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1987 J. Phys. A: Math. Gen. 20 4097

(http://iopscience.iop.org/0305-4470/20/13/018)

J. Phys. A: Math. Gen. **20** (1987) 4097-4108. Printed in the UK

Dynamical invariance algebra of the Hartmann potential

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Received 29 December 1986

Abstract. The 'accidental' degeneracy occurring in the quantum mechanical treatment of the ring-shaped potential $V = -\eta\sigma^2 r^{-1} + \frac{1}{2}q\eta^2\sigma^2(r \sin\theta)^{-2}$ is explained by constructing an su(2) dynamical invariance algebra. The Schrödinger equation is solved in parabolic coordinates written in the framework of the Kustaanheimo-Stiefel transformation and the Hamilton-Jacobi equations are solved in ordinary parabolic coordinates. All finite trajectories are found to be periodic.

1. Introduction and preliminaries

This article is devoted to a group theoretical study of the classical and quantum mechanical motion of a particle in the (ring-shaped) three-dimensional potential

$$V_q = \eta\sigma^2\left(\frac{2a_0}{r} - q\eta\frac{a_0^2}{r^2 \sin^2\theta}\right)\varepsilon_0. \tag{1}$$

In equation (1), θ and r are the polar angle and the radius in spherical coordinates, a_0 and ε_0 stand for the Bohr radius and the ground state energy of the hydrogen atom, respectively. The constants η and σ are two dimensionless positive parameters, ranging from 1 to 10 in applications to quantum chemistry (Hartmann 1972a, b, Hartmann *et al* 1976, Schuch 1978, Hartmann and Schuch 1980). The dimensionless positive parameter q makes it possible to obtain from (1) the potential energy for a hydrogen-like atom with nucleus charge Ze as a limiting case by taking $\eta\sigma^2 = Z$ and $q = 0$ (Kibler and Négadi 1984a, b, c). (Note that the introduction of the parameter q constitutes a convenient alternative to the limiting processes ($\sigma\eta \to 0$, $\sigma^2\eta \to 1$, $\eta \to 0$ and $\sigma \to \infty$) described by Schuch (1978).) The potential V_q, which is invariant under the point symmetry group $C_{\infty v}$, was introduced with $q = 1$ by Hartmann (1972a, b) in view of its application to axial symmetric systems like ring-shaped molecules. The Schrödinger equation for V_1 was solved in spherical coordinates (Hartmann 1972a, b) and the diamagnetic susceptibility of the corresponding ground state was calculated by Hartmann *et al* (1976). The research programme set up by the late Professor Hartmann concerning systems subjected to the potential V_1 culminated with the analytical determination of the corresponding spin-orbit energy in a quasirelativistic approach (Schuch 1978, Hartmann and Schuch 1980).

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0305-4470/87/134097+12$02.50

Recently, the Schrödinger equation for the potential V_q has been converted, by means of the so-called KS transformation (Kustaanheimo and Stiefel 1965), into a coupled pair of two-dimensional non-harmonic oscillators with inverse squared potential (Kibler and Négadi 1984a, b, c). Such an approach permits an easy derivation of the energy of the bound states for a particle moving in the potential V_q. In addition, the system of coupled wave equations arising in the KS treatment is close to the equations one may obtain by directly solving the Schrödinger equation for the potential V_q in ordinary parabolic coordinates. Indeed, the treatments via the KS transformation and via the use of parabolic coordinates are equivalent as we shall show in this paper. In this respect, Gerry (1986) has solved the Schrödinger equation for V_1 in 'squared' parabolic coordinates without using the connection between parabolic coordinates and KS transformation. Finally, let us mention that a Feynman path integral treatment of the Hartmann potential problem has been published very recently (Carpio and Inomata 1986, Sökmen 1986).

The Hartmann potential (1) belongs to the class of potentials exhibiting an 'accidental degeneracy', i.e. a degeneracy of the energy levels not explained by the occurrence of an obvious geometrical symmetry. In fact, the corresponding Hamiltonian in au (atomic units: $\mu = e = \hbar = 1$, $a_0 = 1$, $\varepsilon_0 = -\frac{1}{2}$)

$$H = -\tfrac{1}{2}\Delta + V(\boldsymbol{x}) \tag{2}$$

with V being V_q in au, is invariant under $C_{\infty v}$, in particular under rotations about the z axis, but not any larger point symmetry group. To understand the degeneracy afforded by H in group theoretical terms, it is hence necessary to go beyond point symmetries and to invoke a dynamical invariance group, along the lines of the O(4) group for the hydrogen atom (Pauli 1926, Klein (see Hulthén 1933), Fock 1935, Bargmann 1936). Accidental degeneracy may also be tackled in the framework of groups of canonical transformations, see, e.g., Moshinsky *et al* (1975), Moshinsky and Quesne (1983) and references therein.

