution, they obtain the amount adsorbed:

$$V = V_0 \frac{\Gamma(p+1, ar)}{\Gamma(p+1)} \tag{1}$$

where

$\Gamma(a,b) = \int_0^b r^{a-1} e^{-r} dr$ and $\Gamma(a) = \int_0^\infty e^{-r} r^{a-1} dr$ are incomplete and complete Gamma functions respectively.

2. GAMMA FUNCTION

Among analytic functions, Gamma function $\Gamma(z)$ has infinity poles at $n = 0, -1, -2, \ldots$while it does not have any zeros. It is well known that the Gamma function $\Gamma(z)$for real and positive values of z has a minimum between $z = 1.46$ and 1.47. The value of $\Gamma(z)$at the minimum is relatively insensitive to changes in z[3]. The following infinite definition for the Gamma function, due to Euler, is valid for all complex numbers z except the non-positive integers:

$$\Gamma(z) = \lim_{n\to\infty} \frac{n! n^z}{z(z+1)\ldots(z+n)} = \frac{1}{z} \prod_{n=1}^{\infty} \frac{(1+\frac{1}{n})^z}{1+\frac{z}{n}} \tag{2}$$

As equation (2) shows, $\Gamma(z)$is a meromorphic function, namely analytic except for isolated singularities which are simple poles. The function $\frac{1}{\Gamma(z)}$ has no any poles, instead it has infinity zeroes.

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The notation *Γ(z)* is due to Legendre. If the real part of the complex number z is positive $(Re(z) > 0)$, then the integral

$$\Gamma(z) = \int_{\mathbf{0}}^{\infty} e^{-t} t^{z-1} dt \tag{3}$$

converges absolutely. By integrating by parts, the gamma function satisfies the functional equation:

$$\Gamma(z+1) = z\Gamma(z) \tag{4}$$

While the Gamma function is defined for all complex numbers except the non-positive integers, it is defined via an improper integral that converges only for complex numbers with a positive real part.

The Gamma function has simple poles at *z = -n, n = 0, -1, -2, …* . The residue there is:

$$Res(\Gamma, -n) = \frac{(-1)^n}{n!} \tag{5}$$

This integral function is extended by analytic continuation to all complex numbers except the non-positive integers where the function has simple poles. The Gamma function appears occasionally in physical problems such as the normalization of Coulomb wave functions and the computation of probabilities in statistical mechanics [4].

3. MAIN RESULTS

Although important roles in theory and applications have been played by the gamma function so far, we give the new role which can be extended more in future. We first begin our discussion in one dimension, and then we develop it to two dimensional cases. The main idea is that the position of the infinity simple poles of Gamma function $\Gamma(z)$ can be considered as the position of a chain of semi-infinite of atoms placed at negative part of real axis. What can we tell about infinite (not semi-infinite) of atoms? We demonstrate that the poles' position of product of two Gamma functions $\Gamma(z)\Gamma(1-z)$can indicate the position of infinity atoms from $(-\infty, +\infty)$ along a straight line on Real axis on the complex plane.

The position of poles of $\Gamma(a+z)$: $z = -n - a;\ n = 0,1,2, \dots$.

The position of poles of $\Gamma(b-z)$: $z = n + b;\ n = 0,1,2, \dots$.

Example: 3.1 *Show the position of poles of the following Gamma functions:*

1. Let *a = 0* so the position of poles of $\Gamma(z)$ is at *z = 0, 1, 2…* (See Figure 1- light blue points).

2. Let *b = 1* so the position of poles of $\Gamma(1-z)$ is at *z = 1, 2,…*. (See Figure 1- orange points).

By adding $i = \sqrt{-1}$ or $-i = -\sqrt{-1}$ to each argument of Gamma function we can shift one unit the poles' position of the functions $\Gamma(z)$ and $\Gamma(1-z)$ to down with functions $\Gamma(z+i)$ and $\Gamma(1-z-i)$ or up with functions $\Gamma(z-i)$ and $\Gamma(1-z+i)$ respectively.

In Figure 1 six complex Gamma functions specify all poles on the complex plane. However, we can illustrate the same poles just by three functions instead of distinct six functions. Figure 2 shows the same poles by just three functions which each one is product of two Gamma functions.

