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Determination of the symmetries characterising separable systems in Euclidean spaces

Gregory J Reid

Department of Mathematics and Institute of Applied Mathematics, University of British Columbia, Vancouver V6T 1Y4, Canada

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Abstract. The (additively) separable coordinate systems for the Hamilton-Jacobi equation of classical mechanics, in n-dimensional complex Euclidean space $\mathbb{C}^n$, are characterised explicitly in terms of the Lie symmetry algebra of $\mathbb{C}^n$. Specifically a formula is given by which the n-separation constants, regarded as functions of position and momentum, can be expressed as members of the enveloping algebra of $\mathbb{C}^n$ (i.e. as elements of the vector space spanned by products of the members of the Lie algebra of $\mathbb{C}^n$). By quantising these n integrals of the motion we easily obtain the commuting sets of n partial differential operators characterising the (multiplicatively) separable systems for the corresponding Helmholtz equation. A package including this formula has been implemented in the symbolic language MACSYMA. The resulting program is also capable of calculating many of the time-consuming details (separation equations, etc) of separation on $\mathbb{C}^n$.

1. Introduction

Separation of variables for the Hamilton-Jacobi equation and time-independent Schrödinger equations, in n variables in n-dimensional Euclidean space, is known to be characterisable in terms of the Lie symmetries (rotations and translations) of Euclidean space. As Miller (1977) has shown, the knowledge of such symmetry characterisations enables the easy generation of (special function) identities between the separable solutions. For example, the problem of expanding one separable solution in terms of the separated eigenfunctions arising out of a different separable coordinate system can be reduced to a problem in the representation theory of the Euclidean group.

The calculation of these symmetry characterisations has been achieved in practice by using *ad hoc* techniques, which soon become unmanageable in higher dimensions ($n \geqslant 3$). In this paper we present a formula by which the symmetry characterisations associated with a given separable coordinate system can be calculated explicitly. This formula has been incorporated in a computer program, SEPCAL.V, written in the symbolic language MACSYMA. Other features, such as the calculation of separation equations, have also been incorporated in the program and relieve much of the tedium of the calculations involved in separation of variables.

This paper is concerned with the separable coordinate systems for the time-independent (reduced) Schrödinger equation, in n-dimensional complex Euclidean space $\mathbb{C}^n$:

$$-(\hbar^2/2m)\Delta\psi + (V-E)\psi = 0 \qquad \hbar = h/2\pi \tag{1.1}$$

where E is a non-zero constant, Δ is the Laplace-Beltrami operator

$$\Delta=\frac{1}{\sqrt{g}}\sum_{i,j=1}^{n}\frac{\partial}{\partial x^i}\left(\sqrt{g}\,g^{ij}\frac{\partial}{\partial x^j}\right) \tag{1.2}$$

and $\hbar$ is Planck's constant. The metric in a given coordinate system $z^i=f^i(x^k)$ is $ds^2=g_{ij}\,dx^i\,dx^j$, $g=\det(g_{ij})\neq 0$ and $g^{ik}g_{kj}=\delta^i_j$. The Einstein summation convention will always be assumed unless otherwise stated. We consider equation (1.1) in n-dimensional complex Euclidean space $\mathbb{C}^n$, with complex cartesian coordinates $z^1,\ldots,z^n$, since we will be able to give a uniform treatment of the multitude of various real forms of (1.1) (e.g. the constant potential Klein-Gordon equation).

Equation (1.1) is closely associated with the Hamilton-Jacobi (HJ) equation of classical mechanics for a particle of mass m moving under the influence of a potential $V(x^k)$:

$$H(x^i,p_i)=(1/2m)g^{ij}p_ip_j+V=E. \tag{1.3}$$

Here $p_i=\partial W/\partial x^i$ and W is the Hamilton-Jacobi function or complete integral of (1.3), i.e. $W=W(x^i,\lambda_j)$ is a regular n-parameter family of solutions of (1.3) such that $\det(\partial^2W/\partial x^i\partial\lambda_j)\neq 0$. Once a complete integral is known for (1.3) one can determine the trajectory of a particle by known methods (see Whittaker (1961) ch 10-12 and in particular § 142).