A systematic search for non-relativistic Hamiltonians with dynamical invariance groups was initiated several years ago (Winternitz *et al* 1966, Makarov *et al* 1967). The emphasis was on two- and three-dimensional Hamiltonians of the form (2) allowing integrals of motion quadratic in the momenta. In particular, it was shown (Makarov *et al* 1967) that in three dimensions a Hamiltonian (2) will commute with a pair $\{X_1, X_2\}$ of second-order mutually commuting operators, viz

$$\begin{gathered} X_a = \phi_a^{ij}(\boldsymbol{x}) \frac{\partial}{\partial x^i} \frac{\partial}{\partial x^j} + f_a^i(\boldsymbol{x}) \frac{\partial}{\partial x^i} + h_a(\boldsymbol{x}) \\ [X_1, X_2] = 0 \qquad [X_a, H] = 0 \qquad a = 1, 2 \end{gathered} \tag{3}$$

if and only if $V(\boldsymbol{x})$ allows the separation of variables in the Schrödinger equation. All separable potentials in the three-dimensional Euclidean space are known (Eisenhart 1948); all the corresponding pairs $\{X_1, X_2\}$ of operators were found by Makarov *et al* (1967).

Accidental degeneracy and a corresponding non-Abelian dynamical symmetry group will occur if at least one more operator exists, commuting with H, but not with both X_1 and X_2. The requirement that a further pair, say $\{Y_1, Y_2\}$, of second-order operators satisfying (3) should exist implies that $V(\boldsymbol{x})$ allows the separation of variables in at least two coordinate systems.

Thus, demanding separability in more than one coordinate system, it is possible to generate a class of potentials with 'redundant' sets of quadratic integrals of motion (redundant in the sense that there are more integrals than degrees of freedom). The point is to find physically interesting ones inside this class of potentials.

It turns out that the Hartmann potential belongs to this class. Indeed, any potential of the form (Makarov *et al* 1967)

$$V(\boldsymbol{r})=\frac{\alpha}{r}+\beta\frac{\cos\theta}{r^2\sin^2\theta}+\frac{h(\varphi)}{r^2\sin^2\theta} \tag{4}$$

will allow the separation of variables in both spherical coordinates (cf Landau and Lifshitz 1960)

$$x=r\sin\theta\cos\varphi \qquad y=r\sin\theta\sin\varphi \qquad z=r\cos\theta \tag{5}$$

and parabolic rotational coordinates

$$x=(ab)^{1/2}\cos\varphi \qquad y=(ab)^{1/2}\sin\varphi \qquad z=\tfrac{1}{2}(a-b). \tag{6}$$

(In (4), α and β are constants and h is an arbitrary function of φ.) The corresponding integrals of motion are also known, namely for the coordinates (r, θ, φ)

$$\begin{aligned} X_1&=L_1^2+L_2^2+L_3^2-2\beta\frac{\cos\theta}{\sin^2\theta}-2\frac{1}{\sin^2\theta}h(\varphi) \\ X_2&=L_3^2-2h(\varphi) \end{aligned} \tag{7}$$

and for the coordinates (a, b, φ)

$$\begin{aligned} Y_1&=L_1p_2+p_2L_1-L_2p_1-p_1L_2-2\left(\alpha\frac{a-b}{a+b}+\beta\frac{a^2+b^2}{ab(a+b)}+\frac{a-b}{ab}h(\varphi)\right) \\ Y_2&=L_3^2-2h(\varphi)=X_2. \end{aligned} \tag{8}$$

The translations p_i and rotations L_i in (7) and (8) form a basis for the Euclidean Lie algebra e(3). Our conventions are

$$p_i=\frac{\partial}{\partial x^i} \qquad L_i=-\varepsilon_{ijk}x^jp^k \qquad x^1=x \qquad x^2=y \qquad x^3=z \tag{9}$$

and hence

$$[L_i, L_j]=\varepsilon_{ijk}L_k \qquad [L_i, p_j]=\varepsilon_{ijk}p_k \qquad [p_i, p_j]=0. \tag{10}$$

The pairs $\{X_1, X_2\}$ and $\{Y_1, Y_2\}$ correspond to the separation of variables in spherical and parabolic coordinates, respectively, and we have

$$[X_1, X_2]=[Y_1, Y_2]=0 \qquad [X_1, Y_1]\neq 0. \tag{11}$$

The case of the Hartmann potential is obtained by putting

$$\alpha=-\eta\sigma^2 \qquad \beta=0 \qquad h=\tfrac{1}{2}q\eta^2\sigma^2 \tag{12}$$

in equations (4), (7) and (8). The operator $X_2=Y_2$ can then be replaced by L_3^2, dropping the constant h.

In § 2, we solve the quantum mechanical Hartmann problem making use of the KS transformation, on the one hand, and of the integrals of motion (8) in parabolic coordinates, on the other. The dynamical symmetry algebra explaining the accidental degeneracy is found to be isomorphic to su(2) and investigated in § 3. The classical equations of motion for the Hartmann potential are solved in § 4. It is shown that all orbits that are finite are also periodic, a property shared with other Hamiltonian systems having dynamical symmetry groups. Finally, the conclusions and possible applications are discussed in § 5.