Now suppose that we want to remove a few of substrate atoms and then put impurity atoms instead of them. Figure 3 shows the position of all poles of the functions $\Gamma(1+z)\Gamma(1-z)$, $\Gamma(2+z-i)\Gamma(-z-i)$ and $\Gamma(3+z+i)\Gamma(-1-z+i)$ respectively. The function $\Gamma(1+z)\Gamma(1-z)$ has just one pole less than $\Gamma(z)\Gamma(1-z)$ (there is no pole at *z =i-1*). The function $\Gamma(2+z-i)\Gamma(-z-i)$ has just one pole less than $\Gamma(z+i)\Gamma(1-z-i)$ (there is no pole at *z = i-1*). The function $\Gamma(3+z+i)\Gamma(-1-z+i)$ has just one pole less than $\Gamma(z-i)\Gamma(1-z+i)$ at *z =-i-2*. In other words, the function $\Gamma(1+z)\Gamma(1-z)$ describes a chain of infinite atoms that is broken at *z = 0*.

If we have a different atom (impurity) at *z = 0*, poles' position can be described by the function $\frac{1}{z}$. The position of three impurity atoms is specified in Figure 4. We note that three chains of infinite atoms are broken exactly at the position of these three impurity atoms. So, six functions describe this configuration as shown in Figure 4.

3.1 Complex substrate function

This type of description with gamma functions can be extended into whole plane by introducing the "complex substrate function" as follows

$$f_1 = \prod_{m=-\infty}^{0} \Gamma(z + im)\Gamma(1 - z - im) \tag{6}$$

Poles of the function $f_1$describe the upper semi-infinite at surface of material at atomic scale.

$$f_2 = \prod_{m=0}^{\infty} \Gamma(z + im)\Gamma(1 - z - im) \tag{7}$$

On the other hand, poles of f_2 describe the down semi-infinite at surface of material at atomic scale. Finally, the sum of f_1 and f_2 leads to describe whole surface of substrate material as it is shown in Figure 5.

$$f_1 + f_2 = \prod_{m=-\infty}^{\infty} \Gamma(z + im)\Gamma(1 - z - im) \tag{8}$$

3.2 Complex Impurity function

Being the position of *n* impurity atoms at $= z_1, z_2, \dots, z_n$, we define the impurity function as follows:

$$h = \prod_{q=1}^{n} \frac{1}{z - z_q} \tag{9}$$

3.3 Complex mixed function

Making product of substrate and impurity functions, we define the mixed function as follows:

where m ≠ q; This function describes mathematically the surface of material as it is shown in Figure 5.

$$gh = \prod_{m=-\infty}^{+\infty} \Gamma(z + im)\Gamma(1 - z - im) \prod_{q=1}^{n} \frac{1}{z - z_q} \tag{10}$$

Because at Micro- and Nano-scales we dealt with just the limited surface, so the values of *m* in summation are not infinite. So this mathematical tool is convenient for applying in Micro- and Nano-scales. On the other hand, the Gamma functions can be used in softwares like Maple and Mathematica for doing computations.

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FIGURE

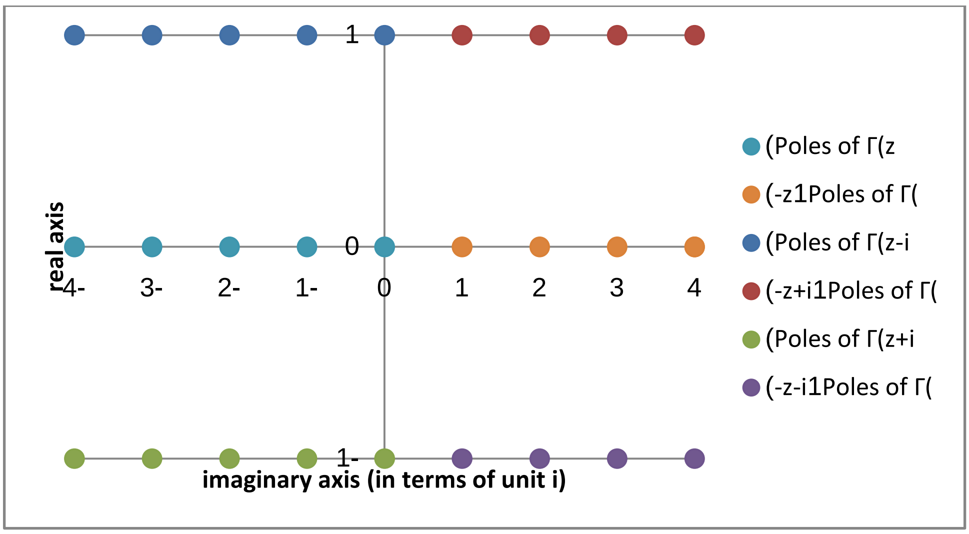

Figure 1: Position of poles of six Gamma functions with different arguments.

