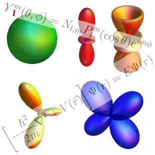
Generating recurrence and ladder-type relations for Orthogonal Polynomials and Special Functions with applications to Quantum Systems

Renato Álvarez-Nodarse



AMS-EMS-SPM Meeting, Porto, 10-13 June 2015

Plan

1. From Quantum Mechanics ...
2. Generating recurrence and ladder-type relations for SF & OP
3. The "discrete" case: SF & OP on linear-type lattices
4. What to do else?

A pure mathematical heresy

Special Functions (SF) appear in (almost) all context of Mathematics and other Sciences.

As Alberto Grunbaum one time said: "*Special functions are to mathematics what pipes are to a house: nobody wants to exhibit them openly but nothing works without them*".

We will show Alberto's statement in the case of Quantum Mechanics.

Solving the Schrödinger Equation

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A usual method for solving the SE is to expand the unknown wave functions $|\Phi\rangle$ in the "finite" basis $\{|\Phi_k\rangle\}_{k=1}^{\infty}$, i.e.,

$$|\Phi\rangle = \sum_{k=1}^{N} C_{Nk}|\Phi_k\rangle\,,$$

that leads to the linear system of equations

$$\sum_{k=1}^{N} C_{Nk}\langle\Phi_m|\mathcal{H}|\Phi_k\rangle = \varepsilon C_{Nm} \quad \Longleftrightarrow \quad \sum_{k=1}^{N} C_{Nk}h_{mk} = \varepsilon C_{Nm}$$

where h_{mk} denotes the matrix elements $h_{mk} = \langle\Phi_m|\mathcal{H}|\Phi_k\rangle$.

From an analytic to an algebraic problem

$$\begin{pmatrix} h_{11} & h_{12} & \dots & h_{1\,N-1} & h_{1\,N} \\ h_{21} & h_{22} & \dots & h_{2\,N-1} & h_{2\,N} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ h_{N-1} & h_{N-1\,2} & \dots & h_{N-1\,N-1} & h_{N-1\,N} \\ h_{N1} & h_{N2} & \dots & h_{N\,N-1} & h_{N\,N} \end{pmatrix} \begin{pmatrix} C_{N1} \\ C_{N2} \\ C_{N3} \\ \vdots \\ C_{N-1N} \\ C_{NN} \end{pmatrix} = \varepsilon \begin{pmatrix} C_{N1} \\ C_{N2} \\ C_{N3} \\ \vdots \\ C_{N-1N} \\ C_{NN} \end{pmatrix} \quad \Rrightarrow$$

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Here we have two non-trivial problem:

1. Compute the matrix elements $\langle \Phi_m | \mathcal{H} | \Phi_k \rangle$ for certain potentials $\mathcal{H} = -\dfrac{\hbar^2}{2m}\Delta + V(x, y, x)$.
2. The matrix H is in general a dense matrix.

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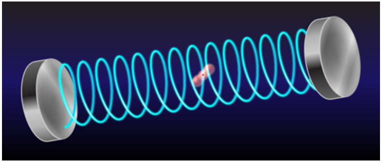
In this talk we will focus on the first problem. In fact, for solving it is convinient to know certain linear relations between **eigenestates Φ_n and its derivatives $\Phi_n^{(k)}$**, namely RR of the form $\mathbf{A_1 \Phi_{n_1}^{(k_1)} + A_2 \Phi_{n_2}^{(k_2)} + A_3 \Phi_{n_2}^{(k_3)} = 0}$



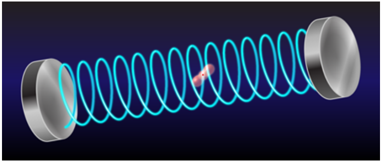
The N-dimensional isotropic harmonic oscillator (IHO) is described by the SE

$$\left(-\Delta + \frac{1}{2}\lambda^2 r^2\right)\Psi = E\Psi, \qquad \Delta = \sum_{k=1}^{N} \frac{\partial^2}{\partial x_k^2}, \quad r = \sqrt{\sum_{k=1}^{n} x_k^2}\,.$$

Its solution has the form $\Psi = R_{nl}^{(N)}(r) Y_{lm}(\Omega_N)$, where $R_{nl}^{(N)}(r)$ is the radial part, usually called the **radial wave functions**, defined by

$$R_{nl}^{(N)}(r) = \mathcal{N}_{nl}^{(N)}\; r^l e^{-\frac{1}{2}\lambda r^2} \mathbf{L_n^{l+\frac{N}{2}-1}}(\lambda \mathbf{r^2}), \;\; \mathcal{N}_{nl}^{(N)} = \sqrt{\frac{2n!\lambda^{l+\frac{N}{2}}}{\Gamma\left(n+l+\frac{N}{2}\right)}},$$

$n = 0, 1, 2, \dots$ and $l = 0, 1, 2, \dots$, are the quantum numbers, $N \geq 3$ the dimension of the space.