2. Energy levels and wavefunctions

2.1. KS transformation and parabolic coordinates

The KS transformation (Kustaanheimo and Stiefel 1965) may be defined through the mapping $\mathbb{R}^4$ (coordinates u_1, u_2, u_3, u_4) $\rightarrow \mathbb{R}^3$ (coordinates x, y, z)

$$x = 2(u_1u_3 - u_2u_4) \qquad y = 2(u_1u_4 + u_2u_3) \qquad z = u_1^2 + u_2^2 - u_3^2 - u_4^2 \tag{13}$$

accompanied by the constraint

$$u_2\,\mathrm{d}u_1 - u_1\,\mathrm{d}u_2 - u_4\,\mathrm{d}u_3 + u_3\,\mathrm{d}u_4 = 0. \tag{14}$$

This transformation has received considerable attention in the recent years and the reader is referred to the paper by Lambert and Kibler (1986) for an exhaustive bibliography. Let us just mention that such a transformation is connected to the theory of spinors (Kustaanheimo and Stiefel 1965) and, therefore, to the algebra of the usual quaternions (Kibler and Négadi 1984c, Cornish 1984, Lambert *et al* 1986) and may be obtained as a particular case of the so-called Hurwitz transformations (Lambert and Kibler 1986, 1987). The KS transformation allows us to write the Laplacian Δ_3 in $\mathbb{R}^3$ as

$$\begin{aligned} \Delta_3 &= \frac{1}{4r}\Delta_4 - \frac{1}{4r^2}X^2 \\ r &= (x^2+y^2+z^2)^{1/2} = u_1^2 + u_2^2 + u_3^2 + u_4^2 \end{aligned} \tag{15}$$

in terms of the Laplacian Δ_4 in $\mathbb{R}^4$ and of the vector field

$$X = u_2\frac{\partial}{\partial u_1} - u_1\frac{\partial}{\partial u_2} - u_4\frac{\partial}{\partial u_3} + u_3\frac{\partial}{\partial u_4} \tag{16}$$

which vanishes when acting on functions $G(x, y, z)$ of class C^1 (Kibler and Négadi 1984d).

A useful link between spherical, parabolic and KS coordinates is given by

$$\begin{aligned} &r = \tfrac{1}{2}(a+b) = \rho_1^2 + \rho_2^2 && r^2\sin^2\theta = ab = 4\rho_1^2\rho_2^2 \\ &a = r(1+\cos\theta) = 2\rho_1^2 && b = r(1-\cos\theta) = 2\rho_2^2 \\ &\varphi = \varphi_1 + \varphi_2 + 2k\pi && (k \in \mathbb{Z}) \end{aligned} \tag{17}$$

where

$$u_1 = \rho_1\cos\varphi_1 \qquad u_2 = \rho_1\sin\varphi_1 \qquad u_3 = \rho_2\cos\varphi_2 \qquad u_4 = \rho_2\sin\varphi_2. \tag{18}$$

2.2. Bound states

The Schrödinger equation for V_q of (1) is in au

$$-\tfrac{1}{2}\Delta_3\psi + \left(-\eta\sigma^2\frac{1}{r} + \tfrac{1}{2}q\eta^2\sigma^2\frac{1}{r^2\sin^2\theta}\right)\psi = E\psi. \tag{19}$$

The KS transformation allows us to convert (19) into the Schrödinger equation for an $\mathbb{R}^4$ isotropic non-harmonic oscillator with an inverse squared potential and subjected to a constraint condition. The latter Schrödinger equation and the constraint condition in turn yield the system (Kibler and Négadi 1984b)

$$-\frac{1}{2}\left(\frac{\partial^2 f}{\partial u_1^2}+\frac{\partial^2 f}{\partial u_2^2}\right)+\left(-4E\rho_1^2+\tfrac{1}{2}q\eta^2\sigma^2\frac{1}{\rho_1^2}\right)f=2(-K+\eta\sigma^2)f \tag{20a}$$

$$-\frac{1}{2}\left(\frac{\partial^2 g}{\partial u_3^2}+\frac{\partial^2 g}{\partial u_4^2}\right)+\left(-4E\rho_2^2+\tfrac{1}{2}q\eta^2\sigma^2\frac{1}{\rho_2^2}\right)g=2(K+\eta\sigma^2)g \tag{20b}$$

$$u_1\frac{\partial f}{\partial u_2}-u_2\frac{\partial f}{\partial u_1}=\mathrm{i}mf \qquad u_3\frac{\partial g}{\partial u_4}-u_4\frac{\partial g}{\partial u_3}=\mathrm{i}mg \tag{20c}$$

where K and m are separation constants while $f(u_1, u_2)$ and $g(u_3, u_4)$ are such that $\psi=fg$. Single-valued solutions of equations (20) are obtained in the form

$$f=v(\rho_1)\exp(\mathrm{i}m_1\varphi_1) \qquad g=w(\rho_2)\exp(\mathrm{i}m_2\varphi_2) \tag{21}$$

where, owing to (20c), we have

$$m_1=m_2=m\in\mathbb{Z}. \tag{22}$$

Furthermore, (20a) reduces to the following differential equation:

$$\frac{\mathrm{d}^2v}{\mathrm{d}\rho_1^2}+\frac{1}{\rho_1}\frac{\mathrm{d}v}{\mathrm{d}\rho_1}+\left(4(-K+\eta\sigma^2)+8E\rho_1^2-\frac{M^2}{\rho_1^2}\right)v=0 \tag{23}$$

