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General Orthogonality for Orthogonal Polynomials

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The bound state wave functions for all the known exactly solvable potentials can be expressed in terms of orthogonal polynomials because the polynomials always satisfy the boundary conditions with a proper weight function. The orthogonality of polynomials is of great importance because the orthogonality characterizes the wave functions and consequently the quantum system. Though the orthogonality of orthogonal polynomials has been known for hundred years, the known orthogonality is found to be inadequate for polynomials appearing in some exactly solvable potentials, for example, Ginocchio potential. For those potentials a more general orthogonality is defined and algebraically derived. It is found that the general orthogonality is valid with a certain constraint and the constraint is very useful in understanding the system.

Key Words : Orthogonality, Solvable potentials, Orthogonal polynomials

Introduction

Nowadays it is a textbook knowledge that there are exactly solvable one-dimensional quantum systems whose wave functions are orthogonal polynomials. The one-dimensional systems are almost trivially simple to solve but their implications for understanding the quantum chemistry are immense. The classical orthogonal polynomials include the Jacobi polynomials, the Hermite polynomials, the Laguerre polynomials, the Legendre polynomials and so on. For example, the harmonic oscillator potential, which is frequently used to determine harmonic vibrational frequencies of a molecule, has wave functions of the Hermite polynomials ($H_n(z)$). The wave functions of rotational motion of a rigid body involve the associated Legendre polynomials ($P_l^{(m)}(z)$). The associated Laguerre polynomials ($L_n^{(\alpha)}(z)$) are used for Coulomb potential (*e.g.* hydrogen atom) and also for Morse potential (*e.g.* anharmonic vibrational motion).[1]

The orthogonal polynomials are, as its name implicates, orthogonal to each other with a proper weight function. The bound sate wave functions are expressed in terms of the orthogonal polynomials. The orthogonality of wave functions for a bound state ensures the existence of the state, which helps one to find or characterize the bound states of a system.

Mathematically the classical orthogonal polynomials $f_n(z)$ are solutions to the following differential equation[2]

$$\left[g_2(z)\frac{d^2}{dz^2} + g_1(z)\frac{d}{dz} + a_n\right]f_n(z) = 0 \tag{1}$$

where the functions $g_2(z)$ and $g_1(z)$ are independent of n and a_n is a constant depending on n, the degree of function $f_n(z)$. n is a nonnegative integer, *i.e.* $n = 0, 1, 2,...$ This form of differential equation (sometimes called Sturm-Liouville equation) can have solution functions $f_n(z)$ when particular forms of $g_2(z)$, $g_1(z)$, and a_n are provided. There are basically three types of solution functions, i.e. polynomials. The set of $g_2(z) = 1-z^2$, $g_1(z) = \beta-\alpha-(\alpha+\beta+2)z$, and $a_n = n(n+\alpha+\beta+1)$ produces solution functions of $f_n(z) = P_n^{(\alpha,\beta)}(z)$, called the Jacobi polynomials. The associated Laguerre polynomials $f_n(z) = L_n^{(\alpha)}(z)$ with $g_2(z) = z$, $g_1(z) = \alpha + 1 - z$, and $a_n = n$, and the Hermite polynomials $f_n(z) = H_n(z)$ with $g_1(z) = 1$, $g_1(z) = -2z$, and $a_n = 2n$. The well known polynomials like Legendre, Laguerre, Chevyshev, or Gegenbauer polynomials are subclasses of one of the three basic types of polynomials.

The polynomials $f_n(z)$ are called the orthogonal polynomials if

$$\int_a^b w(z)f_n(z)f_m(z)dz = 0 \quad (n\neq m;\ n,m = 0,1,2,...), \tag{2}$$

on the interval $a\leq z\leq b$, with respect to the weight function $w(z)$,

$$w(z) = \frac{1}{g_2(z)}\exp\left(\int\frac{g_1(z)}{g_2(z)}dz\right). \tag{3}$$

This 'usual orthogonality' (Eqs. (2) and (3)) has been known for a long time and widely used to characterize the properties of $f_n(z)$.

