

Advanced Studies in Theoretical Physics
Vol. 9, 2015, no. 3, 145 - 154
HIKARI Ltd, www.m-hikari.com
<http://dx.doi.org/10.12988/astp.2015.516>

A G -function Form of Radial States in Carbon and Hydrogen Atoms: Absorption or Emission of Radiation

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Abstract

The Meijer's G -functions (MGFs) are an admirable family of functions which each of them is determined by finitely many indices. Analytic manipulations and numerical computations involving Meijer's G -functions have been provided by the software packages such as *Mathematica*, *Maple*, and *Matlab*. Recently, MGFs are obtained as the solution of Schrödinger equation as well as diffusion equation, and reaction-diffusion equation by using modified separation of variables method. It was also shown that MGFs are the radial functions of the Hydrogen atom. The radial functions such as R_{20} and R_{21} have crucial role in making superposition of orbitals and the formation of chemical bonds such as SP^2 hybridization. In this paper we deduce some useful relations upon which the radial functions can be represented by summation of a number of Meijer's G -functions. As a result, MGFs may be utilized in describing carbon nanotubes, absorption and emission of radiation such as X-rays and γ -rays.

Keywords: Meijer's G -function, Schrödinger equation, Bohr operator, Radial functions.

1 INTRODUCTION

The Meijer's G -functions are a remarkable family of functions of one variable, each of them determined by finitely many indices. They play a crucial role in a certain useful mathematical enterprise. When we look at conceptually, they are both attractive and attractive, and have remarkable closure properties. The implementation of Meijer's G -function in Mathematica constitutes an additional utility for analytic manipulations and numerical computations involving this special function [4]. Most of the software packages such as *Maple* (Maple 2011), *Mathematica* (Wolfram 2011), and *Matlab* (Matlab 2011) provide computations involving Meijer's G -functions. Additionally, Maple can provide a means to understand the relationships among Meijer's G -functions and other functions. Considering the well-known applications of MGF, it is obvious that MGF is a useful tool in mathematical physics because of its analytical properties, and more because it can be expressed as a finite sum of generalized hypergeometric functions [7,10,22]. In [16-18] MGFs are obtained as solution of physical problems by introducing modified separation of variables (MSV) method. Being MGFs as the solution form of Schrödinger equation [16,19] especially Hydrogen atom, a new door has been opened for obtaining new results in the present paper. We aim that MGFs may be utilized in describing carbon nanotubes, absorption and emission of radiation [1,8,15]. Because many deduced results from atomic physics can be generalized to nuclear physics, we may expect MGFs to be even the wave functions of parent and daughter nuclei. As a result, we may properly describe α , β , and γ -decays for which the first steps have been done in [20,21]. Meijer's G -functions are the solution of Schrödinger equation, depending on dimensionality, it is opened a new way to describe quantum dots or clusters 0D, quantum wire 1D, quantum well, thin film or layer 2D, and bulk material 3D in terms of G -functions [5,9,13,23].

Regarding to radial functions we now refer to their role in the formation of chemical bonds. The ability of a single carbon atom to form up to four strong covalent bonds makes it a key player in organic chemistry and hence a cornerstone in the formulation of biological tissue. It is a well-known fact that atoms are most stable when the s, p orbitals of the outer shell are occupied (octet rule). This is known as hybridization which is done most efficiently by making superposition of the symmetric $2s, 2p_1, 2p_0$, and $2p_{-1}$ orbitals as follows [6].

$$\begin{aligned} \mathbf{s}(\mathbf{r}) &\equiv 2s = R_{20}Y_0^0, \\ p_x(\mathbf{r}) &\equiv 2p_1 - 2p_{-1} = R_{21}Y_1^1 - R_{21}Y_{-1}^1, \\ p_y(\mathbf{r}) &\equiv 2p_1 + 2p_{-1} = R_{21}Y_1^1 + R_{21}Y_{-1}^1, \\ p_z(\mathbf{r}) &\equiv 2p_0 = R_{21}Y_1^0. \end{aligned}$$

The sp^2 hybridization consists of the following superpositions of $s(\mathbf{r})$, $p_x(\mathbf{r})$, and $p_y(\mathbf{r})$. This type of hybridization is relevant to the formation of graphene and carbon nanotubes [6].