where

$$M^2=m^2+q\eta^2\sigma^2. \tag{24}$$

Relation (20b) gives a differential equation similar to (23). The two differential equations so obtained may be readily solved in terms of the confluent hypergeometric function ${}_1F_1$. The resulting function $\psi=\exp(\mathrm{i}m\varphi)v(\rho_1)w(\rho_2)$ may be completely written in parabolic coordinates due to (17) and (22). This leads to a function ψ of a, b and φ which must belong to $L^2(\mathbb{R}^3)$. The condition for $\psi(a, b, \varphi)$ to be square integrable implies that $E\equiv E_N$ is quantised according to

$$\begin{aligned}&E_N=-\frac{1}{2N^2}\eta^2\sigma^4\\ &N=|M|+n_1+n_2+1 \qquad n_1\in\mathbb{N} \qquad n_2\in\mathbb{N}\\ &|M|=(m^2+q\eta^2\sigma^2)^{1/2} \qquad m\in\mathbb{Z}\end{aligned} \tag{25}$$

a result already obtained in this form (Kibler and Négadi 1984b). Finally, the normalised wavefunction $\psi\equiv\psi_{n_1n_2m}$ is given by (up to a phase factor)

$$\begin{aligned}\psi_{n_1n_2m}&(a, b, \varphi)\\ &=N_{n_1n_2m}\exp(\mathrm{i}m\varphi)\exp[-\tfrac{1}{2}\varepsilon(a+b)](\varepsilon_a\varepsilon_b)^{|M|/2}\\ &\quad\times{}_1F_1(-n_1;|M|+1;\varepsilon a)\,{}_1F_1(-n_2;|M|+1;\varepsilon b)\\ N_{n_1n_2m}&=\frac{(N\pi)^{-1/2}\varepsilon^{3/2}}{[\Gamma(|M|+1)]^2}\left(\frac{\Gamma(n_1+|M|+1)\Gamma(n_2+|M|+1)}{n_1!\,n_2!}\right)^{1/2}\\ \varepsilon&=(-2E_N)^{1/2}\end{aligned} \tag{26}$$

which compares with the expression derived by Gerry (1986) in 'squared' parabolic coordinates (our result differs from the one of Gerry (1986) by a factor $N^{-1/2}$).

It is to be observed that the wavefunctions and eigenvalues obtained in § 2.2 yield, in the particular case for which $q=0$ and $\eta\sigma^2=Z$, well known results for a hydrogen-like atom of atomic number Z. In this limiting case, M and N must be replaced by the azimuthal (m) and principal (n) quantum numbers, respectively, and the non-negative integers n_1 and n_2 (or n_r and n'_r in the notation of Kibler and Négadi (1984a)) coincide with the usual parabolic quantum numbers.

2.3. Relation to a set of commuting operators

According to the general philosophy of the group theoretical approach to variable separation (Winternitz and Friš 1965, Miller 1977, Miller *et al* 1981), the wavefunctions $\psi_{n_1n_2m}$ that are separated in parabolic rotational coordinates should be the common eigenfunctions of a complete set of commuting second-order operators. This set is $\{H, Y_1, Y_2\}$, where H is the Hamiltonian occurring in (19) and Y_1 and Y_2 follow from (8) by taking (12) into account. More precisely, in parabolic coordinates we obtain

$$H=-\frac{2}{a+b}\left[\frac{\partial}{\partial a}\left(a\frac{\partial}{\partial a}\right)+\frac{\partial}{\partial b}\left(b\frac{\partial}{\partial b}\right)\right]-\frac{1}{2ab}\frac{\partial^2}{\partial\varphi^2}-2\eta\sigma^2\frac{1}{a+b}+\frac{1}{2}q\eta^2\sigma^2\frac{1}{ab}$$

$$Y_1=-4\frac{ab}{a+b}\left(\frac{\partial^2}{\partial a^2}-\frac{\partial^2}{\partial b^2}\right)-\frac{4}{a+b}\left(b\frac{\partial}{\partial a}-a\frac{\partial}{\partial b}\right)+\frac{a-b}{ab}\frac{\partial^2}{\partial\varphi^2}+2\eta\sigma^2\frac{a-b}{a+b}-q\eta^2\sigma^2\frac{a-b}{ab} \tag{27}$$

$$Y_2=\frac{\partial^2}{\partial\varphi^2}=L_3^2$$

(we drop the constant $-q\eta^2\sigma^2$ in the definition of Y_2). As a matter of fact, we have

$$H\psi_{EKm}=E\psi_{EKm}\qquad Y_1\psi_{EKm}=(-2K)\psi_{EKm}\qquad L_3^2\psi_{EKm}=-m^2\psi_{EKm} \tag{28}$$

where ψ_{EKm} coincides with $\psi_{n_1n_2m}$ and E with E_N. The eigenvalues of the operator Y_1 are nothing but (up to the factor -2) the possible values of the separation constant K of (20*a*) and (20*b*). The square integrability of the wavefunction $\psi_{n_1n_2m}$ of equation (26) requires that $(1,2\equiv +,-)$