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$n=0,1,2,\ldots$ and $l=0,1,2,\ldots,$ are the quantum numbers, $N\geq 3$ the dimension of the space. $\mathbf{L}_{\mathbf{n}}^{\alpha}(\mathbf{z})$ are the **Laguerre** OP.

How to obtain RR for the $R_{nl}^{(N)}(r)$ functions?

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Use $L_n^{l+\frac{N}{2}-1}(\lambda r^2) = \left(\mathcal{N}_{n,l}^{(N)}\right)^{-1} r^{-l} e^{\frac{1}{2}\lambda r^2} R_{nl}^{(N)}(r)$ substitute and symplify.

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Teorema (Cardoso & RAN, JPA 2003 RR à la carte)

Let $R_{nl}^{(N)}(r)$, $R_{n+n_1,l+l_1}^{(N)}(r)$ *and* $R_{n+n_2,l+l_2}^{(N)}(r)$ *be 3 different radial functions of the N-th dimensional I.H.O.,* $n_1, n_2, l_1, l_2 \in \mathbb{Z}$

- *If* $\min(n+n_1, n+n_2, l+l_1, l+l_2) \geq 0 \Longrightarrow \exists$ *non-vanishing polynomials* A_0, A_1, *and* A_2, *such that* **(General TTRR)**

$$\mathbf{A_0(r)R_{n,l}^{(N)}(r) + A_1(r)R_{n+n_1,l+l_1}^{(N)}(r) + A_2(r)R_{n+n_2,l+l_2}^{(N)}(r) = 0}.$$

- *If* $\min(n+n_1, l+l_1) \geq 0$ *and* $(n_1)^2 + (l_1)^2 \neq 0 \Longrightarrow \exists \neq 0$ *polynomials* A_0, A_1, *and* A_2, *s.t.* **(ladder-type RR)**

$$\mathbf{A_0(r)R_{n,l}^{(N)}(r) + A_1(r)\frac{d}{dr}R_{n,l}^{(N)}(r) + A_2(r)R_{n+n_1,l+l_1}^{(N)}(r) = 0}.$$

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Proof: It is based on an old Lemma by Nikiforov and Uvarov proved in their classical book *Special Functions of Mathematical Physics: A Unified Introduction with Applications* (published for the first time in 1972).

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Using this technique, it is very simple to obtain concrete relations between three different *radial functions* of the I.H.O.

Let see some examples.

Example of application

From the relation between $R^{(N)}_{n,l}(r)$ and $L_n^{l+\frac{N}{2}-1}(\lambda r^2)$

$$A_0 R^{(N)}_{n,l} + A_1 R^{(N)}_{n+n_1,l+l_1} + A_2 R^{(N)}_{n+n_2,l+l_2} = 0$$

$$\Updownarrow$$

$$C_0 L_n^{l+\frac{N}{2}-1} + C_1 L_{n+n_1}^{(l+l_1)+\frac{N}{2}-1} + C_2 L_{n+n_2}^{(l+l_2)+\frac{N}{2}-1} = 0$$

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- Now we substitute $n_1 = -1$, $n_2 = 1$, $l_1 = l_2 = 0$ and $\alpha = l + \frac{N}{2} - 1 \Rightarrow$

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Comparing it with the TTRR $\Rightarrow$ $C_0 = s - (2n + \alpha + 1)$, $C_1 = n + \alpha$ and $C_2 = n + 1$. Coming back to $R^{(N)}_{n,l}$

$$\sqrt{n\left(n+l+\frac{N}{2}-1\right)} R^{(N)}_{n-1,l}(r) + \left[\lambda r^2 - \left(2n+l+\frac{N}{2}\right)\right] R^{(N)}_{n,l}(r) + \sqrt{(n+1)\left(n+l+\frac{N}{2}\right)} R^{(N)}_{n+1,l}(r) = 0.$$

Another example of application: ladder operators

$$A_0 R_{n,l}^{(N)}(r) + A_1 \frac{d}{d\,r} R_{n,l}^{(N)}(r) + A_2 R_{n+n_1,l+l_1}^{(N)}(r) = 0$$

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$$B_0 L_n^{l+\frac{N}{2}-1}(s) + B_1 L_{n-1}^{l+\frac{N}{2}}(s) + B_2 L_{n+n_1}^{(l+l_1)+\frac{N}{2}-1}(s) = 0$$