$$\begin{aligned} sp_a^2 &\equiv \sqrt{\frac{4}{6}}s(\mathbf{r}) + \sqrt{\frac{2}{6}}p_x(\mathbf{r}), \\ sp_b^2 &\equiv \sqrt{\frac{2}{6}}s(\mathbf{r}) - \sqrt{\frac{1}{6}}p_x(\mathbf{r}) + \sqrt{\frac{3}{6}}p_y(\mathbf{r}), \\ sp_c^2 &\equiv \sqrt{\frac{2}{6}}s(\mathbf{r}) - \sqrt{\frac{1}{6}}p_x(\mathbf{r}) - \sqrt{\frac{3}{6}}p_y(\mathbf{r}), \end{aligned}$$

It is seen that radial functions such as $R_{20}(r)$; $R_{21}(r)$ have crucial role in making superposition of orbitals. The last part of the Schrödinger equation to be solved concerns the radial coordinate r . The size of the atomic orbitals is not well defined due to the statistical nature of the wavefunction. It is only characterized fully by calculating all the expectation values $\langle r^k \rangle$ for any power k . Since the potential behaves as $\frac{1}{r}$ it is natural to estimate the size of the orbitals by calculating $\langle \frac{1}{r} \rangle$.

$$\langle \frac{1}{r} \rangle_{nlm} = \int_0^\infty dr r^2 \frac{1}{r} |R_{nl}|^2 = \frac{1}{n^2} \frac{1}{r_B}.$$

For the ground state ψ_{100} of the Hydrogen atom we find (with $Z = 1$) the ground state energy E_0 and the size r_B to be

$$r_B = r_{Z=1} = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2} = 0.053nm \quad \& \quad E_0 = E_{Z=1} = -\frac{m_e e^4}{32\pi^2\epsilon_0^2\hbar^2} = -13.6ev,$$

where r_B is Bohr radius.

The content of this paper is divided into two main sections. In the first section, the definition of MGFs, some of their properties are recalled. Second section gives our results by introducing Bohr operator and then in the format of two theorems we represent Radial functions of the Hydrogen atom as MGFs by deducing Eq. (3.11). In fact, Bohr operator acts as photon which gives energy to electron and changing Radial functions with regarding selection rules (absorption), and vice versa in the process of emission.

2 MEIJER'S *G*-FUNCTIONS

The *G*-function was introduced by Cornelis Simon Meijer (1936) as a very general function intended to include all elementary functions and most of the known special functions, for instance:

- $\sin x = \sqrt{\pi} G_{0,2}^{1,0}(\frac{x^2}{4} |_{\frac{1}{2}, 0}^-)$; $\cos x = \sqrt{\pi} G_{0,2}^{1,0}(\frac{x^2}{4} |_{0, \frac{1}{2}}^-)$
- $\ln x = G_{2,2}^{1,2}(x-1 |_{1,0}^{1,1})$; $J_\nu(x) = G_{0,2}^{1,0}(\frac{x^2}{4} |_{\frac{\nu}{2}, -\frac{\nu}{2}}^-)$

We begin with the definition of Meijer G -function.

Definition 2.1 *A definition of the Meijer G -function is given by the following path integral in the complex plane, called Mellin-Barnes type integral [2,3,11,12,14]:*

$$G_{p,q}^{m,n}(\mathbf{a}_p, \dots, \mathbf{a}_p | \mathbf{b}_1, \dots, \mathbf{b}_q | z) = \frac{1}{2\pi i} \int_L \frac{\prod_{j=1}^m \Gamma(b_j - s) \prod_{j=1}^n \Gamma(1 - a_j + s)}{\prod_{j=m+1}^q \Gamma(1 - b_j + s) \prod_{j=n+1}^p \Gamma(a_j - s)} z^s ds. \quad (2.1)$$

Here, L is a suitable closed contour in the complex plane; 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 $\Gamma(1 - a_k + s), k = 1, \dots, n$. We follow usual convention that the empty product equals 1.

Choosing $m = 1, n = 0, p = 0$ and $q = 1$, we have

$$G_{0,1}^{1,0}(\bar{} |_{b_1} | z) = \frac{1}{2\pi i} \int_L \Gamma(b_1 - s) z^s ds. \quad (2.2)$$

Or in more general in terms of elementary function is (see[11])

$$G_{0,1}^{1,0}(\bar{} |_{\frac{\beta}{\alpha}} | \eta z^\alpha) = \eta^{\frac{\beta}{\alpha}} z^\beta e^{-\eta z^\alpha} \quad (2.3)$$

Based on the definition, the following basic properties are easily derived:

$$z^\alpha G_{p,q}^{m,n}(\mathbf{a}_p | \mathbf{b}_q | z) = G_{p,q}^{m,n}(\mathbf{a}_p + \alpha | \mathbf{b}_q + \alpha | z), \quad (2.4)$$

where the multiplying term z^α changes the parameters of the G -function. The key to a conceptual understanding of a G -function is the differential equation that it satisfies.