For example, the usual orthogonality for the associated Laguerre polynomials is explicitly, from Eqs. (2) and (3),

$$\int_0^\infty z^\alpha \exp(-z)L_n^{(\alpha)}(z)L_m^{(\alpha)}(z)dz = 0 \quad (n\neq m) \tag{4}$$

where α is a constant. Note that $L_n^{(\alpha)}(z)$ and $L_m^{(\alpha)}(z)$ are solutions to the differential equation (Eq. 1) with the same α. Now a question of interest is if $L_n^{(\alpha)}(z)$ and $L_m^{(\alpha')}(z)$ are orthogonal to each other when $\alpha\neq\alpha'$. The new orthogonality for the associated Laguerre polynomials may look like

$$\int_0^\infty w(z)L_n^{(\alpha)}(z)L_m^{(\alpha')}(z)dz = 0 \quad (n\neq m;\ \alpha\neq\alpha'). \tag{5}$$

This new orthogonality called 'general orthogonality' can be written as in the universal form of

$$\int_a^b w(z) f_n^{(\alpha)}(z) f_m^{(\alpha')}(z) dz = 0 \quad (n \neq m;\ \alpha \neq \alpha'). \tag{6}$$

The polynomials are denoted as $f_n^{(\alpha)}$ instead of $f_n(z)$ in order to show α-dependence of the polynomials explicitly. Obviously the general orthogonality is not applicable to polynomials like the Hermite polynomials which do not have a constant α in its differential equation.

For a long time the 'general orthogonality' has not attracted much attention simply because a potential requiring the general orthogonality was not encountered. To our knowledge Ginocchio first introduced the general orthogonality but he presented it only for the Gegenbauer polynomials without detailed mathematical proof.[3] In the present work the general orthogonality for any polynomials depending on a constant is derived without any approximation. Two examples of the associated Laguerre and the Gegenbauer polynomials are presented in order to show the importance of the general orthogonality and its relationship with Morse potential and Ginocchio potential which are frequently used for real chemical or physical quantum systems.

Derivation of General Orthogonality

When $\alpha \neq \alpha'$, obviously there is no relationship between $f_n^{(\alpha)}$ and $f_m^{(\alpha')}(z)$. $f_n^{(\alpha)}$ belongs to the set of $\{f_n^{(\alpha)}(z);\ n = 0,1,2,...\}$ and $f_m^{(\alpha')}(z)$ belonging to $\{f_n^{(\alpha')}(z);\ n = 0,1,2,...\}$. The two sets are distinct from each other. Therefore, if a general orthogonality Eq. (6) should exist, the two constants α and α' should be related to each other. From our previous study on the determination of Ginocchio potential,[4] we learned that a proper relationship between the constants α and α' could be obtained if both α and α' depend on n. Therefore, α in $f_n^{(\alpha)}(z)$ is set to be α_n, *i.e.* $f_n^{(\alpha_n)}(z) = f_n^{(\alpha)}(z)$ and α' in $f_m^{(\alpha')}(z)$ is set to be α_m, *i.e.* $f_m^{(\alpha')}(z) = f_m^{(\alpha_m)}(z)$, which unambiguously exhibits the n-dependence of α.

α always appears in the $g_1(z)$ term in Eq. (1) and is no longer independent of n so that $g_1(z;n)$ notation is used. Now the differential equation of interest is

$$\left[g_2(z)\frac{d^2}{dz^2} + g_1(z;n)\frac{d}{dz} + a_n\right] f_n^{(\alpha_n)}(z) = 0. \tag{7}$$

It is well known that the eigenfunctions of Schrödinger equation are always orthogonal. To exploit this fact, let's transform Eq. (7) to a form of Schrödinger equation.

Let

$$f_n^{(\alpha_n)}(z) = \frac{\Psi_n(z)}{h_n(z)}, \tag{8}$$

then Eq. (7) is

$$\begin{aligned} &g_2(z)\Psi_n''(z) + \left[-2g_2(z)\frac{h_n'(z)}{h_n(z)} + g_1(z;n)\right]\Psi_n'(z) \\ &+\left[-g_2(z)\frac{h_n''(z)}{h_n(z)} + 2g_2(z)\left(\frac{h_n'(z)}{h_n(z)}\right)^2 - g_1(z;n)\frac{h_n'(z)}{h_n(z)} + a_n\right]\Psi_n(z) = 0 \end{aligned} \tag{9}$$

where $\Psi_n'(z) = \frac{d}{dz}\Psi_n(z)$ and $h_n''(z) = \frac{d^2}{dz^2}h_n(z)$, *etc.* Here $\Psi_n(z)$ and $h_n(z)$ are any arbitrary functions.