$$n_{1,2}=-\frac{1}{2}\left(\frac{\pm K-\eta\sigma^2}{(-2E)^{1/2}}+|M|+1\right) \tag{29}$$

be two non-negative integers and this is only possible if the constant K satisfies

$$|K|<\eta\sigma^2. \tag{30}$$

2.4. Discussion of degeneracies

The energy levels as given by (25) are obviously degenerate. For N and m fixed, the degree of degeneracy

$$\mathrm{d}(N,m)=N-|M| \tag{31}$$

is the same as for a two-dimensional isotropic harmonic oscillator. Observe that for N and $|m|$ fixed, the degree of degeneracy $\mathrm{d}(N,m)$ should be replaced by

$$\mathrm{d}'(N,|m|)=[2-\delta(m,0)]\,\mathrm{d}(N,m) \tag{32}$$

in view of the two possibilities for the angular momentum component m. In this regard, we note that confusion between $d'(N, |m|)$ and $d(N, m)$ exists in some previous works (Hartmann and Schuch 1980, Kibler and Négadi 1984b). However, the basic degeneracy to be understood corresponds, in the final analysis, to equation (31). This degeneracy is explained by the existence of a dynamical invariance algebra of type su(2), to be discussed below.

Finally, let us mention that truly accidental degeneracies may exist for some specific energy levels if the parameters q, η and σ of the Hartmann potential satisfy a particular relation. To be specific, the energy levels associated to the triplets (m, n_1, n_2) and (m', n_1', n_2') with $m' \neq m$ are degenerate if

$$4q\eta^2\sigma^2 = \frac{1}{I^2}[I^2 - (m+m')^2][I^2 - (m-m')^2] \tag{33}$$

where the integer $I = n_1' + n_2' - n_1 - n_2$ is different from zero for $m' \neq m$. We shall not deal with this kind of degeneracy here.

3. Dynamical invariance algebra

To simplify notation we put

$$z_1 = \varepsilon a \qquad z_2 = \varepsilon b \tag{34}$$

and rewrite the obtained bound state wavefunctions (26) as

$$\psi_{n_1 n_2 m}(a, b, \varphi) = N_{n_1 n_2 m} H_{n_1 M}(z_1) H_{n_2 M}(z_2) \exp(im\varphi) \tag{35}$$

where

$$H_{n_i M}(z_i) = \exp(-z_i/2) z_i^{|M|/2} {}_1F_1(-n_i; |M|+1; z_i) \qquad i = 1, 2. \tag{36}$$

Using the recursion relations for the confluent hypergeometric series (Gradshteyn and Ryzhik 1980) we construct raising and lowering operators for the wavefunctions $\psi_{n_1 n_2 m}$. As a result, the operators

$$b_i^{\pm} = \mp z_i \frac{\partial^2}{\partial z_i^2} + (z_i \mp 1)\frac{\partial}{\partial z_i} \pm \frac{M^2}{4z_i} + \frac{1}{2} \mp \frac{z_i}{4} \qquad i = 1, 2 \tag{37}$$

act on $\psi_{n_1 n_2 m}$ in the following manner:

$$\begin{aligned}
b_1^+ \psi_{n_1 n_2 m} &= \left(\frac{N+1}{N}\right)^2 [(n_1+1)(n_1+|M|+1)]^{1/2} \psi_{n_1+1, n_2, m} \\
b_1^- \psi_{n_1 n_2 m} &= -\left(\frac{N-1}{N}\right)^2 [n_1(n_1+|M|)]^{1/2} \psi_{n_1-1, n_2, m} \\
b_2^+ \psi_{n_1 n_2 m} &= \left(\frac{N+1}{N}\right)^2 [(n_2+1)(n_2+|M|+1)]^{1/2} \psi_{n_1, n_2+1, m} \\
b_2^- \psi_{n_1 n_2 m} &= -\left(\frac{N-1}{N}\right)^2 [n_2(n_2+|M|)]^{1/2} \psi_{n_1, n_2-1, m}.
\end{aligned} \tag{38}$$

The operators $b_i^{\mp}$ $(i = 1, 2)$ change the energy E_N (by one unit in $N = |M| + n_1 + n_2 + 1$). The four bilinear forms $b_i^+ b_j^-$ (i and $j = 1, 2$), on the other hand, will commute with the Hamiltonian H and hence leave invariant the subspace associated with E_N.

Directly from (38) we obtain

$$([b_1^+, b_1^-]+[b_2^+, b_2^-])\psi_{n_1n_2m} = 2N\psi_{n_1n_2m} \tag{39a}$$

$$([b_1^+, b_1^-]-[b_2^+, b_2^-])\psi_{n_1n_2m} = 2(n_1-n_2)\psi_{n_1n_2m} \tag{39b}$$

and we see that the operators

$$N_i = \tfrac{1}{2}([b_i^+, b_i^-]-|M|-1) \qquad i=1,2 \tag{40}$$

play the role of 'number of quanta' operators since

$$N_i\psi_{n_1n_2m} = n_i\psi_{n_1n_2m} \qquad i=1,2. \tag{41}$$

The invariants N_i ($i=1,2$) are two operators of second order (in the derivatives). Two further invariants are $b_1^-b_2^+$ and $b_1^+b_2^-$, which may be seen to be of fourth order. Applied to the wavefunction $\psi_{n_1n_2m}$, they change its normalisation. To compensate for this we make use of the number operators (40) and construct the triplet of operators

$$\begin{aligned} J_3 &= \tfrac{1}{2}(N_2-N_1) \\ J_+ &= -b_1^-b_2^+[(N_1+|M|)(N_2+|M|+1)]^{-1/2} \\ J_- &= -b_1^+b_2^-[(N_1+|M|+1)(N_2+|M|)]^{-1/2}. \end{aligned} \tag{42}$$