3 MAIN RESULTS

The Bohr radius, symbolized r_B , is the mean radius of the orbit of an electron around the nucleus of a hydrogen atom at its ground state (lowest-energy level). We define the Bohr operator to change the mean radius of the orbit for electron. (for example $r_B \rightarrow 2r_B$)

The Bohr operator

Generally, an operator acting on a function maps it into another function.

Definition 3.1 *The Bohr operator is represented by \hat{B} and defined as follows:*

$$\hat{B}\left[\left(\frac{1}{r_B}\right)^{\frac{3}{2}}G_{0,1}^{1,0}\left(-\left|\frac{r}{r_B}\right.\right)\right] = \left[\left(\frac{1}{2r_B}\right)^{\frac{3}{2}}G_{0,1}^{1,0}\left(-\left|\frac{r}{2r_B}\right.\right)\right] \quad (3.1)$$

The meaning of square \hat{B}^2 of the Bohr operator \hat{B} is obvious:

$$\hat{B}^2\left[\left(\frac{1}{r_B}\right)^{\frac{3}{2}}G_{0,1}^{1,0}\left(-\left|\frac{r}{r_B}\right.\right)\right] = \hat{B}\left[\left(\frac{1}{2r_B}\right)^{\frac{3}{2}}G_{0,1}^{1,0}\left(-\left|\frac{r}{2r_B}\right.\right)\right] = \left[\left(\frac{1}{3r_B}\right)^{\frac{3}{2}}G_{0,1}^{1,0}\left(-\left|\frac{r}{3r_B}\right.\right)\right]$$

The operator \hat{B}^n is formed by \hat{B} acting n times:

$$\hat{B}^n\left[\left(\frac{1}{r_B}\right)^{\frac{3}{2}}G_{0,1}^{1,0}\left(-\left|\frac{r}{r_B}\right.\right)\right] = \hat{B}\hat{B}\hat{B}\dots\hat{B}\left[\left(\frac{1}{r_B}\right)^{\frac{3}{2}}G_{0,1}^{1,0}\left(-\left|\frac{r}{r_B}\right.\right)\right] = \hat{B}^{n-1}\left(\hat{B}\left[\left(\frac{1}{r_B}\right)^{\frac{3}{2}}G_{0,1}^{1,0}\left(-\left|\frac{r}{r_B}\right.\right)\right]\right)$$

with $r_B = \frac{4\pi\epsilon_0\hbar^2}{me^2}$, where r_B is the Bohr radius.

Theorem 3.1 *Let $R_{10} = 2\left(\frac{1}{r_B}\right)^{\frac{3}{2}}e^{-\frac{r}{r_B}} = 2\left(\frac{1}{r_B}\right)^{\frac{3}{2}}G_{0,1}^{1,0}\left(-\left|\frac{r}{r_B}\right.\right)$ be the ground radial state of the Hydrogen atom, then the operators $\hat{B}\left(\frac{r}{r_B}\right)$ and $\hat{B}^2\left(\frac{r}{r_B}\right)^2$ map the radial function R_{10} into multiple of R_{21} and of R_{32} , respectively.*

Proof 1 *From (2.3) and (2.4) for $\alpha = 1$ we have*

$$\left(\frac{r}{r_B}\right)e^{-\frac{r}{r_B}} = \left(\frac{r}{r_B}\right)G_{0,1}^{1,0}\left(-\left|\frac{r}{r_B}\right.\right) = G_{0,1}^{1,0}\left(-\left|\frac{r}{r_B}\right.\right)$$

so

$$\left(\frac{r}{r_B}\right)R_{10} = 2\left(\frac{1}{r_B}\right)^{\frac{3}{2}}\left(\frac{r}{r_B}\right)e^{-\frac{r}{r_B}} \quad (3.2)$$

Affecting \hat{B} on (3.2) gives

$$\hat{B}\left[\left(\frac{r}{r_B}\right)R_{10}\right] = \hat{B}\left[2\left(\frac{1}{r_B}\right)^{\frac{3}{2}}\left(\frac{r}{r_B}\right)e^{-\frac{r}{r_B}}\right] = 2\left(\frac{1}{2r_B}\right)^{\frac{3}{2}}\left(\frac{r}{2r_B}\right)e^{-\frac{r}{2r_B}} = \sqrt{3}R_{21}$$