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Since L_n^{α} and $(L_n^{\alpha})'$ are l.i. $\Rrightarrow B_0 = 0$, $B_1 = -B_2$. Thus choosing $B_2 = 1$

$$\left[\frac{d}{dr} + \lambda r - \frac{l}{r}\right] R_{n,l}^{(N)}(r) = -2\sqrt{\lambda n} R_{n-1,l+1}^{(N)}(r).$$

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For other SF (not OP) [Cardoso, Fernandes & RAN, ETNA 2009]

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The starting point is the hyp. eq. on a lattice $x(s)$

$$\sigma(s)\frac{\Delta}{\Delta x(s-\frac{1}{2})}\left[\frac{\nabla y(s)}{\nabla x(s)}\right]+\tau(s)\frac{\Delta y(s)}{\Delta x(s)}+\lambda y(s)=0$$

$$\Delta f(s)=f(s+1)-f(s),\quad \nabla f(s)=\Delta f(s-1),\quad \deg\sigma\leq 2,\, \deg\tau\leq 1$$

$$x(s)=\mathbf{c_1(q)q^s}+\mathbf{c_2(q)q^{-s}}\quad \text{or}\quad x(s)=\mathbf{c_1 s^2}+\mathbf{c_2 s}.$$

What about the linear-type lattices? (Discrete QM)

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Teorema (RAN & Cardoso JMAA 2013)

Let $x(s)$ be a linear-type lattice $x(s)=q^s$ or $x(s)=s$. Then, any three functions $y_{\nu_i}^{(k_i)}(s)$, $i=1,2,3$, are connected by a linear relation

$$\sum_{i=1}^{3}B_i(s)y_{\nu_i}^{(k_i)}(s)=0,\qquad y_n^{(k)}(s):=\Delta^{(k)}y_n(s)$$

where the $B_i(s)$, $i=1,2,3$, are polynomials.

The simplest corollaries

Corollary (three-term recurrence relation)

$$A_1(s)y_\nu(s) + A_2(s)y_{\nu+1}(s) + A_3(s)y_{\nu-1}(s) = 0,$$

where the coefficients $A_i(s)$, $i = 1, 2, 3$, *are polynomials.*

Corollary (Δ and ∇-ladder-type relations)

$$B_1(s)y_\nu(s) + B_2(s)\frac{\Delta y_\nu(s)}{\Delta x(s)} + B_3(s)y_{\nu+m}(s) = 0, \qquad m \in \mathbb{Z},$$

$$C_1(s)y_\nu(s) + C_2(s)\frac{\nabla y_\nu(s)}{\nabla x(s)} + C_3(s)y_{\nu+m}(s) = 0, \qquad m \in \mathbb{Z},$$

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Special important cases: $m = 1$ and $m = -1$

These operators are usually called **raising** and **lowering** operators, respectively.

In [RAN, Atakishiyev, Costas, JPA 2005 & ETNA 2007] we have construct some discrete **quantum** oscillators associated with several OP on discrete variables.

For these systems the *wave functions* are

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We can use the same idea: To write $P_n(z) = \dfrac{d_n}{\sqrt{\rho(z)\Delta x(s-1/2)}}\psi_n(z)$; and

then use the RR $\displaystyle\sum_{i=1}^{3} B_i(s) P_{n_i}^{(k_i)}(s) = 0$ to obtain the RR for ψ_n

Δ-Ladder operators for Charlier oscillator [Atakishiyev & Suslov 1990]

The wave function is: $\psi_n^\mu(z) = \sqrt{\dfrac{e^{-\mu}\mu^{z-n}}{\Gamma(z+1)n!}}\, C_n^\mu(z)$

$$\left[\sqrt{\mu}B_1 + \left(\sqrt{z+1} - \sqrt{\mu}\right) B_2\right] \psi_n^\mu(z) + B_2\sqrt{z+1}\Delta\psi_n^\mu(z)$$

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- Case $m = -1$

$$\searrow \quad \left(\sqrt{z+1} - \sqrt{\mu}\right)\psi_n^\mu(z) + \sqrt{z+1}\Delta\psi_n^\mu(z) - \sqrt{n}\,{\psi_{n-1}}^\mu(z) = 0$$

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- Caso $m = 1$

$$\nearrow \quad \left[(\mu - z)(\mu + n - z) - \mu(\sqrt{\mu} - \sqrt{z+1})\right]\psi_n^\mu(z)$$

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♦ RAN and J. L. Cardoso: Recurrence relations for discrete hypergeometric functions. J. Difference Equations. Appl. 11 (2005) 829-850

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For more complicated examples

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What about the general quadratic lattice $x(s) = c_1 q^s + c_2 q^{-s} + c_3$?

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Thanks