In general, the introduction in (42) of the negative square roots of operators may pose mathematical problems. We shall, however, only apply the operators J_3 and $J_\pm$ on a subspace of eigenfunctions associated to given values of the energy E_N and the angular momentum projection m. Then, the operators N_i ($i=1,2$) are just non-negative numbers and we have

$$\begin{aligned} J_3\psi_{n_1n_2m} &= \tfrac{1}{2}(n_2-n_1)\psi_{n_1n_2m} \\ J_+\psi_{n_1n_2m} &= [n_1(n_2+1)]^{1/2}\psi_{n_1-1,n_2+1,m} \\ J_-\psi_{n_1n_2m} &= [(n_1+1)n_2]^{1/2}\psi_{n_1+1,n_2-1,m}. \end{aligned} \tag{43}$$

Equations (43) are the canonical relations for the SU(2) infinitesimal generators and they provide a representation of su(2) with angular momentum $j=\tfrac{1}{2}(n_1+n_2)$ and third component $m_j=\tfrac{1}{2}(n_2-n_1)$. The commutation relations of J_3 and $J_\pm$ (when applied to $\psi_{n_1n_2m}$ with n_1+n_2 and m fixed) are clearly the appropriate ones, viz $[J_+, J_-]=2J_3$ and $[J_3, J_\pm]=\pm J_\pm$.

The next step is to relate the invariants N_i ($i=1,2$) to the Hamiltonian H and the integral of motion Y_1. Writing Y_1, H, N_1 and N_2 in parabolic coordinates, we prove that

$$Y_1 = (-2E)^{1/2}([b_1^+, b_1^-]-[b_2^+, b_2^-]). \tag{44}$$

From (39a) we obtain an expression for the Hamiltonian H which can be combined with (44). Finally, we are left with

$$H = -\frac{2\eta^2\sigma^4}{([b_1^+, b_1^-]+[b_2^+, b_2^-])^2} \qquad Y_1 = 2\eta\sigma^2\frac{[b_1^+, b_1^-]-[b_2^+, b_2^-]}{[b_1^+, b_1^-]+[b_2^+, b_2^-]} \tag{45}$$

as far as H and Y_1 act on a subspace associated to given values of N and m. The relation between the energy E_N and the separation constant K, on the one hand, and the numbers of quanta n_i ($i=1,2$), on the other, is directly deducible from (39) and (45). We thus obtain

$$E_N = -\eta^2\sigma^4\frac{1}{2N^2} \qquad K = -\eta\sigma^2\frac{n_1-n_2}{N} \qquad N=|M|+n_1+n_2+1. \tag{46}$$

At this point, we may establish contact with the KS treatment of § 2. It can be shown that

$$[b_i^+, b_i^-] = \tfrac{1}{2}(-2E)^{-1/2} h_i \qquad i = 1, 2 \tag{47}$$

where

$$\begin{aligned} h_1 &= -\frac{1}{2}\left(\frac{\partial^2}{\partial u_1^2} + \frac{\partial^2}{\partial u_2^2}\right) - 4E(u_1^2 + u_2^2) + \tfrac{1}{2}q\eta^2\sigma^2 \frac{1}{u_1^2 + u_2^2} \\ h_2 &= -\frac{1}{2}\left(\frac{\partial^2}{\partial u_3^2} + \frac{\partial^2}{\partial u_4^2}\right) - 4E(u_3^2 + u_4^2) + \tfrac{1}{2}q\eta^2\sigma^2 \frac{1}{u_3^2 + u_4^2} \end{aligned} \tag{48}$$

are the two Hamiltonians occurring in the Schrödinger equations (20*a*) and (20*b*) for the two coupled isotropic non-harmonic oscillators.

The considerations of § 3 are based on the use of the wavefunctions separated in parabolic coordinates. Thus the operator Y_1 plays a privileged role. An equivalent realisation of the dynamical invariance algebra su(2) could be obtained in spherical coordinates. The corresponding raising and lowering operators would then be related to the operator X_1 of (7) and (12) (and, of course, to the Hamiltonian H) but the connection with the KS treatment would yield relations less simple than (47).