The relationship between (1.3) and (1.1) is one of quantisation. A close relationship also exists in the case of separation of variables (see Kalnins and Miller 1982). Every multiplicatively separable system for (1.1), i.e. every coordinate system $\{x^k\}$ in which (1.1) admits a solution of form

$$\psi(x^k)=\prod_{i=1}^{n}\psi_i(x^i;c_1,\ldots,c_n) \tag{1.4}$$

is an additively separable system for the HJ equation (1.3), i.e. one in which the HJ equation admits a solution of the form

$$W(x^k)=\sum_{i=1}^{n}W_i(x^i;\lambda_1,\ldots,\lambda_n). \tag{1.5}$$

The c_i and λ_i are the separation constants for (1.1) and (1.3) respectively. The $\lambda_i=g_i(x^k,p_k)$ are often called constants of the motion since their value depends only on the particular trajectory followed by a particle, although they may vary from trajectory to trajectory.

Benenti and Francaviglia (1980) have shown that if $\{x^k\}$ is a separable system for the HJ equation (1.3) with $V\neq 0$ then it is also a separable system for (1.3) with $V=0$. Henceforth, therefore, we will restrict ourselves to the study of the free-particle case $V=0$ for (1.1) (now the Helmholtz equation) and the HJ equation (1.3).

The Helmholtz equation (1.1) and the HJ equation (1.3) both share the same Lie symmetry group, that of the underlying Euclidean space (see Eisenhart 1949). The $n(n+1)/2$ infinitesimal generators of its Lie algebra $\mathcal{L}_n=\{\mathcal{Q}_r\colon r=1,2,\ldots,n(n+1)/2\}$ can be taken as

$$\begin{aligned}&\mathcal{Q}_j=\mathcal{P}_j=\frac{\hbar}{i}\frac{\partial}{\partial z^j}\\ &\mathcal{Q}_s=\mathcal{M}_{jk}=\frac{\hbar}{i}\left(z^j\frac{\partial}{\partial z^k}-z^k\frac{\partial}{\partial z^j}\right)\qquad j<k;\ j,k=1,\ldots,n\end{aligned} \tag{1.6}$$

where $s = n + \frac{1}{2}(k-1)(k-2) + j$, $\mathrm{i} = \sqrt{-1}$ and the commutation relations are

$$[\mathscr{P}_j, \mathscr{P}_k] = 0 \qquad [\mathscr{P}_j, \mathscr{M}_{kl}] = \frac{\hbar}{\mathrm{i}}(\delta_{jk}\mathscr{P}_l - \delta_{jl}\mathscr{P}_k)$$
$$[\mathscr{M}_{ij}, \mathscr{M}_{kl}] = \frac{\hbar}{\mathrm{i}}(\delta_{jk}\mathscr{M}_{il} + \delta_{il}\mathscr{M}_{jk} + \delta_{jl}\mathscr{M}_{ki} + \delta_{ik}\mathscr{M}_{lj}). \tag{1.7}$$

It has long been known that if a variable x^α does not appear explicitly in equations (1.1) and (1.3) then $\psi_\alpha = \exp(cx^\alpha)$ in (1.4) and $W_\alpha = \lambda x^\alpha$ in (1.5). Thus $(\partial\psi/\partial x^\alpha) = c\psi$, $\partial W/\partial x^\alpha = P_\alpha = \lambda$ and $\partial/\partial x^\alpha$ corresponds to a Lie symmetry for these equations, and as such is a linear combination of the $\mathscr{Q}_l$ in $\mathscr{L}_n$. The simplest examples include two-dimensional cartesian coordinates ($x^\alpha = x$) and polar coordinates ($x^\alpha = \theta$).

