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POLYNOMIALS OF A DISCRETE VARIABLE, DYNAMICAL SYMMETRIES AND QUANTUM MECHANICS

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Abstract

In the case of exactly solvable problems, the dynamical symmetries give a group theoretical setting for the Lanczos method. They will be used to obtain recurrence relations for classical orthogonal polynomials of a discrete variable. Specifically, the one-dimensional harmonic oscillator and the radial part of the Schrödinger equation for the three-dimensional harmonic oscillator and the hydrogen atom are shown to provide an algebraic interpretation of the Charlier and Meixner polynomials respectively. As a byproduct, realizations of the oscillator and su(1,1) algebras in terms of finite difference operators can be constructed. The connection with coherent states is also mentioned.

Difference equations play an important rôle in physics: besides being naturally suited to the description of discrete physical systems, they appear whenever a differential equation is discretized on a lattice. It is therefore natural to investigate their symmetry properties, in the hope that such a study be as fruitful as it was in the case of differential equations. Amongst the questions that come to mind, is the following: how can one construct realizations of Lie algebras in terms of operators acting on functions of a discrete variable, and what are, then, the relevant functions? The purpose of this talk is to show that such a program can be realized [1] within the context of elementary quantum mechanics, and that the functions spanning irreducible representation spaces are classical orthogonal polynomials of a discrete variable [2].

Our starting point will be the Lanczos method [3] which, given a self-adjoint Hamiltonian H and a state u_0 that is not an eigenstate of H, provides a set of orthogonal functions $\{u_0, u_1, u_2, ...\}$, and two sets of numbers $\{a_0, a_1, ...\}$ and $\{b_1, b_2, ...\}$ such that the three-term recurrence relation

$$Hu_n = b_n u_{n-1} + a_n u_n + b_{n+1} u_{n+1} \tag{1}$$

holds. Expanding solutions ψ_E of the eigenvalue problem $H\psi_E = E\psi_E$ on the Lanczos basis,

$$\psi_E = \sum_n P_n(E) u_n \,, \tag{2}$$

one readily obtains a recurrence representation of the Schrödinger equation ,

$$EP_n(E) = a_n P_n(E) + b_{n+1} P_{n+1}(E) + b_n P_{n-1}(E) \,. \tag{3}$$

Now, for exactly solvable problems, dynamical symmetries allow one to derive analytical expressions for the sets $\{u_n\}$, $\{a_n\}$ and $\{b_n\}$. The three-term recurrence relation (3) then defines orthogonal polynomials $P_n(E)$ and one may view Eq.(2) as an addition law for the

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u_n's and the P_n's. In particular, for Hamiltonians with a discrete spectrum, one deals with polynomials $P_n(E_k)$ of a discrete variable E_k.

In order to illustrate these considerations, let us apply them to the Hamiltonian of a one-dimensional harmonic oscillator, $H = \frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2$, which can be rewritten as $H = A^\dagger A + \frac{1}{2}$ in terms of the usual creation and annihilation operators $A^\dagger = \frac{1}{\sqrt{2}}[-\frac{d}{dx} + x]$ and $A = \frac{1}{\sqrt{2}}[\frac{d}{dx} + x]$. This system can be solved exactly, because it has a symmetry algebra, the oscillator algebra, which is formed of the generators A, $A^\dagger$, H and I, with the commutation relations

$$[A, A^\dagger] = I, \quad [H, A^\dagger] = A^\dagger, \quad [H, A] = -A, \quad [I, \bullet] = 0. \tag{4}$$

A Lanczos basis can be constructed by introducing the set of eigenvectors $\{\tilde{u}_n\}$ of the Hamiltonian $\tilde{H} = \frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}(x-a)^2$ for a shifted harmonic oscillator. Just as H, $\tilde{H}$ can be written in a factorized manner, $\tilde{H} = \tilde{A}^\dagger \tilde{A} + \frac{1}{2}$, with $\tilde{A}^\dagger = A^\dagger - a/\sqrt{2}$ and $\tilde{A} = A - a/\sqrt{2}$. As usual,

$$\tilde{H}|\tilde{u}_n >= (n + \tfrac{1}{2})|\tilde{u}_n >, \quad \tilde{A}^\dagger|\tilde{u}_n >= \sqrt{n+1}|\tilde{u}_{n+1} >, \quad \tilde{A}|\tilde{u}_n >= \sqrt{n}|\tilde{u}_{n-1} > . \tag{5}$$

It is worth noticing that $\tilde{u}_0$, the first state of the Lanczos basis, obeys the relation $\tilde{A}|\tilde{u}_o >= 0$, so that the relation between A and $\tilde{A}$ implies $A|\tilde{u}_0 >= \frac{a}{\sqrt{2}}|\tilde{u}_0 >$. Thus, $\tilde{u}_0$ is a coherent state of the unshifted oscillator, restricted to a real eigenvalue of A.