4. Classical equations of motion

The Hamilton-Jacobi equation for the Hartmann potential allows the separation of variables in spherical and parabolic coordinates. The (classical) Hamilton function H_{cl} for V_q is in parabolic coordinates

$$H_{\mathrm{cl}} = \frac{2}{a+b}(ap_a^2 + bp_b^2) + \frac{1}{2ab}p_\varphi^2 - 2\eta\sigma^2\frac{1}{a+b} + \tfrac{1}{2}q\eta^2\sigma^2\frac{1}{ab} \tag{49}$$

where p_a, p_b and p_φ are the classical momenta, canonically conjugated to a, b and φ, respectively. Since H_{cl} is time independent and φ is a cyclical variable, and since we know that the Hamilton-Jacobi equation separates, we shall look for the action S in the form

$$S = S_0(a, b, \varphi) - Et = S_1(a) + S_2(b) + m\varphi - Et \tag{50}$$

where we have put

$$p_\varphi = m = \text{constant.} \tag{51}$$

The Hamilton-Jacobi equation then becomes

$$\frac{2}{a+b}\left[a\left(\frac{\partial S_0}{\partial a}\right)^2 + b\left(\frac{\partial S_0}{\partial b}\right)^2\right] + \frac{1}{2ab}\left(\frac{\partial S_0}{\partial \varphi}\right)^2 - 2\eta\sigma^2\frac{1}{a+b} + \tfrac{1}{2}q\eta^2\sigma^2\frac{1}{ab} = E. \tag{52}$$

Using (50) we obtain two ordinary first-order differential equations

$$\begin{aligned} 2a\left(\frac{\mathrm{d}S_1}{\mathrm{d}a}\right)^2 + \frac{M^2}{2a} - Ea &= -K + \eta\sigma^2 \\ 2b\left(\frac{\mathrm{d}S_2}{\mathrm{d}b}\right)^2 + \frac{M^2}{2b} - Eb &= K + \eta\sigma^2 \end{aligned} \tag{53}$$

where K is a separation constant and $M^2 = m^2 + q\eta^2\sigma^2$ as in § 3 (except, of course, that m and K are not quantised). The solutions to (53) can be written as

$$\begin{aligned} S_1 &= \tfrac{1}{2}(-2E)^{1/2} \int \frac{1}{a}[(a-\xi_1)(\xi_2-a)]^{1/2}\,\mathrm{d}a \\ S_2 &= \tfrac{1}{2}(-2E)^{1/2} \int \frac{1}{b}[(b-\eta_1)(\eta_2-b)]^{1/2}\,\mathrm{d}b \end{aligned} \tag{54}$$

where $(1, 2 \equiv -, +)$

$$\begin{aligned} \xi_{1,2} &= (-2E)^{-1}\{\eta\sigma^2 - K \mp [(-K+\eta\sigma^2)^2 + 2M^2E]^{1/2}\} \\ \eta_{1,2} &= (-2E)^{-1}\{\eta\sigma^2 + K \mp [(K+\eta\sigma^2)^2 + 2M^2E]^{1/2}\}. \end{aligned} \tag{55}$$

The case of bounded motion corresponds to

$$-(\mp K + \eta\sigma^2)^2/2M^2 \leqslant E < 0 \qquad |K| < \eta\sigma^2 \tag{56}$$

and restricting ourselves to this case we have

$$0 < \xi_1 \leqslant a \leqslant \xi_2 \qquad 0 < \eta_1 \leqslant b \leqslant \eta_2. \tag{57}$$

The integrals in equation (54) can easily be evaluated. However, it is better to write the equations of motion directly by putting

$$\frac{\partial S}{\partial E} = \beta_1 \qquad \frac{\partial S}{\partial K} = \beta_2 \qquad \frac{\partial S}{\partial m} = \beta_3 \tag{58}$$

with $\beta_i = \text{constant}$ $(i = 1, 2, 3)$. The equations so obtained yield integrals which can be calculated and after some manipulation we obtain that the trajectories in parabolic coordinates are given by

$$\begin{aligned} &[(a-\xi_1)(\xi_2-a)]^{1/2} + [(b-\eta_1)(\eta_2-b)]^{1/2} - \tfrac{1}{2}(\xi_1+\xi_2)\sin^{-1}\left(\frac{2a-\xi_1-\xi_2}{\xi_2-\xi_1}\right) \\ &\qquad -\tfrac{1}{2}(\eta_1+\eta_2)\sin^{-1}\left(\frac{2b-\eta_1-\eta_2}{\eta_2-\eta_1}\right) = -2(-2E)^{1/2}(\beta_1+t) \end{aligned} \tag{59a}$$

$$\sin^{-1}\left(\frac{2a-\xi_1-\xi_2}{\xi_2-\xi_1}\right) - \sin^{-1}\left(\frac{2b-\eta_1-\eta_2}{\eta_2-\eta_1}\right) = -2(-2E)^{1/2}\beta_2 \tag{59b}$$

$$\varphi + \frac{m}{2|M|}\left[\sin^{-1}\left(2\frac{\xi_1\xi_2}{\xi_2-\xi_1}\frac{1}{a} - \frac{\xi_1+\xi_2}{\xi_2-\xi_1}\right) + \sin^{-1}\left(2\frac{\eta_1\eta_2}{\eta_2-\eta_1}\frac{1}{b} - \frac{\eta_1+\eta_2}{\eta_2-\eta_1}\right)\right] = \beta_3. \tag{59c}$$

