

G-Function Solutions for Schrödinger Equation in Cylindrical Coordinates System

Amir Pishkoo^{1,2}, Maslina Darus²

¹Nuclear Science Research School, NSTRI, Tehran, Iran

²School of Mathematical Sciences, Faculty of Science and Technology,
Universiti Kebangsaan Malaysia, Selangor, Malaysia

Email: apishkoo@gmail.com, maslina@ukm.my

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ABSTRACT

In this paper, the Schrödinger equation is solved by Modified separation of variables (MSV) method suggested by Pishkoo and Darus. Using this method, Meijer's G -function solutions are derived in cylindrical coordinate system for quantum particle in cylindrical can. All elementary functions and most of the special functions which are the solution of extensive problems in physics and engineering are special cases of Meijer's G -functions.

KEYWORDS

Meijer's G -Function; Partial Differential Equation; Modified Separation of Variables; Schrödinger Equation

1. Introduction

Perhaps, Cornelis Simon Meijer (1936) was the first to introduce the G -function in mathematics. This very general function intended to include most of the known special functions as particular cases; and for a long time, many studies have been done involving this type of functions. These functions have a lot of practical applications in the fields of mathematical physics, theoretical physics, mathematical analysis, etc.

Meijer's G -functions are defined as Mellin-Barnes contour integrals which have been in existence for over 60 years [1-5]. Meijer's G -function satisfies the linear ordinary differential equation (LODE) of the generalised hypergeometric type whose order is equal to $\max(p; q)$ [6-8]. This fact triggered us to verify the equality conditions between Meijer's G -function's LODE and some partial differential equations governing physical phenomena. In physics, we have many ordinary and partial differential equations, in which their solutions are elementary functions, special functions or a combination of both of them. Thus, Meijer's G -functions can be the solution for many physical problems if the equality requirement between Meijer's G -function's LODE and those differential equations are verified. As such, we seek to deduce the solution of physical problems explicitly in terms of Meijer's G -functions.

Our previous works had focused on the introduction of the Modified separation of variables method (MSV), and applying it to solve partial differential equation related to the Reaction-Diffusion process [9], Laplace's diffusion and Schrödinger equations [10-12] which led to representing its solution in terms of Meijer's G -functions. The Cartesian coordinate system is used to derive their solutions. However, in this paper, we obtain G -function solutions for the same problem related to Schrödinger equation, solved by "separation of variables (SV)" in [13], by using modified separation of variables (MSV) method and cylindrical coordinates system as follows.

2. Meijer's G -Function

We begin with the definition of Meijer's G -function as the following:

Definition 1 A definition of the Meijer's G -function is given by the following path integral in the complex plane, called Mellin-Barnes type integral:

$$G_{p,q}^{m,n} \left(\begin{matrix} a_1, \dots, a_p \\ b_1, \dots, b_q \end{matrix} \middle| z \right) = \frac{1}{2\pi i} \int_L \frac{\prod_{j=1}^m \Gamma(b_j - s) \prod_{j=1}^n \Gamma(1 - a_j + s)}{\prod_{j=m+1}^q \Gamma(1 - b_j + s) \prod_{j=n+1}^p \Gamma(a_j - s)} z^s ds. \quad (1.1)$$

Here, the integers $m; n; p; q$ are called "orders" of the G -function, or the components of the order $(m; n; p; q)$; a_j and b_j are called "parameters" and in general, they are complex numbers. The definition holds under the following assumptions: $0 \leq m \leq q$ and $0 \leq n \leq p$, where m, n, p , and q are integer numbers. Subtracting parameters $a_j - b_k \neq 1, 2, 3, \dots$ for $k = 1, \dots, n$ and $j = 1, 2, \dots, m$ imply that no pole of any $\Gamma(b_j - s), j = 1, \dots, m$ coincides with any pole of any $\Gamma(1 - a_k + s), k = 1, \dots, n$.

Exercise 1 Using (1.1), we obtain the follows $G_{0,2}^{1,0}; G_{1,2}^{1,1}; G_{1,1}^{1,1}$: see [14]

$$G_{0,2}^{1,0} = \frac{1}{2\pi i} \int_L \frac{\Gamma(b_1 - s) z^s}{\Gamma(1 - b_2 + s)} ds. \quad (1.2)$$

$$G_{1,2}^{1,1} = \frac{1}{2\pi i} \int_L \frac{\Gamma(b_1 - s) \Gamma(1 - a_1 + s) z^s}{\Gamma(1 - b_2 + s)} ds. \quad (1.3)$$

$$G_{1,1}^{1,1} = \frac{1}{2\pi i} \int_L \Gamma(b_1 - s) \Gamma(1 - a_1 + s) z^s ds. \quad (1.4)$$

The Meijer's G -function $y(z) = G_{p,q}^{m,n} \left(z \middle| \begin{matrix} a_j \\ b_k \end{matrix} \right)$ satisfies the linear ordinary differential equation of the generalised hypergeometric type

$$\left[(-1)^{p-m-n} z \prod_{j=1}^p \left(z \frac{d}{dz} - a_j + 1 \right) - \prod_{k=1}^q \left(z \frac{d}{dz} - b_k \right) \right] y(z) = 0, \quad (1.5)$$

whose order is equal to $\max(p, q)$.