Not so widely known is the fact that every separable system for (1.1) and (1.3) can also be characterised (see Kalnins and Miller 1980) in terms of the Lie algebra of $\mathbb{C}^n$ but now in a more complicated way. The simplest examples include separation for the two-dimensional Helmholtz equation in elliptic and parabolic coordinates, systems in which no obvious continuous Lie symmetry is present.

Specifically, for the HJ equation in $\mathbb{C}^n$, Kalnins and Miller (1980) have shown, albeit implicitly, that each of the n-separation constants λ_i can be expanded in terms of the enveloping algebra of $\mathbb{C}^n$ (the vector space spanned by symmetrised products of members of $\mathscr{L}_n$). A similar characterisation but now in terms of n commuting symmetry operators for the Helmholtz equation can be obtained by mapping the constants of the motion into the corresponding symmetry operators, essentially a process of quantisation.

The fruitful relationship between symmetry and separation of variables has motivated an intensive series of investigations (see, e.g., Miller *et al* (1981) and references cited therein) to classify the separable systems for the common partial differential equations of mathematical physics and to give their accompanying symmetry characterisations. A particularly arduous part of the work has been to find the enveloping algebra members characterising the separation. In some cases, such as for orthogonal separable systems on real n-dimensional Euclidean spaces and the real n-sphere (see Kalnins 1986, Reid 1986) general formulae have been derived using limiting techniques. In general, however, no direct technique is known, and the results have to be derived by inspection, an approach which soon becomes impossible in higher dimensions. For example, in Kalnins and Miller (1979) the operators characterising the separable coordinate systems (3.20) and (3.21) have defied calculation by hand.

In this paper we present an explicit formula (theorem 2.1) for calculating the enveloping algebra members characterising the separation.

2. Determination of the symmetries characterising separable systems for the Hamilton–Jacobi equation

The principal result of this section is the formula given in theorem 2.1. This formula determines the constants of the motion arising from separation of variables for the HJ equation (1.3) with $V = 0$, explicitly in terms of the enveloping algebra of $\mathbb{C}^n$.

One way of solving the equations of motion for a classical particle moving under the influence of a potential $V(x^k)$ is to find n constants or integrals of the motion.

Thus one seeks n independent quantities K_j such that $\mathrm{d}K_j/\mathrm{d}t = 0$ where $\mathrm{d}/\mathrm{d}t$ is the total time derivative following the particle along its trajectory. This is equivalent in Hamilton's formalism to finding $K_j(x^i, p_i)$:

$$\{H, K_j\} = 0 \qquad j = 1, 2, \ldots, n \tag{2.1}$$

where $\{\,,\}$ is the Poisson bracket and is defined by

$$\{F, G\} = \sum_{i=1}^{n} \left(\frac{\partial F}{\partial p_i} \frac{\partial G}{\partial x^i} - \frac{\partial F}{\partial x^i} \frac{\partial G}{\partial p_i} \right). \tag{2.2}$$

One method for finding such constants of the motion is the method of separation of variables. The most elementary constants of the motion are the first-order constants of the motion which are those functions λ_α linear in the momentum:

$$\lambda_\alpha = a^i_{(\alpha)} P_i \tag{2.3}$$

that commute with H via the Poisson bracket. As already mentioned these correspond directly to geometric symmetries of the manifold and to the simplest possible type of variable separation. Indeed this correspondence can be taken as

$$\mathcal{Q}_j \leftrightarrow Q_j \tag{2.4}$$

with

$$\mathcal{P}_j \leftrightarrow \frac{\partial W}{\partial z^j} = P_j \qquad \text{and} \qquad \mathcal{M}_{ij} \leftrightarrow M_{ij} = z^i P_j - z^j P_i. \tag{2.5}$$

A coordinate-dependent set of necessary and sufficient conditions for (1.3) to be additively separable in orthogonal coordinates (i.e. $g_{ij} = 0$ for $i \neq j$) was given by Stäckel (1891) and later Levi-Civita (1904) considered the general (non-orthogonal) problem. In principle a solution to the general problem (g_{ij} not necessarily orthogonal) was found by Dall'Acqua (1909, 1912) resulting in four classes of separable coordinates, but his results are rather difficult to apply. However, it was only recently that Benenti and Francaviglia (1980), using Dall-Acqua's results, were able to give a complete solution to the separation of variables problem for (1.3) in terms of the local coordinates x^k. (Dall'Acqua's four classes of separable coordinates reduce to three under the definition of equivalence used by Benenti and Francaviglia.)

