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A new realisation of dynamical groups and factorisation method

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Abstract. A new method of algebraisation of quantum mechanical eigenvalue equations is presented. In this method the dynamical algebra is represented on the space of group matrix elements. The ladder operators of the dynamical algebra are obtained from Infeld-Hull-Miller factorisations. The method is used to study the first Pöschl-Teller equation even in the non-symmetric case. The energy spectrum and the exact normalised solutions are obtained in agreement with the results of non-algebraic methods.

1. On different algebraisation methods

It is known that the matrix element of a representation of the rotation group, $D^J_{mn}(\theta, \phi)$, plays a double role in quantum mechanics. It can represent a wavefunction, and thus a state, namely a rotational state of angular momentum J and with angular momentum components m and n along the space-fixed and body-fixed axes. It can also represent a transformation of a state into another state, and thus the matrix element of an observable. The identification of states with rotations can be understood if we think that *all* states of a rotator are obtained from some reference state by *all* possible rotations. In this work, we generalise this idea so that wavefunctions are in fact identified with the matrix elements of group elements in some representation. The differential operators of the wave equation act in the space of these matrix elements $V^S_{n'n}(g)$, where $g \in G$, $V^S(g)$ is its representation and $V^S_{nn'}$ are the matrix elements of $V(g)$ in the representation S with respect to a basis of states $\{n\}$. The observables, being elements of the Lie algebra of G or its enveloping algebra, act on $V^S_{n'n}(g)$ so that the Lie algebra is itself represented on the space of matrix elements of G.

By now Lie algebraic methods are commonly used to algebraise the wave equation or Hamiltonian representing a physical system (Barut 1972, Wybourne 1974). (For more recent examples see Arima and Iachello (1979), Jackiw (1980) and Frank and Wolf (1984).) There exist primarily two methods of algebraisation. In the first method, dating back to Casimir (1931a, b), the physical equation is expressed in terms of Casimir products of the operators which close under a Lie algebra. For one-dimensional problems which require a Lie algebra of rank one the corresponding bound state, scattering state and zero-energy solutions are respectively obtained by using unitary representations of SO(3), SO(2, 1) and E(2).

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The second method is very suitable for three-dimensional problems (Barut 1967, Fronsdal 1967, Nambu 1967). In this BFN method the physical equation is expressed as a linear form on the Lie algebra, e.g. $[(1-E)\Gamma_0+(1+E)\Gamma_4+c]|\psi\rangle=0$, where c is a constant and where $\Gamma_0=L_{56}$, $\Gamma_4=L_{46}$ and another operator $S=L_{45}$ form an SO(2, 1) subalgebra of SO(4, 2). The dynamical symmetry of the physical system is provided by the subgroup $SO(3)\otimes SO(2,1)\subset SO(4,2)$. The diagonalisation of the operators Γ_0, Γ_4 and $\Gamma_0+\Gamma_4$ gives, respectively, the corresponding bound states, scattering states and zero-energy solutions. In a most degenerate unitary representation of SO(4, 2) it can be easily seen that the operators Γ_0, Γ_4 and $\Gamma_0+\Gamma_4$ are respectively given by the square root of the quadratic Casimir products of the algebras of the subgroups SO(4), SO(3, 1) and E(3) and the local isomorphisms such as $SO(4)\sim SO(3)\otimes SO(3)$ enable us to express the fourth-order linear differential equations of these quadratic forms as perfect squares of second-order linear differential equations. In this sense the BFN method is a unified generalisation of the earlier method due to Casimir. The lesson we learn from both methods is that for algebraisation the physical equations are expressed in terms of the invariant elements in the universal enveloping algebra of a Lie algebra or a Lie subalgebra.