Choosing appropriate values for $m; n; p; q$, orders of G -functions, Equation (1.5) can be changed to complex first and second order linear differential equations. The following section discusses the properties of the solutions of complex first and second order differential equations, and then studies the properties of coefficient functions of these differential equations in the complex plane.

We start with using Modified separation of variables method (MSV) in cylindrical coordinates system as follows:

3. The G -Function Solutions for the Schrödinger Equation

When the geometry of the boundaries is cylindrical, the appropriate coordinate system is the cylindrical one. Separation of variables leads to ODEs in which certain constants (eigenvalues) appear. Different choices of signs for these constants can lead to different functional forms of the general solution. Thus general form of the solution is indeterminate. However, once the boundary conditions are imposed, the unique solutions will emerge regardless of the initial functional form of the solutions. Writing $\Phi(\rho, \varphi, z)$ as a product of three functions, $\Phi(\rho, \varphi, z) = R(\rho)S(\varphi)Z(z)$ and a separation of variables transforms Laplace's equation, $\nabla^2 \Phi(\rho, \varphi, z) = 0$, into three ODEs:

$$\frac{d}{d\rho} \left(\rho \frac{dR}{d\rho} \right) + \left(k^2 \rho - \frac{m^2}{\rho} \right) R = 0,$$

$$\frac{d^2 S}{d\varphi^2} + m^2 S = 0, \quad \frac{d^2 Z}{dz^2} - k^2 Z = 0,$$

where in anticipation of the correct BCs, we have written the constants as k^2 and $-m^2$ with m an integer.

$$S(z) = A \sin mz + B \cos mz$$

is a combination of two independent solutions deduced by “separation of variables method” or

$$S(z) = AG_{0,2}^{1,0} \left(\frac{m^2}{4} z^2 \Big|_{\frac{1}{2}, 0}^- \right) + BG_{0,2}^{1,0} \left(\frac{m^2}{4} z^2 \Big|_{0, \frac{1}{2}}^- \right).$$

is a combination of two independent solutions deduced by “modified separation of variables method”. Similarly

$$Z(z) = C \sinh kz + D \cosh kz$$

is a combination of two independent solutions deduced by “separation of variables method” or

$$Z(z) = CG_{0,2}^{1,0} \left(-\frac{k^2}{4} z^2 \Big|_{\frac{1}{2}, 0}^- \right) + DG_{0,2}^{1,0} \left(-\frac{k^2}{4} z^2 \Big|_{0, \frac{1}{2}}^- \right).$$

is a combination of two independent solutions deduced by “modified separation of variables method”.

1) For $m = 1, n = 0, p = 0, q = 2$, (1.5) reduces to

$$\left[-z - \left(z \frac{d}{dz} - b_2 \right) \left(z \frac{d}{dz} - b_1 \right) \right] G_{0,2}^{1,0} \left(z \Big|_{b_1, b_2}^- \right) = 0.$$

By changing $z \rightarrow \alpha z^2$, we have

$$\left[-\alpha z^2 - \left(\frac{z}{2} \frac{d}{dz} - b_2 \right) \left(\frac{z}{2} \frac{d}{dz} - b_1 \right) \right] G_{0,2}^{1,0} \left(\alpha z^2 \Big|_{b_1, b_2}^- \right) = 0.$$

By multiplying both sides of the equation by -4 , we have

$$\left[z^2 \frac{d^2}{dz^2} + (1 - 2(b_1 + b_2)) z \frac{d}{dz} + 4\alpha z^2 + 4b_1 b_2 \right] G_{0,2}^{1,0} \left(\alpha z^2 \Big|_{b_1, b_2}^- \right) = 0.$$

On the other hand, let Bessel equation

$$\left[z^2 \frac{d^2}{dz^2} + z \frac{d}{dz} + z^2 - \nu^2 \right] J_\nu(z) = 0.$$

The conditions for equivalence or these two differential equations are

$$b_1 + b_2 = 0, 4\alpha = 1, 4b_1 b_2 = -\nu^2 \Rightarrow b_1 = \frac{\nu}{2}, b_2 = \frac{-\nu}{2}, \alpha = \frac{1}{4},$$

and its solutions is

$$J_\nu(z) = G_{0,2}^{1,0} \left(\frac{1}{4} z^2 \Big|_{\frac{\nu}{2}, \frac{-\nu}{2}}^- \right) \ \& \ J_{-\nu}(z) = G_{0,2}^{1,0} \left(\frac{1}{4} z^2 \Big|_{\frac{-\nu}{2}, \frac{\nu}{2}}^- \right).$$