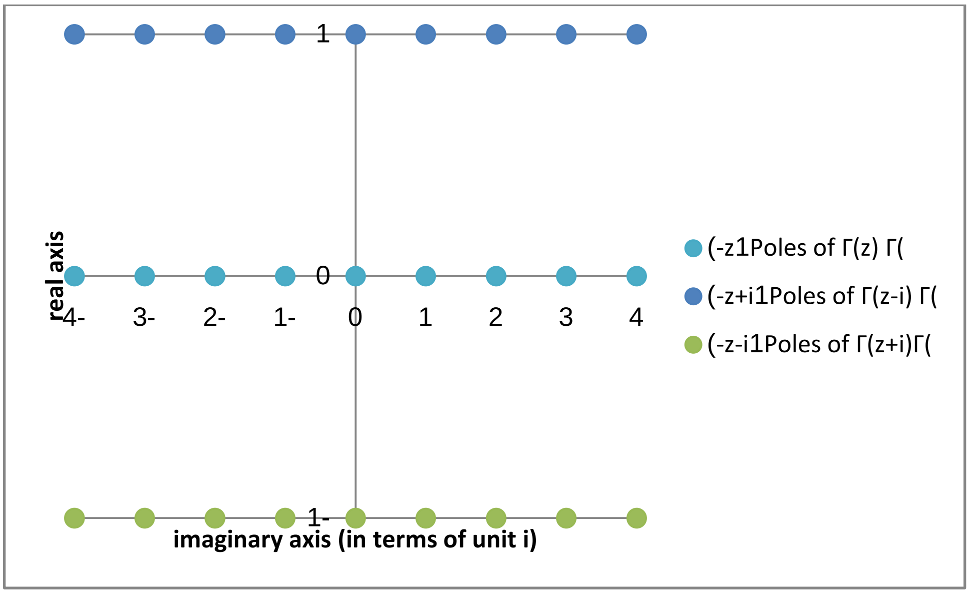

Figure 2: Position of poles of tuple product of Gamma functions with different arguments.

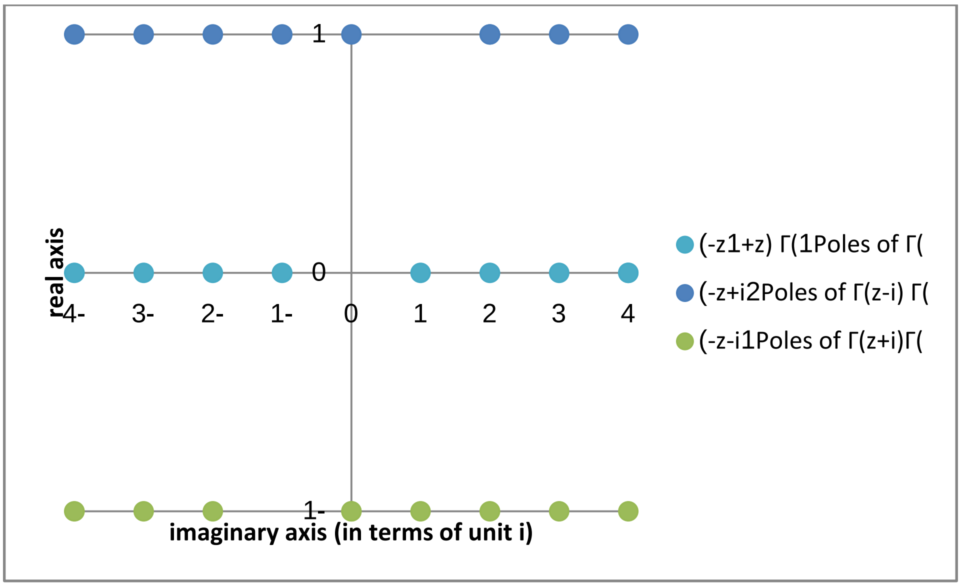

Figure 3: Position of poles of tuple product of Gamma functions with different arguments.