The two methods mentioned above are generally successful to algebraise physical equations which are Kummerian and have scalar- or vector-valued solutions mostly expressible in terms of ${}_1F_1$ confluent hypergeometric functions of one variable. The physical actions corresponding to such problems seem to be generally path integrable (Coish 1956). However, for complex composite systems such as diatomic or polyatomic molecules there are several physical equations, e.g., Pöschl-Teller equations, which are ${}_2F_1$ hypergeometric functions of one variable. Such physical equations can be algebraised (Frank and Wolf 1984) using the methods mentioned above *for special cases* by invoking certain symmetries such that the *Gaussian form* degenerates into a Kummerian form or into a simple Gaussian form with two parameters and the solutions correspond to a column or a row vector of general matrix-valued solutions. In this paper we propose a method to algebraise *the general Gaussian type physical equations.*

We use Infeld-Hull factorisations and their algebraic versions given by Miller (1964, 1968) and express the physical equations in terms of products of 'ladder' operators of certain group matrix elements (Biedenharn and Louck 1981, Miller 1964, 1968, Schneider and Wilson 1979). The ladder operators of basis functions have already been used (Schrödinger 1940, 1941a, b, Coish 1956, Hadinger *et al* 1974) within the scope of the two methods mentioned earlier. However, the method we propose here requires the ladder operators of group matrix elements. In this paper we demonstrate this new method for the first Pöschl-Teller equation involving trigonometric angles. The discussion of the second Pöschl-Teller equation and of the Morse-Rosen equation both involving hyperbolic angles and unitary representations of SO(2, 1) is presented in the following paper (Barut *et al* 1987b).

2. Lie algebra action on group matrix elements

The first Pöschl-Teller equation is

$$\left[\frac{\partial^2}{\partial r^2}-a^2\left(\frac{\kappa(\kappa-1)}{\sin^2 ar}+\frac{\lambda(\lambda-1)}{\cos^2 ar}\right)+\frac{2ME}{\hbar^2}\right]\psi=0 \qquad (1)$$

$$\kappa,\lambda>1 \qquad r\in[0,\pi/2a] \qquad a=\text{parameter.}$$

The equation remains unchanged under $\kappa \to -\kappa + 1$ and $\lambda \to -\lambda + 1$ and its exact normalised solution has been obtained using analytic methods (Nieto 1978) for the symmetric case $\kappa = \lambda$ and using coherent state formulation (Nieto *et al* 1981). Under a change of parameters, $\kappa = m + g + \frac{1}{2}$, $\lambda = m - g + \frac{1}{2}$, $\beta = 2ar$, equation (1) becomes

$$\left[\frac{\partial^2}{\partial\beta^2} - \frac{1}{4}\left(\frac{(m+g+\frac{1}{2})(m+g-\frac{1}{2})}{\sin^2\beta/2} + \frac{(m-g+\frac{1}{2})(m-g-\frac{1}{2})}{\cos^2\beta/2}\right) + \Lambda\right]\psi = 0 \qquad \Lambda \equiv ME/2a^2\hbar^2 \qquad \beta \in [0, \pi]. \tag{2}$$

There are two quantum numbers, m and g, in this equation. Following an Infeld-Hull-Miller factorisation (Coulson and Joseph 1967, Joseph 1967) of type A we define

$$\begin{aligned} L_m^+\psi_m &\equiv \exp(i\alpha)\left(-\frac{\partial}{\partial\beta} + \tfrac{1}{2}(m+g+\tfrac{1}{2})\cot\frac{\beta}{2} - \tfrac{1}{2}(m-g+\tfrac{1}{2})\tan\frac{\beta}{2}\right)\psi_m \\ &\equiv [\Lambda - (m+\tfrac{1}{2})^2]^{1/2}\psi_{m+1} \\ L_m^-\psi_m &\equiv \exp(-i\alpha)\left(\frac{\partial}{\partial\beta} + \tfrac{1}{2}(m+g-\tfrac{1}{2})\cot\frac{\beta}{2} - \tfrac{1}{2}(m-g-\tfrac{1}{2})\tan\frac{\beta}{2}\right)\psi_m \\ &\equiv [\Lambda - (m-\tfrac{1}{2})^2]^{1/2}\psi_{m-1} \\ L_m^3\psi_m &\equiv -i(\partial/\partial\alpha)\psi_m = m\psi_m \end{aligned} \tag{3}$$

where we have introduced a new angle $\alpha \in [0, 2\pi)$. The operators $L_m^{\pm}$ and L_m^3 form an SO(3) algebra satisfying the relations

$$[L_m^+, L_m^-] = 2L_m^3 \qquad [L_m^{\pm}, L_m^3] = \mp L_m^{\pm}.$$

The action of the Casimir product

$$C_m\psi_m = (L_m^+L_m^- + L_m^3L_m^3 - L_m^3)\psi_m = (L_m^-L_m^+ + L_m^3L_m^3 + L_m^3)\psi_m$$