From (2.3) and (2.4) for $\alpha = 2$ we have

$$\left(\frac{r}{r_B}\right)^2e^{-\frac{r}{r_B}} = \left(\frac{r}{r_B}\right)^2G_{0,1}^{1,0}\left(-\left|\frac{r}{r_B}\right.\right) = \left(\frac{r}{r_B}\right)G_{0,1}^{1,0}\left(-\left|\frac{r}{r_B}\right.\right) = G_{0,1}^{1,0}\left(-\left|\frac{r}{2r_B}\right.\right)$$

$$\left(\frac{r}{r_B}\right)^2 R_{10} = 2\left(\frac{1}{r_B}\right)^{\frac{3}{2}}\left(\frac{r}{r_B}\right)^2 e^{-\frac{r}{r_B}} \quad (3.3)$$

Affecting \hat{B} on (3.3) gives

$$\hat{B}\left(\frac{r}{r_B}\right)^2 R_{10} = \left(\frac{1}{2r_B}\right)^{\frac{3}{2}} 2\left(\frac{r}{2r_B}\right)^2 e^{-\frac{r}{2r_B}} \quad (3.4)$$

Affecting \hat{B} for the second time on (3.3) gives

$$\hat{B}^2\left[\left(\frac{r}{r_B}\right)^2 R_{10}\right] = \hat{B}\left[\left(\frac{1}{2r_B}\right)^{\frac{3}{2}} 2\left(\frac{r}{2r_B}\right)^2 e^{-\frac{r}{2r_B}}\right] = \left(\frac{1}{3r_B}\right)^{\frac{3}{2}} 2\left(\frac{r}{3r_B}\right)^2 e^{-\frac{r}{3r_B}} = \frac{3\sqrt{10}}{2} R_{32}$$

In more general it can be deduced that $\hat{B}^n\left(\frac{r}{r_B}\right)^n$ maps the ground radial state R_{10} into multiple of radial state $R_{n+1,n}$ such that

$$\hat{B}^n\left(\frac{r}{r_B}\right)^n R_{10} = \hat{B}^n\left[\left(\frac{r}{r_B}\right)^n 2\left(\frac{1}{r_B}\right)^{\frac{3}{2}} e^{-\frac{r}{r_B}}\right] = 2\left[\frac{1}{(n+1)r_B}\right]^{\frac{3}{2}} \left[\frac{r}{(n+1)r_B}\right]^n e^{-\frac{r}{(n+1)r_B}} \quad (3.5)$$

Theorem 3.2 Let $R_{10} = 2\left(\frac{1}{r_B}\right)^{\frac{3}{2}} e^{-\frac{r}{r_B}} = 2\left(\frac{1}{r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}\left(\bar{0} \mid \frac{r}{r_B}\right)$ be the ground radial state of the Hydrogen atom, then the radial function R_{21} , R_{20} , R_{32} , R_{31} , and R_{30} may be written in terms of linear combination of $G_{0,1}^{1,0}$ with different value of parameters:

$$R_{21} = a_1\left(\frac{1}{2r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}\left(\bar{1} \mid \frac{r}{2r_B}\right), \quad (3.6)$$

where $a_1 = \frac{2}{\sqrt{3}}$.

$$R_{20} = b_0\left(\frac{1}{2r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}\left(\bar{0} \mid \frac{r}{2r_B}\right) + b_1\left(\frac{1}{2r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}\left(\bar{1} \mid \frac{r}{2r_B}\right), \quad (3.7)$$

where $b_0 = 2$ and $b_1 = 2$.

$$R_{32} = c_1\left(\frac{1}{3r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}\left(\bar{2} \mid \frac{r}{3r_B}\right), \quad (3.8)$$

where $c_1 = \frac{4}{3\sqrt{10}}$.

$$R_{31} = d_1\left(\frac{1}{3r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}\left(\bar{1} \mid \frac{r}{3r_B}\right) + d_2\left(\frac{1}{3r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}\left(\bar{2} \mid \frac{r}{3r_B}\right), \quad (3.9)$$

where $d_1 = \frac{8}{3\sqrt{2}}$ and $d_2 = \frac{4}{3\sqrt{2}}$.

$$R_{30} = e_0\left(\frac{1}{3r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}\left(\bar{0} \mid \frac{r}{3r_B}\right) + e_1\left(\frac{1}{3r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}\left(\bar{1} \mid \frac{r}{3r_B}\right) + e_2\left(\frac{1}{3r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}\left(\bar{2} \mid \frac{r}{3r_B}\right), \quad (3.10)$$

where $e_0 = 2$, $e_1 = -4$ and $e_2 = \frac{4}{3}$.