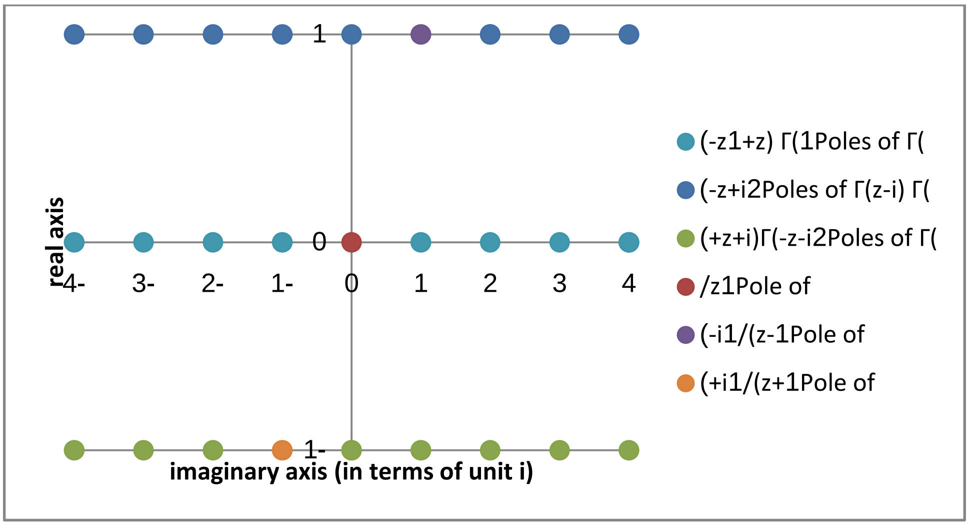

Figure 4: Position of poles of Gamma functions with different arguments.

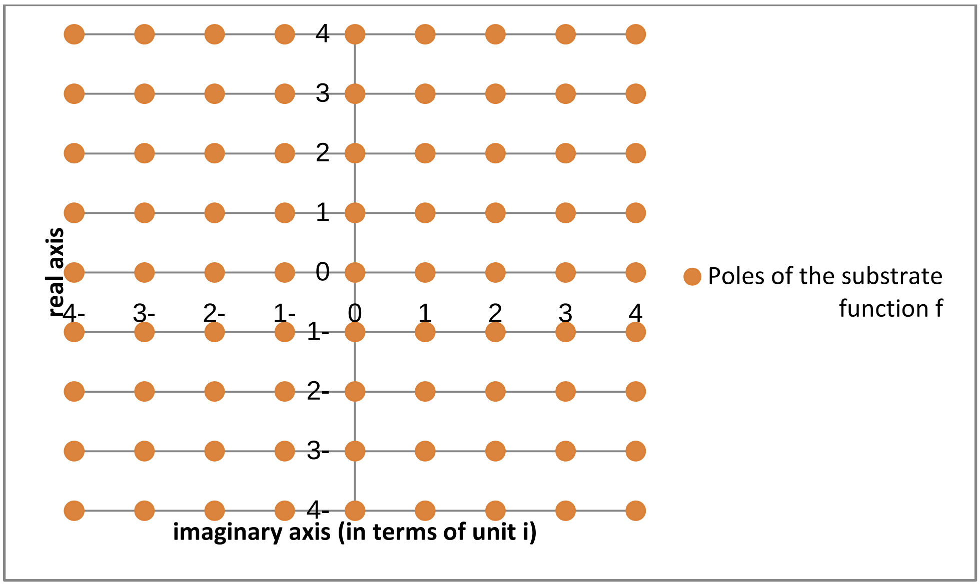

Figure 5: Position of atoms of substrate material

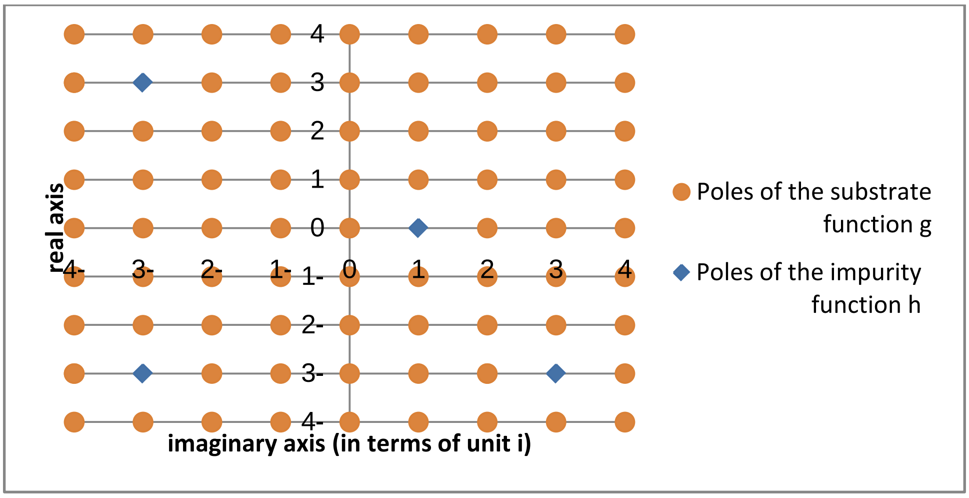

Figure 6: Position of atoms of substrate and impurity material.

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