turns out to be simply

$$C_m\psi_m = (\Lambda - \tfrac{1}{4})\psi_m \equiv l(l+1)\psi_m.$$

if we denote the eigenvalues of C_m by $l(l+1)$ we obtain

$$\Lambda = (l+\tfrac{1}{2})^2.$$

Hence

$$E_n = \frac{2\alpha^2\hbar^2}{M}(l+\tfrac{1}{2})^2 = \frac{\alpha^2\hbar^2}{2M}(\kappa + \lambda + 2n)^2 \tag{4}$$

where we have set $l = m + n$ and n is an integer between 0 and $2l$. The energy spectrum (4) is precisely the well known spectrum first obtained by Pöschl and Teller. Equation (2) can be written in the algebraic form

$$[C_m - l(l+1)]\psi_m = 0. \tag{5}$$

Setting

$$L_m^{\pm} = L_m^1 \pm iL_m^2 \tag{6}$$

we obtain the SO(3) generators

$$
\begin{aligned}
L_m^1 &= -\mathrm{i}\cos\alpha\cot\beta\frac{\partial}{\partial\alpha}-\mathrm{i}\sin\alpha\frac{\partial}{\partial\beta}-\mathrm{i}\frac{\cos\alpha}{\sin\beta}\frac{\partial}{\partial r}+\frac{\mathrm{i}}{2}\sin\alpha\cot\beta \\
L_m^2 &= -\mathrm{i}\sin\alpha\cot\beta\frac{\partial}{\partial\alpha}+\mathrm{i}\cos\alpha\frac{\partial}{\partial\beta}-\mathrm{i}\frac{\sin\alpha}{\sin\beta}\frac{\partial}{\partial r}-\frac{\mathrm{i}}{2}\cos\alpha\cot\beta \\
L_m^3 &= -\mathrm{i}\frac{\partial}{\partial\alpha} \\
[L_m^i, L_m^j] &= \mathrm{i}L_m^k \qquad i,j,k \text{ cyclic.}
\end{aligned}
\tag{7}
$$

So far the g dependence of ψ has not been considered. Equation (2) can also be obtained from (1) by interchanging m and g such that $\kappa = g+m+\frac{1}{2}$, $\lambda = g-m+\frac{1}{2}$. Again by factorisation of type A we define

$$
\begin{aligned}
L_g^+\psi_g &= -\exp(\mathrm{i}\gamma)\left(-\frac{\partial}{\partial\beta}+\tfrac{1}{2}(g+m+\tfrac{1}{2})\cot\frac{\beta}{2}-\tfrac{1}{2}(g-m+\tfrac{1}{2})\tan\frac{\beta}{2}\right)\psi_g \\
&= [\Lambda-(g+\tfrac{1}{2})^2]^{1/2}\psi_{g+1} \\
L_g^-\psi_g &= -\exp(-\mathrm{i}\gamma)\left(\frac{\partial}{\partial\beta}+\tfrac{1}{2}(g+m-\tfrac{1}{2})\cot\frac{\beta}{2}-\tfrac{1}{2}(g-m-\tfrac{1}{2})\tan\frac{\beta}{2}\right)\psi_g \\
&= [\Lambda-(g-\tfrac{1}{2})^2]^{1/2}\psi_{g-1} \\
L_g^3\psi_g &= -\mathrm{i}\frac{\partial}{\partial r}\psi_g = g\psi_g
\end{aligned}
\tag{8}
$$

where we have again introduced a new variable $\gamma\in[0,2\pi)$. The operators $L_g^{\pm}$ and L_g^3 form an SO(3) algebra satisfying the relations

$$[L_g^+, L_g^-] = 2L_g^3 \qquad [L_g^{\pm}, L_g^3] = \mp L_g^{\pm}.$$

The Casimir operator is now

$$C_g\psi_g = (L_g^+L_g^- + L_g^3L_g^3 - L_g^3)\psi_g = (L_g^-L_g^+ + L_g^3L_g^3 + L_g^3)\psi_g$$