Proof 2 Choosing $z = r$, $\alpha = 1$, $\beta = 0$, and $\eta = \frac{1}{2r_B}$ in (2.3) gives

$$G_{0,1}^{1,0}(\bar{0} | \frac{r}{2r_B}) = e^{-\frac{r}{2r_B}}$$

$$R_{21} = \left(\frac{1}{2r_B}\right)^{\frac{3}{2}} \frac{1}{\sqrt{3}} \left(\frac{r}{2r_B}\right) e^{-\frac{r}{2r_B}} = \left(\frac{1}{2r_B}\right)^{\frac{3}{2}} \frac{2}{\sqrt{3}} \left(\frac{r}{2r_B}\right) G_{0,1}^{1,0}(\bar{0} | \frac{r}{2r_B})$$

Thus we have

$$R_{21} = \frac{2}{\sqrt{3}} \left(\frac{1}{2r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}(\bar{1} | \frac{r}{2r_B})$$

$$R_{20} = b_0 \left(\frac{1}{2r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}(\bar{0} | \frac{r}{2r_B}) + b_1 \left(\frac{1}{2r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}(\bar{1} | \frac{r}{2r_B})$$

$$R_{32} = c_2 \left(\frac{1}{3r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}(\bar{2} | \frac{r}{3r_B})$$

$$R_{31} = d_1 \left(\frac{1}{3r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}(\bar{1} | \frac{r}{3r_B}) + d_2 \left(\frac{1}{3r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}(\bar{2} | \frac{r}{3r_B})$$

$$R_{30} = e_1 \left(\frac{1}{3r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}(\bar{2} | \frac{r}{3r_B}) + e_2 \left(\frac{1}{3r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}(\bar{1} | \frac{r}{3r_B}) + e_3 \left(\frac{1}{3r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}(\bar{0} | \frac{r}{3r_B})$$

Finally, we can suggest the following general formula

$$R_{nl} = \sum_{k=l}^{n-1} a_k \left(\frac{1}{nr_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}(\bar{k} | \frac{r}{nr_B}), \quad (3.11)$$

where n is principal quantum number, l is azimuthal quantum number which its value ranges from 0 to $n - 1$.

Example 3.1 Find the expression for radial function R_{60} in terms of Meijer's G-functions

Since $n=6$ and $l = 0$, using (4.8) gives

$$\begin{aligned} R_{60} &= \sum_{k=0}^5 c_k \left(\frac{1}{6r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}(\bar{k} | \frac{r}{6r_B}) \\ &= c_0 \left(\frac{1}{6r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}(\bar{0} | \frac{r}{6r_B}) + c_1 \left(\frac{1}{6r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}(\bar{1} | \frac{r}{6r_B}) + c_2 \left(\frac{1}{6r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}(\bar{2} | \frac{r}{6r_B}) + \\ &\quad c_3 \left(\frac{1}{6r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}(\bar{3} | \frac{r}{6r_B}) + c_4 \left(\frac{1}{6r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}(\bar{4} | \frac{r}{6r_B}) + c_5 \left(\frac{1}{6r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}(\bar{5} | \frac{r}{6r_B}) \end{aligned}$$

Example 3.2 Find the expression for radial function R_{52} in terms of Meijer's G -functions

Since $n = 5$ and $l = 2$, using (4.8) gives

$$\begin{aligned} R_{52} &= \sum_{k=2}^4 d_k \left(\frac{1}{5r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}\left(-\left|\frac{r}{5r_B}\right.\right) \\ &= d_2 \left(\frac{1}{5r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}\left(2\left|\frac{r}{5r_B}\right.\right) + d_3 \left(\frac{1}{5r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}\left(3\left|\frac{r}{5r_B}\right.\right) + d_4 \left(\frac{1}{5r_B}\right)^{\frac{3}{2}} G_{0,1}^{1,0}\left(4\left|\frac{r}{5r_B}\right.\right) \end{aligned}$$

4 CONCLUSION

The radial functions such as R_{20} and R_{21} have crucial role in making superposition of orbitals and the formation of chemical bonds such as SP^2 hybridization. Using of operator method by introducing Bohr operator, we show that radial functions can be represented with summation of Meijer's G -functions. Absorption or emission of photons can be occurred mathematically through changing in combination of Meijer's G -functions.

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Received: February 1, 2015; Published: March 5, 2015