The three-term recurrence relation (1) for this problem follows immediately from the relation between H and $\tilde{H}$,

$$H = \tilde{H} + \frac{a}{\sqrt{2}}\left(\tilde{A}^\dagger + \tilde{A}\right) + \frac{a^2}{2}, \tag{6}$$

and from Eqs. (5):

$$H|\tilde{u}_n >= \left(n + \tfrac{1}{2}(1 + a^2)\right)|\tilde{u}_n > + \frac{a}{\sqrt{2}}\left(\sqrt{n}\,|\tilde{u}_{n-1} > + \sqrt{n+1}|\tilde{u}_{n+1} >\right). \tag{7}$$

Let us now introduce in the Schrödinger equation, $H|\psi_k >= (k + \frac{1}{2})|\psi_k >$, the expansion of ψ_k on the Lanczos basis,

$$|\psi_k >= \sum_{n=0}^{\infty}\left(\frac{\sqrt{2}}{a}\right)^n \frac{1}{\sqrt{n!}}\,\nu(k)\,P_n(k)\,|\tilde{u}_n >, \tag{8}$$

$\nu(k)$ being a normalisation factor to be determined presently. Using (1) and the orthogonality of the $\tilde{u}$'s, we easily get the recurrence relation

$$P_{n+1}(k) = \left(k - n - \frac{a^2}{2}\right)P_n(k) - n\frac{a^2}{2}P_{n-1}(k). \tag{9}$$

that defines [2] the Charlier polynomials $C_n^{(a^2/2)}(k) \equiv P_n(k)$. These polynomials of a discrete variable obey the orthogonality relations

$$\sum_{k=0}^{\infty} C_m^{(\alpha)}(k)\,C_n^{(\alpha)}(k)\,\frac{e^{-\alpha}\,\alpha^k}{k!} = \alpha^n\,n!\,\delta_{mn} \tag{10}$$

as well as the dual ones

$$\sum_{n=0}^{\infty} C_n^{(\alpha)}(k)\,C_n^{(\alpha)}(l)\,\frac{e^{-\alpha}\,\alpha^{-n}}{n!} = \alpha^{-k}\,k!\,\delta_{kl}. \tag{11}$$

The normalisation condition $\|\psi\|^2 = 1$ yields the factor

$$\nu(k) = e^{-a^2/4}\left(\frac{a}{\sqrt{2}}\right)^k \frac{1}{\sqrt{k!}}, \tag{12}$$

as a consequence of (11).

At this point, it is a simple matter to construct a realization of the oscillator algebra in terms of the forward difference operator

$$T_k f(k) \equiv f(k+1). \tag{13}$$

and its inverse T_k^{-1}. Indeed, rewriting (9) in terms of Charlier polynomials, and introducing (8) in the relations $A|\psi_k >= \sqrt{k}|\psi_{k-1} >$ and $A^\dagger|\psi_k >= \sqrt{k+1}|\psi_{k+1} >$, we get three equations,

$$\begin{aligned}
(k - n - \alpha)C_n^{(\alpha)}(k) - \alpha n C_{n-1}^{(\alpha)}(k) &= C_{n+1}^{(\alpha)}(k), \\
(T_k - 1)C_n^{(\alpha)}(k) &= n C_{n-1}^{(\alpha)}(k), \qquad \alpha \equiv a^2/2 \\
(kT_k^{-1} - \alpha)C_n^{(\alpha)}(k) &= C_{n+1}^{(\alpha)}(k),
\end{aligned} \tag{14}$$

which provide the starting point for constructing such a realization. Since k, T_k and kT_k^{-1} are operators acting on functions of the discrete variable k, we will denote them by $\hat{k}$, $\hat{T}_k$ and $\hat{k}\hat{T}_k^{-1}$, so as to avoid any confusion. These operators obey the commutation relations

$$[\hat{T}_k, \hat{k}\hat{T}_k^{-1}] = I, \quad [\hat{k}, \hat{k}\hat{T}_k^{-1}] = \hat{k}\hat{T}_k^{-1}, \quad [\hat{k}, \hat{T}_k] = -\hat{T}_k. \tag{15}$$

Thus, the identification

$$\hat{T}_k \sim A, \quad \hat{k}\hat{T}_k^{-1} \sim A^\dagger, \quad \hat{k} \sim H, \tag{16}$$

provides an isomorphism with the oscillator algebra, and from Eqs.(14) the Charlier polynomials are seen to span a representation of this algebra . Using (10) to construct normalized polynomials $|n >\equiv (\alpha^n n!)^{-\frac{1}{2}}C_n^{(\alpha)}(k)$, one can define matrix elements of operators $\hat{O}(k)$ between these polynomials,

$$< m|\hat{O}(k)|n > \equiv \sum_{k=0}^{\infty}\frac{\alpha^k\,e^{-\alpha}}{k!\sqrt{\alpha^{m+n}\,m!\,n!}}C_m^{(\alpha)}\hat{O}(k)C_n^{(\alpha)}(k). \tag{17}$$