which has the same eigenvalues as C_m, equation (5),

$$C_g\psi_g = (\Lambda-\tfrac{1}{4})\psi_g \equiv l(l+1)\psi_g$$

with

$$\Lambda = (l+\tfrac{1}{2})^2 \qquad l = g+n \qquad n\in\mathbb{N}.$$

Hence again

$$E_n = \frac{\alpha^2\hbar^2}{2M}(\kappa+\lambda+2n)^2. \tag{9}$$

Thus (2) can be written as the alternate algebraic form

$$[C_g - l(l+1)]\psi_g = 0. \tag{10}$$

We define $L_g^{\pm} \equiv L_g^1 \mp \mathrm{i}L_g^2$ and obtain the corresponding generators

$$\begin{aligned} L_g^1 &= \mathrm{i}\frac{\cos\gamma}{\sin\beta}\frac{\partial}{\partial\alpha} + \mathrm{i}\sin\gamma\frac{\partial}{\partial\beta} + \mathrm{i}\cos\gamma\cot\beta\frac{\partial}{\partial\gamma} - \frac{\mathrm{i}}{2}\cot\beta\sin\gamma \\ L_g^2 &= -\mathrm{i}\frac{\sin\gamma}{\sin\beta}\frac{\partial}{\partial\alpha} + \mathrm{i}\cos\gamma\frac{\partial}{\partial\beta} - \mathrm{i}\sin\gamma\cot\beta\frac{\partial}{\partial\gamma} - \frac{\mathrm{i}}{2}\cot\beta\cos\gamma \\ L_g^3 &= -\mathrm{i}\frac{\partial}{\partial\gamma} \\ [L_g^i, L_g^j] &= -\mathrm{i}L_g^k \qquad i, j, k \text{ cyclic.} \end{aligned} \tag{11}$$

The negative sign associated with the commutation relations is due to the definition of $L_g^{\pm}$ and was first noticed by Casimir. In fact our L_g^i and L_m^i are similar to Casimir's Q and P operators, respectively. From (7) and (11) we conclude that

$$\begin{aligned} &[L_m^i, L_g^j] = 0 \qquad i, j = 1, 2, 3 \\ &L_g^i = \sum_j R_{ji}(\alpha, \beta, \gamma) L_m^j \end{aligned}$$

where

$$R(\alpha,\beta,\gamma) = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} -\cos\beta & 0 & \sin\beta \\ 0 & 1 & 0 \\ -\sin\beta & 0 & -\cos\beta \end{pmatrix}\begin{pmatrix} \cos\gamma & -\sin\gamma & 0 \\ \sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{12}$$

Thus the solutions to (1) turn out to be the eigenfunctions satisfying

$$\begin{aligned} &C_m\psi = C_g\psi = l(l+1)\psi \qquad \psi = \exp(-\mathrm{i}m\alpha)\exp(-\mathrm{i}g\gamma)\psi_{m,g}(\beta) \\ &L_m^3\psi = m\psi \\ &L_g^3\psi = g\psi. \end{aligned} \tag{13}$$

Physically, $\boldsymbol{L}_m$ is the angular momentum vector referred to the space-fixed frame while $\boldsymbol{L}_g$ is the angular momentum vector referred to the body-fixed frame of a rigid body (e.g. a diatomic molecule) with its centre of mass fixed in space.

From (3) and (8) we obtain the following recurrence relations (by putting $\alpha = 0$ ($\gamma = 0$) and by adding L^+ and L^-):

$$\begin{aligned} &\left(\frac{g + m\cos\beta}{\sin\beta}\right)\psi_{m,g}(\beta) \\ &\qquad = \tfrac{1}{2}[(l-m)(l+m+1)]^{1/2}\psi_{m+1,g}(\beta) + \tfrac{1}{2}[(l+m)(l-m+1)]^{1/2}\psi_{m-1,g}(\beta) \\ &\left(\frac{m + g\cos\beta}{\sin\beta}\right)\psi_{m,g}(\beta) \\ &\qquad = -\tfrac{1}{2}[(l-g)(l+g+1)]^{1/2}\psi_{m,g+1}(\beta) - \tfrac{1}{2}[(l+g)(l-g+1)]^{1/2}\psi_{m,g-1}(\beta) \end{aligned}$$