Further transformation of Eq. (9) using

$$[h_n(z)]^2 = [\varphi(z)]^{-1/2}\exp\left[\int \frac{g_1(z;n)}{g_2(z)}dz\right] \tag{10}$$

yields the equation of

$$\begin{aligned} &g_2(z)\Psi_n''(z) + \frac{1}{2}g_2(z)\frac{d\ln\varphi(z)}{dz}\Psi_n'(z) \\ &+ g_2(z)\begin{bmatrix} -\frac{1}{2}\frac{d}{dz}\left(\frac{g_1(z;n)}{g_2(z)}\right) - \frac{1}{4}\left(\frac{g_1(z;n)}{g_2(z)}\right)^2 + \frac{a_n}{g_2(z)} \\ +\frac{1}{4}\left(\frac{d^2\ln\varphi(z)}{dz^2}\right) + \frac{1}{16}\left(\frac{d\ln\varphi(z)}{dz}\right)^2 \end{bmatrix}\Psi_n(z) = 0. \end{aligned} \tag{11}$$

As mentioned before, two constants $\alpha(=\alpha_n)$ and $\alpha'(=\alpha_m)$ should be related to each other. Let's define a new function $V(z)$ as

$$V(z) = \varphi(z)\begin{bmatrix} \frac{1}{2}\frac{d}{dz}\left(\frac{g_1(z;n)}{g_2(z)}\right) + \frac{1}{4}\left(\frac{g_1(z;n)}{g_2(z)}\right)^2 - \frac{a_n}{g_2(z)} \\ -\frac{1}{4}\left(\frac{d^2\ln\varphi(z)}{dz^2}\right) - \frac{1}{16}\left(\frac{d\ln\varphi(z)}{dz}\right)^2 + \frac{E_n}{\varphi(z)} \end{bmatrix}. \tag{12}$$

Here E_n is a constant depending on n and more importantly the function $V(z)$ is assumed to be independent of n. Eq. (12) can be rewritten as

$$[\varphi(z)]^{-1} = (E_n - E_m)^{-1}\begin{bmatrix} \frac{1}{2}\frac{d}{dz}\left(\frac{g_1(z;m) - g_1(z;n)}{g_2(z)}\right) + \frac{1}{4}\left(\frac{g_1(z;m)}{g_2(z)}\right)^2 \\ -\frac{1}{4}\left(\frac{g_1(z;n)}{g_2(z)}\right)^2 + \frac{a_n - a_m}{g_2(z)} \end{bmatrix}. \tag{13}$$

The n-independence of $V(z)$ (or equivalently n-independence of $\varphi(z)$) guarantees and produces the relationship between α and α'. We call it 'Constraint 1'. This constraint will be clarified by examining the examples in the next section. Inserting Eq. (12) into Eq. (11), one obtains

$$\left[\varphi(z)\frac{d^2}{dz^2} + \frac{1}{2}\frac{d\varphi(z)}{dz}\frac{d}{dz} - V(z) + E_n\right]\Psi_n(z) = 0. \tag{14}$$

Let $\varphi(z)$ be a square of the derivative of z with respect to x, *i.e.*

$$\varphi(z) = \left(\frac{dz}{dx}\right)^2. \tag{15}$$

Since a function is replaced with a derivative, the function $\varphi(z)$ should be smooth and continuous (without singularity) through the interval $a \le z \le b$. This condition brings about another constraint (Constraint 2). Inserting Eq. (15) into Eq. (14), one obtains the Schrödinger equation, *i.e.*

$$\left[-\frac{d^2}{dx^2}+V(x)\right]\Psi_n(x)=E_n\Psi_n(x)\,. \tag{16}$$

$\Psi_n(x)$ are eigenfunctions of the Schrödinger equation (Eq. 16) so that $\Psi_n(x)$ are always orthogonal, *i.e.*, for $E_m \neq E_n$ (or $m \neq n$),

$$\int_{a'}^{b'}\Psi_n(x)\Psi_m(x)dx=\int_a^b\Psi_n(z)\Psi_m(z)\left(\frac{dz}{dx}\right)^{-1}dz=0 \tag{17}$$

where $\Psi_n(x=a')=\Psi_n(z=a)$. Using Eqs. (8), (10) and (15), Eq. (17) can be rewritten as

$$\int_a^b[\varphi(z)]^{-1}\exp\left[\frac{1}{2}\int\frac{g_1(z;n)+g_1(z;m)}{g_2(z)}dz\right]f_n^{(\alpha_n)}(z)f_m^{(\alpha_m)}(z)dz=0\,. \tag{18}$$

Eq. (18) is a new orthogonality which we call the 'general orthogonality'.