The left-hand sides of (59b) and (59c) are seen to be constants of motion. The time dependence is in (59a). Note that the variables $a(t)$ and $b(t)$ in formulae (59a) and (59b) can be separated and we obtain the transcendental equation

$$\begin{aligned} &\{-(\xi_2-\xi_1) - (\eta_2-\eta_1)\cos[2(-2E)^{1/2}\beta_2]\}\cos\rho \\ &\qquad + (\eta_2-\eta_1)\sin[2(-2E)^{1/2}\beta_2]\sin\rho + (\xi_1+\xi_2+\eta_1+\eta_2)\rho \\ &\quad = 4(-2E)^{1/2}(\beta_1+t) - 2(-2E)^{1/2}\beta_2(\eta_1+\eta_2) \end{aligned} \tag{60}$$

giving ρ as a function of time, where

$$\sin\rho = \frac{2a-\xi_1-\xi_2}{\xi_2-\xi_1}. \tag{61}$$

Thus, $a(t)$, $b(t)$ and $\varphi(t)$ are given by

$$a(t)=\tfrac{1}{2}[\xi_1+\xi_2+(\xi_2-\xi_1)\sin\rho]$$
$$b(t)=\tfrac{1}{2}\{\eta_1+\eta_2+(\eta_2-\eta_1)\sin[\rho+2(-2E)^{1/2}\beta_2]\}$$
$$\varphi(t)=\beta_3+\frac{m}{2|M|}\left(\sin^{-1}\frac{\xi_2-\xi_1+(\xi_1+\xi_2)\sin\rho}{\xi_1+\xi_2+(\xi_2-\xi_1)\sin\rho}+\sin^{-1}\frac{\eta_2-\eta_1+(\eta_1+\eta_2)\sin[\rho+2(-2E)^{1/2}\beta_2}{\eta_1-\eta_2+(\eta_2-\eta_1)\sin[\rho+2(-2E)^{1/2}\beta_2]}\right). \tag{62}$$

The final result that we wish to stress is that all the trajectories described by (59*a*, *b*, *c*), i.e. all the finite trajectories, are periodic. To prove this, use (59*b*) to eliminate $\sin^{-1}[(2b-\eta_1-\eta_2)/(\eta_2-\eta_1)]$ from (59*a*), evaluate the obtained expression for the times t and $t+T$ and subtract the two expressions. The requirement

$$a(t+T)=a(t) \qquad b(t+T)=b(t) \tag{63}$$

implies that

$$T=2\pi\eta\sigma^2(-2E)^{-3/2} \tag{64}$$

is the period of the motion (remember that $\mu=1$).

5. Concluding remarks

The present paper complements earlier quantum mechanical studies of the Hartmann potential in spherical coordinates (Hartmann 1972a), KS coordinates (Kibler and Négadi 1984a) and parabolic coordinates (Gerry 1986). The KS approach developed in § 2 completes the endeavour undertaken by Kibler and Négadi (1984a) and constitutes an alternative to the treatment in squared parabolic coordinates given by Gerry (1986). The dynamical invariance algebra and the classical equations of motion for the Hartmann system are, to our knowledge, treated for the first time in this paper.

Several possible applications and open problems should be mentioned. The Hartmann potential takes its origin in the quantum chemistry of ring-shaped molecules. The fact that the corresponding Hamiltonian admits a dynamical invariance group should be useful in the calculation of quantities other than energy levels. We have in mind objects of physicochemical interest, such as various transition matrix elements.

An important property that the Hartmann system shares with other systems that exhibit accidental degeneracy of quantum levels is the periodicity of all finite classical trajectories. We recall that in three space dimensions the only spherically symmetric potentials with this property are, according to Bertrand's (1873) famous theorem, the Newton potential $1/r$ and the harmonic oscillator potential r^2. A question of practical interest is whether the periodicity of finite orbits in the Hartmann potential field can be put to good use. More specifically, could an electrostatic system, creating a ring-shaped potential of the form (1), be employed to confine charged particles in a stable manner? The set of periodic trajectories for the Hartmann potential is clearly stable with respect to perturbations of the initial conditions. Stability with respect to interactions between different particles or aggregates of particles, moving in such a potential, remains to be investigated.

An open conceptual question is related to the dynamical invariance group of the Hartmann Hamiltonian and similar systems having more integrals of motion than degrees of freedom. The three second-order operators X_1, X_2 and Y_1 of equations

(7)-(11) generate an infinite-dimensional Lie algebra since the commutators $[X_1, Y_1]$, $[X_1, [X_1, Y_1]]$, $[Y_1, [X_1, Y_1]]$, etc, are all linearly independent. It would be interesting to determine the structure of this Lie algebra and its relation to well understood infinite-dimensional Lie algebras, such as Kac-Moody or loop algebras (Kac 1984).

Acknowledgments

The authors are indebted to Dr T Tauth for illuminating discussions of possible macroscopic applications of the Hartmann system. They also thank T Négadi for discussions and attracting their attention to the paper by Carpio and Inomata (1986). One of the authors (MK) acknowledges helpful comments made by Dr D Schuch. The other author (PW) thanks the Institut de Physique Nucléaire de Lyon for its hospitality during the work on this project. His research is partially supported by NSERC of Canada and the Fonds FCAR du Gouvernement du Québec.

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