and subtracting $L^+ - L^-$

$$\begin{aligned} &\left(\frac{\partial}{\partial\beta} - \tfrac{1}{2}\cot\beta\right)\psi_{m,g}(\beta) \\ &\qquad = -\tfrac{1}{2}[(l-m)(l+m+1)]^{1/2}\psi_{m+1,g}(\beta) + \tfrac{1}{2}[(l+m)(l-m+1)]^{1/2}\psi_{m-1,g}(\beta) \\ &\qquad = \tfrac{1}{2}[(l-g)(l+g+1)]^{1/2}\psi_{m,g+1}(\beta) - \tfrac{1}{2}[(l+g)(l-g+1)]^{1/2}\psi_{m,g-1}(\beta). \end{aligned} \tag{14}$$

The crucial observation is now to compare (14) with the recurrence relations for Wigner functions given by (Biedenharn and Louck 1981, Schneider and Wilson 1979)

$$\begin{aligned}
&\left(\frac{m-m'\cos\theta}{\sin\theta}\right)d^l_{m',m}(\theta)\\
&\qquad=\tfrac{1}{2}[(l-m')(l+m'+1)]^{1/2}d^l_{m'+1,m}(\theta)+\tfrac{1}{2}[(l+m')(l-m'+1)]^{1/2}d^l_{m'-1,m}(\theta)\\
&\left(\frac{m'-m\cos\theta}{\sin\theta}\right)d^l_{m',m}(\theta)\\
&\qquad=-\tfrac{1}{2}[(l-m)(l+m+1)]^{1/2}d^l_{m',m+1}(\theta)-\tfrac{1}{2}[(l+m)(l-m+1)]^{1/2}d^l_{m',m-1}(\theta)
\end{aligned}\tag{15}$$

$$\begin{aligned}
\frac{\partial}{\partial\theta}d^l_{m',m}(\theta)&=\tfrac{1}{2}[(l-m')(l+m'+1)]^{1/2}d^l_{m'+1,m}(\theta)-\tfrac{1}{2}[(l+m')(l-m'+1)]^{1/2}d^l_{m'-1,m}(\theta)\\
&=-\tfrac{1}{2}[(l-m)(l+m+1)]^{1/2}d^l_{m',m+1}(\theta)+\tfrac{1}{2}[(l+m)(l-m+1)]^{1/2}d^l_{m',m-1}(\theta)
\end{aligned}$$

which gives us immediately the exact normalised solutions

$$\psi_{m,g}(\beta)=\left(\frac{2l+1}{2}\right)^{1/2}\sin^{1/2}\beta\, d^l_{m,g}(\pi-\beta)$$

with the property

$$\begin{aligned}
&\int_0^\pi \psi^*_{m',g'}(\beta)\psi_{m,g}(\beta)\,\mathrm{d}\beta=\delta_{m',m}\delta_{g',g}\\
&\int_0^\pi d^{l*}_{m',n'}(\theta)d^l_{m,n}(\theta)\sin\theta\,\mathrm{d}\theta=\left(\frac{2}{2l+1}\right)\delta_{m',m}\delta_{n',n}.
\end{aligned}\tag{16}$$

Furthermore the solutions obtained above satisfy the correct boundary conditions on the infinite walls of the potential 'hole': ${}_m\psi_g(0)={}_m\psi_g(\pi)=0$.

In order to express the solutions in a more explicit form we use the following relations:

$$\begin{aligned}
&d^l_{m',m}(\theta)=(-1)^{m'-m}d^l_{m,m'}(\theta)\qquad d^l_{m',m}(\pi-\theta)=(-1)^{m'-l}d^l_{m',-m}(\theta)\\
&d^l_{m',m}(\theta)=\left[\binom{l-m}{l-m'}\binom{l+m'}{l+m}\right]^{1/2}(-\tan\tfrac{1}{2}\theta)^{m'-m}(\cos\tfrac{1}{2}\beta)^{2m'}\\
&\qquad\times{}_2F_1[m'-l,\,m'+l+1;\,m'-m+1;\,\sin^2\tfrac{1}{2}\theta]
\end{aligned}\tag{17}$$

with

$$\binom{\alpha+h}{n}{}_2F_1[-n,\,1+\alpha+\beta+n;\,1+\alpha;\,x]=P_n^{\alpha,\beta}(1-2x).$$