Therefore, the final form of general orthogonality is

$$\int_a^b w(z)\,f_n^{(\alpha)}(z)f_m^{(\alpha')}(z)dz=0 \quad (n\neq m) \tag{19}$$

where

$$w(z)=[\varphi(z)]^{-1}\exp\left[\frac{1}{2}\int\frac{g_1(z;n)+g_1(z;m)}{g_2(z)}dz\right] \tag{20}$$

and $[\varphi(z)]^{-1}$ in Eq. (13). Recall that the above orthogonality is valid when the two constraints are satisfied, *i.e.*, combining Constraints 1 and 2, the function $\varphi(z)$ (Eq. 13) should be independent of n and smoothly continuous on $[a,b]$. When $g_1(z;n)=g_1(z)$, *i.e.* $g_1(z)$ is independent of n, one immediately sees that the 'usual orthogonality' (Eqs. 2 and 3) is recovered.

We would like to mention an interesting notion emerging from the above derivation process. As well known, the quantum mechanical interpretation of the Schrödinger equation (Eq. 16) is that $V(x)$ is a potential function, $\Psi_n(x)$ wave functions, and E_n eigenenergies. It implies that once a differential equation of the form (Eq. 1) is exactly solved, the Schrödinger equation for a quantum system having a potential $V(x)$ can be exactly solved. A detailed work on this subject will be reported in the near future.

Usage of General Orthogonality

Let us apply the 'general orthogonality' to the associated Laguerre polynomials for which the differential equation is

$$\left[g_2(z)\frac{d^2}{dz^2}+g_1(z;n)\frac{d}{dz}+a_n\right]f_n^{(\alpha_n)}(z)=0 \tag{21}$$

where, $f_n^{(\alpha_n)}(z)=L_n^{(\alpha_n)}(z)$, $g_2(z)=z$, $g_1(z;n)=\alpha_n+1-z$, and $a_n=n$. The orthogonality limits are $a=0$ and $b=\infty$. Evaluating $\varphi(z)$ (Eq. 13), one obtains

$$[\varphi(z)]^{-1}=\frac{(\alpha_m)^2-(\alpha_n)^2}{4(E_n-E_m)}\left[1+\frac{2(\alpha_n-\alpha_m+2n-2m)}{(\alpha_m)^2-(\alpha_n)^2}z\right]z^{-2}\,. \tag{22}$$

Since $\varphi(z)$ should be independent of n (Constraint 1), one can set

$$\lambda=\frac{(\alpha_m)^2-(\alpha_n)^2}{2(\alpha_n-\alpha_m+2n-2m)} \tag{23}$$

where λ is a number (independent of n). Also Constraint 2, *i.e.* $\varphi(z)$ should be smooth and continuous, requires that $\lambda \geq 0$. The coefficient in front of the bracket in Eq. (22) will be canceled out later. Then the general orthogonality is, by evaluating Eqs. (19) and (20),

$$\int_0^\infty(1+\lambda^{-1}z)z^{(\alpha+\alpha'-2)/2}\exp(-z)L_n^{(\alpha)}(z)L_m^{(\alpha')}(z)dz=0 \quad (n\neq m;\alpha\neq\alpha') \tag{24}$$

where

$$(\alpha+\lambda)^2+4\lambda n=(\alpha'+\lambda)^2+4\lambda m\,. \tag{25}$$

Eq. (25) is a constraint determined by using Eq. (23). Recall that $\alpha\equiv\alpha_n$ and $\alpha'\equiv\alpha_m$.

The most well known example of a potential having the associated Laguerre polynomials as wave functions is Morse potential. The eigenfunctions of Morse potential have been correctly assumed to be orthogonal since the pioneering work of Morse.[5] In the present work we have explicitly shown how the associated Laguerre polynomials can be orthogonal even when $\alpha\neq\alpha'$.

Ginocchio found a new class of exactly solvable potentials called 'Ginocchio potentials' which resemble the potentials appearing in the mean field study of an atomic nucleus.[3,6] Due to its formal simplicity Ginocchio potentials have been utilized widely. For example, they were used to test various theoretical approximations involving one dimensional potentials.[7,8] Furthermore Ginocchio first introduced the 'general orthogonality' and its exact form for Ginocchio potentials.[3]