4. Quantum Particle in a Cylindrical Can

Exercise 2 Considering a quantum particle in a cylindrical can, for an atomic particle of mass μ confined in a cylindrical can of length L and radius a , the relevant Schrödinger equation is

$$i \frac{\partial \Psi}{\partial t} = -\frac{\hbar}{2\mu} \left[\frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial \Psi}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2 \Psi}{\partial \phi^2} + \frac{\partial^2 \Psi}{\partial z^2} \right].$$

Let us solve this equation subject to the BCs that $\Psi(\rho, \phi, z, t)$ vanishes at the sides of the can by using

MSV method.

Here is the steps: A separation of variables,

$$\Psi(\rho, \varphi, z, t) = R(\rho)S(\varphi)Z(z)T(t),$$

leads to the following ODEs:

$$\frac{dT}{dt} = -i\omega T, \quad \frac{d^2Z}{dz^2} + \lambda Z = 0, \quad \frac{d^2S}{d\varphi^2} + m^2 S = 0, \tag{1.6}$$

$$\frac{d^2R}{d\rho^2} + \frac{1}{\rho} \frac{dR}{d\rho} + \left(\frac{2\mu}{\hbar} \omega - \lambda - \frac{m^2}{\rho^2} \right) R = 0. \tag{1.7}$$

The second DE, the Z equation, along with its BCs, constitutes an S-L system with G -function solutions.

$$Z(z) = G_{0,2}^{1,0} \left(-\frac{k^2 \pi^2}{4L^2} z^2 \middle|_{\frac{1}{2}, 0}^- \right) \lambda = \frac{k\pi^2}{L} \text{ for } k = 1, 2, \dots.$$

Since the extra condition of periodicity is usually imposed on the potential for variable φ , the third DE, in terms of Meijer's G -functions, has the general solution.

$$S(\varphi) = CG_{0,2}^{1,0} \left(\frac{m^2}{4} \varphi^2 \middle|_{\frac{1}{2}, 0}^- \right) + DG_{0,2}^{1,0} \left(\frac{m^2}{4} \varphi^2 \middle|_{0, \frac{1}{2}}^- \right).$$

If we let $\frac{2\mu\omega}{\hbar} - \frac{k\pi^2}{L} \equiv b^2$, then the solution of the last equation that is well-behaved is at $\rho = 0$ and is $G_{0,2}^{1,0} \left(\frac{1}{4} b^2 \rho^2 \middle|_{\frac{m}{2}, \frac{-m}{2}}^- \right)$. From the last BC, $R(a) = 0$, we obtain the quantisation condition $b = \frac{x_{mn}}{a}$ for $n = 1, 2, \dots$.

Then, the energy eigenvalues are

$$E_{kmn} \equiv \hbar\omega_{kmn} = \frac{-\hbar^2}{2\mu} \left[\left(\frac{k\pi}{L} \right)^2 + \frac{x_{mn}^2}{a^2} \right].$$

t component: for $m = 1, n = 0, p = 0, q = 1$, (1.5) is reduced to:

$$\left[-z - \left(z \frac{d}{dz} - b_1 \right) \right] G_{0,1}^{1,0} \left(z \middle|_{b_1}^- \right) = 0.$$

On the other hand, $\frac{dT}{dt} + i\omega T = 0$ with changing variable $t \rightarrow z$.

The condition for the equivalence of these two differential equations is given by the solution of t -component. Thus, the general solution can be written as

$$\Psi(\rho, \varphi, z) = \sum_{m=0, k=1, n=1}^{\infty} G_{0,2}^{1,0} \left(\frac{1}{4} \frac{x_{mn}^2}{a} \rho^2 \middle|_{\frac{m}{2}, \frac{-m}{2}}^- \right) G_{0,2}^{1,0} \left(-\frac{k^2 \pi^2}{4L^2} z^2 \middle|_{\frac{1}{2}, 0}^- \right) \cdot \left[C_{kmn} G_{0,2}^{1,0} \left(\frac{m^2}{4} \varphi^2 \middle|_{\frac{1}{2}, 0}^- \right) + D_{kmn} G_{0,2}^{1,0} \left(\frac{m^2}{4} \varphi^2 \middle|_{0, \frac{1}{2}}^- \right) \right], \tag{1.8}$$

$$\& \Psi(\rho, \varphi, z, t) = \Psi(\rho, \varphi, z) G_{0,1}^{1,0} \left(i\omega_{kmn} t \middle|_0^- \right).$$

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