Finally we obtain the solution in terms of the original parameters r, κ, λ ($\beta=2\alpha r$, $m=\frac{1}{2}(\kappa+\lambda-1)$, $g=\frac{1}{2}(\kappa-\lambda)$, $l=\frac{1}{2}(\kappa+\lambda-1+2n)$ as

$$\begin{aligned}
\psi(r)&=(-1)^{n+\kappa-1/2}\left[2\alpha(\kappa+\lambda+2n)\binom{\kappa+n-\frac{1}{2}}{n}\binom{\kappa+\lambda+n-1}{\lambda+n-\frac{1}{2}}\right]^{1/2}\\
&\qquad\times(\sin\alpha r)^\kappa(\cos\alpha r)^\lambda{}_2F_1[-n,\,\kappa+\lambda+n;\,\kappa+\tfrac{1}{2};\,\sin^2\alpha r]\\
&=(-1)^{n+\kappa-1/2}\left[2\alpha(\kappa+\lambda+2n)\frac{n!(\kappa+\lambda+n-1)!}{(\kappa+n-\frac{1}{2})!(\lambda+n-\frac{1}{2})!}\right]^{1/2}\\
&\qquad\times(\sin\alpha r)^\kappa(\cos\alpha r)^\lambda P_n^{\kappa-1/2,\lambda-1/2}(1-2\sin^2\alpha r).
\end{aligned}\tag{18}$$

The term $\sqrt{2}\alpha$ enters through the normalisation with respect to r. The final solution obtained above agrees exactly with the results of Nieto (1978).

Note that the Euler angles (α, β, γ) are related to the spherical polar coordinates as follows:

$$\begin{aligned} &\sin\theta\cos\phi\sin\omega = \sin\tfrac{1}{2}\beta\sin\tfrac{1}{2}(\gamma-\alpha) \\ &\sin\theta\sin\phi\sin\omega = \sin\tfrac{1}{2}\beta\cos\tfrac{1}{2}(\gamma-\alpha) \\ &\cos\theta\sin\omega = \cos\tfrac{1}{2}\beta\sin\tfrac{1}{2}(\gamma+\alpha) \\ &\cos\omega = \cos\tfrac{1}{2}\beta\cos\tfrac{1}{2}(\gamma+\alpha). \end{aligned} \tag{19}$$

For a sphere of unit radius we have

$$\cos\beta = \cos 2\theta \qquad \sin\beta = \sin 2\theta. \tag{20}$$

In the special symmetric case $\kappa = \lambda$, we have $g = 0$ in (16) and in (18) we have the limit

$${}_2F_1(-n, \kappa+\lambda+n; \kappa+\tfrac{1}{2}; \sin^2\alpha r) \to \frac{n!}{(2\kappa)_n} C_n^{\kappa}(1-2\sin^2\alpha r)$$

$$P_n^{\kappa-1/2,\lambda-1/2}(1-2\sin^2\alpha r) \to \frac{(\kappa+\frac{1}{2})_n}{(2\kappa)_n} C_n^{\kappa}(1-2\sin^2\alpha r).$$

3. On the quantisation of coupling constants

The two Lie algebras we found, $\{L_m\}$ and $\{L_g\}$ forming an $SU(2)\times SU(2)$ with a common Casimir operator, go beyond the spectrum-generating algebra of our starting problems (1). This is not the dynamical Lie algebra whose single representation gives all the energy states of the system. Rather we have a family of systems with *quantised coupling constants* κ and λ, as some kind of periodic table, and an $SU(2)\times SU(2)$ representation contains states of the same energy E from different systems in the family. In order to describe different energy levels we have to take a direct sum of representations of $SU(2)\times SU(2)$, thus going to the larger dynamical group $SO(4, 2)$, which contains operators changing the energy, or what we called the l quantum number of the algebras (3) or (8). Nevertheless, the algebra $SU(2)\times SU(2)$ allows us to find the spectrum and eigenfunctions of our problem. This sort of coupling constant quantisation appears in a number of other problems, such as the Kepler problem in a curved space (Barut and Wilson 1985) and Morse oscillator (Barut *et al* 1987a) and will be discussed again in the non-compact case in the following paper (Barut *et al* 1987b).

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