The wave functions for Ginocchio potentials are the Gegenbauer polynomials. Now we drive the orthogonality by using our general form of orthogonality, Eqs. (19) and (20). For the Gegenbauer polynomials, $f_n^{(\alpha_n)}(z)=C_n^{(\alpha_n)}(z)$, $g_2(z)=1-z^2$, $g_1(z;n)=-(2\alpha_n+1)z$, and $a_n=n(n+2\alpha_n)$. The orthogonality limits are $a=-1$ and $b=1$. Evaluating $\varphi(z)$ (Eq. 13), one obtains

$$[\varphi(z)]^{-1}=\frac{n(n+2\alpha_n)+\alpha_n-m(m+2\alpha_m)-\alpha_m}{E_n-E_m}$$
$$\otimes\left[1+\left(\frac{-(\alpha_n)^2+\alpha_n+(\alpha_m)^2-\alpha_m}{n(n+2\alpha_n)+\alpha_n-m(m+2\alpha_m)-\alpha_m}-1\right)z^2\right](1-z^2)^{-2}\,. \tag{26}$$

Again $\varphi(z)$ should be independent of n (Constraint 1), *i.e.*

$$\lambda^{-2}=\frac{-(\alpha_n)^2+\alpha_n+(\alpha_m)^2-\alpha_m}{n(n+2\alpha_n)+\alpha_n-m(m+2\alpha_m)-\alpha_m} \tag{27}$$

where λ is a number. Also Constraint 2 requires that $\lambda^2>0$.

The general orthogonality is, by evaluating Eqs. (19) and (20),

$$\int_{-1}^{1} [1+(\lambda^{-2}-1)z^2](1-z^2)^{(\alpha+\alpha'-3)/2} C_n^{(\alpha)}(z) C_m^{(\alpha')}(z) dz = 0 \quad (n \neq m; \alpha \neq \alpha') \tag{28}$$

where

$$\left[\left(\alpha-\frac{1}{2}\right)\lambda^2+\frac{1}{2}+n\right]^2-(1-\lambda^2)n(n+1) = \left[\left(\alpha'-\frac{1}{2}\right)\lambda^2+\frac{1}{2}+m\right]^2-(1-\lambda^2)m(m+1). \tag{29}$$

It is the exactly same form as the general orthogonality for Gegenbauer polynomials presented in Ginocchio's work.[3]

What is the constant λ? When $\alpha = \alpha'$ and $\lambda \to \infty$, Eq. (28) becomes

$$\int_{-1}^{1} (1-z^2)^{\alpha-1/2} C_n^{(\alpha)}(z) C_m^{(\alpha)}(z) dz = 0 \quad (n \neq m). \tag{30}$$

It is the usual orthogonality for the Gegenbauer polynomials which are the wave functions for a certain potential, for example, Scarf I potential. Recall that Scarf I potential does not have the λ in it.[7] Ginocchio potentials whose wave functions are also the Gegenbauer polynomials have the λ (as an extra parameter) in it. The present derivation clearly explains why the general orthogonality (Eq. 28) should be applied to Ginocchio potentials, not the usual orthogonality (Eq. 30).

We have shown how the 'general orthogonality' for the associated Laguerre and the Gegenbauer polynomials can be determined by using the general form in Eqs. (19) and (20). It clearly confirms that there exists the 'general orthogonality' for certain polynomials. Probably the application of this formalism to Jacobi polynomials $P_n^{(\alpha,\beta)}(z)$ is very interesting because they have two constants α and β. However, we do not discuss about it at this moment because the *most general form* of potentials having Jacobi polynomials in their wave functions is not known yet even though various (but particular) forms of potentials having Jacobi polynomials have been reported.[7,9]

Conclusion

The general orthogonality for certain orthogonal polynomials is derived (Eqs. 19 and 20). The orthogonality is found to be valid when a certain constraint (or requirement) is satisfied, *e.g.* Eq. (25) for the associated Laguerre polynomials or Eq. (29) for the Gegenbauer polynomials. The constraint is related to the eigenenergies E_n and the wave functions $\Psi_n(x)$ of the corresponding Schrödinger equation (Eq. 16), which, in turn, provides a clue to finding the exactly solvable potential $V(x)$. Another words, for some exactly solvable potentials the 'usual orthogonality' is not valid, instead the 'general orthogonality' condition should be used.

Finally we would like to point out two interesting questions unanswered in the present work. The first question is – Can the general orthogonality for Jacobi polynomials be similarly derived? Since there are various exactly solvable potentials having Jacobi-like polynomials, the question should be answered. The second question is on $\varphi(z)$, *i.e.* Eq. (15). The derivative function has been assumed to be independent of n so that we could find an algebraic expression for the constraint. If the derivative function $\varphi(z)$ depends on n, will one still be able to determine or find an expression for the constraint? The answers to the two questions are perhaps "yes". A continuing study on the questions is under way.

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