It is then easy to obtain from (14) the following representation of $\hat{k}$, $\hat{T}_k$ and $\hat{k}\hat{T}_k^{-1}$ in terms of infinite matrices:

$$\begin{aligned}
< m|\hat{k}|n > &= \sqrt{\alpha(n+1)}\,\delta_{m\,n+1} + (n+\alpha)\,\delta_{m\,n} + \sqrt{\alpha n}\,\delta_{m\,n-1}, \\
< m|\hat{T}_k|n > &= \delta_{m\,n} + \sqrt{\frac{n}{\alpha}}\,\delta_{m\,n-1}, \\
< m|\hat{k}\hat{T}_k^{-1}|n > &= \alpha\delta_{m\,n} + \sqrt{\alpha(n+1)}\,\delta_{m\,n+1}.
\end{aligned} \tag{18}$$

Quite obviously, (16) is not the only possible identification. Had we chosen, rather, $A \sim \alpha^{\frac{1}{2}}(\hat{T}_k - 1)$, $A^\dagger \sim \alpha^{-\frac{1}{2}}(\hat{k}\hat{T}_k^{-1} - \alpha)$ and $H \sim (\hat{k} - \alpha\hat{T}_k - \hat{k}\hat{T}_k^{-1} + \alpha + 1/2)$, we would have recovered the standard representation of the oscillator algebra.

A similar analysis can be performed for other problems. The radial part of the Hamiltonian for a three-dimensional harmonic oscillator $H_r = H + K$, where $H = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2}$, and $K = \frac{1}{2}r^2$, has a su(1,1) dynamical symmetry. In a Cartan basis, the generators of this symmetry are $\mathcal{R} \equiv H_r/2 = \frac{1}{2}(K+H)$ and $L_\pm = \frac{1}{2}(K-H) \pm iD$, with $D \equiv \frac{i}{2}\left(r\frac{d}{dr} + \frac{1}{2}\right)$. The scale transformation $r \to \omega r$, $\mathcal{R} \to \tilde{\mathcal{R}} = \frac{1}{2}(\omega^2 K + \omega^{-2} H)$ and $L_\pm \to \tilde{L}_\pm = \frac{1}{2}(\omega^2 K - \omega^{-2} H) \pm iD$ is an inner automorphism of this algebra. Proceeding as in the one-dimensional case, we expand the eigensolutions of $\mathcal{R}|k;l>= (d+k)|k;l>$ on the Lanczos basis formed by those of $\tilde{\mathcal{R}}|\widetilde{n;l}>= (d+n)|\widetilde{n;l}>$,

$$|k;l>= \mu(k) \sum_{n=0}^{\infty} \left(\frac{1-\tau_+}{\tau_-}\right)^n [n!\,(2d)_n]^{-1/2} Q_n(k) |\widetilde{n;l}>, \tag{19}$$

where $\tau_\pm = \frac{1}{2}(\omega^{-2} \pm \omega^2)$, $d = \frac{1}{2}(l + 3/2)$, $(2d)_n = 2d(2d+1)...(2d+n-1)$, and $\mu(k)$ is a normalisation factor. The coefficients Q_n can be shown to obey the recurrence relation

$$\frac{\tau_+ - 1}{\tau_+ + 1} Q_{n+1}(k) = \frac{2}{\tau_+ + 1}\left(\tau_+ n - k + d(\tau_+ - 1)\right) Q_n(k) - n(n+2d-1) Q_{n-1}(k), \tag{20}$$

which defines [2] the Meixner polynomials of the first kind $m_n(k; 2d, c) \equiv Q_n(k)$, with $c \equiv \frac{\tau_+ - 1}{\tau_+ + 1}$. The identification

$$\hat{k} + d \sim \mathcal{R}, \quad \hat{k}\hat{T}_k^{-1} \sim L_+, \quad (\hat{k} + 2d)\hat{T}_k \sim L_-, \tag{21}$$

provides a realization of su(1,1) in terms of difference operators, and the Meixner polynomials span representations of this algebra. Finally, the states $|\widetilde{0;l}>$, which initiate the Lanczos basis for each value of l, are the su(1,1) coherent states $|\widetilde{0;l}>\sim e^{\sqrt{c}L_+}|0;l>$.

In order to apply such an analysis to the radial part of the Schrödinger equation for the Coulomb problem, $\left[-\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + \frac{Z}{r}\right]\psi = E\psi$, one has to consider separately the attractive and the repulsive cases. For bound states of the hydrogen problem ($Z < 0$), the change of variable $r \to x = (-8E_{nl})^{1/2} r$ transforms the Schrödinger equation into $R(x) y_{nl} = (d+n) y_{nl}$, with $R(x) \equiv -x\frac{d^2}{dx^2} + \frac{l(l+1)}{x^2} + \frac{x}{4}$ and $d = l+1$. The operators $L_\pm(x) = R(x) - \frac{x}{2} \pm x\frac{d}{dx}$ and R are the generators of a su(1,1) algebra, and one is faced with a problem analogous to that of the three-dimensional oscillator, involving Meixner polynomials. Of course, one does not expect to encounter polynomials of a discrete variable in the repulsive case ($Z > 0$), which involves only a continuous spectrum. However, by exploiting the dynamical algebra of the problem in the above manner, one can easily derive the expansion of Coulomb wave functions in terms of Laguerre and Pollaczek polynomials [4].

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