Kalnins and Miller (1981) have found a complete theory which characterises all the separable coordinate systems for the HJ equation (1.3) (with $V = 0$) in a coordinate-free manner. In their theory this is accomplished by focusing on the properties of the separation constants λ_k. In particular they find that the λ_k satisfy

$$\lambda_k = a^{ij}_{(k)}(x^l) p_i p_j \qquad \lambda_1 = H \tag{2.6a}$$

$$\{\lambda_k, \lambda_l\} = 0 \qquad k, l = 1, 2, \ldots, n. \tag{2.6b}$$

(Simply replace λ_α in (2.3) by λ_α^2 to see that the λ_α can be represented in the form (2.6).) Explicit formulae for the $a^{ij}_{(l)}$ are given in Kalnins and Miller (1981). From (2.1) it follows that the $a^{(l)}_{ij}$ must satisfy Killing's equations:

$$a^{(l)}_{ij;k} + a^{(l)}_{jk;i} + a^{(l)}_{ki;j} = 0 \tag{2.7}$$

where $;k$ denotes covariant differentiation with respect to x^k (see § 39 of Eisenhart (1949)). Thus the $a^{(l)}_{ij}$ are second-order Killing tensors and the λ_l are second-order constants of the motion.

From (2.1) it follows that any product of two first-order constants of the motion will be a second-order constant of the motion. The natural question arises as to whether the vector space spanned by products of the first-order constants of the motion (i.e. the enveloping algebra) coincides with the vector space formed by all second-order constants of the motion. For spaces of constant curvature this is true as has been shown by Katzin and Levine (1965). The same result for flat spaces was demonstrated by Thomas (1946). For related work see Delong (1982) and Hauser and Malhiot (1975).

The connection between the Euclidean group and separation of variables for the HJ equation is now clear. For each of the separation constants in (1.5) it is possible to find coefficients of expansion $A^{lm}_{(k)}$:

$$\lambda_k = A^{lm}_{(k)}\{Q_l, Q_m\}_S \tag{2.8}$$

where $\{Q_l, Q_m\}_S = \frac{1}{2}(Q_lQ_m + Q_mQ_l) = Q_lQ_m$ is the symmetrised product of Q_l and Q_m. One difficulty remains: how do we calculate the $A^{lm}_{(k)}$ in (2.8)? Our answer is given by the following theorem.

Theorem 2.1. Suppose that $\lambda(x^k, p_k) = a^{ij}(x^k)p_ip_j$ is a second-order constant of the motion in $\mathbb{C}^n$, and that the x^k are connected to complex cartesian coordinates by $z^i = f^i(x^k)$ then

$$\begin{aligned}\lambda = 4\sum_{r=1}^{n-3}\sum_{s=r+1}^{n-2}\sum_{t=s+1}^{n-1}\sum_{u=t+1}^{n} &(A^{rt}_{su}\{M_{rs}, M_{tu}\}_S + A^{rs}_{tu}\{M_{rt}, M_{su}\}_S)\\
&+\sum_{r=1}^{n-2}\sum_{s=r+1}^{n-1}\sum_{u=s+1}^{n}(2A^{rr}_{su}\{M_{rs}, M_{ru}\}_S + 4A^{rs}_{su}\{M_{rs}, M_{su}\}_S + 2A^{rs}_{uu}\{M_{ru}, M_{su}\}_S\\
&-2B^{rs}_{u}\{M_{ru}, P_s\}_S - 2B^{ru}_{s}\{M_{rs}, P_u\}_S)\\
&+\sum_{r=1}^{n-1}\sum_{s=r+1}^{n}(A^{rr}_{ss}M^2_{rs} + 2B^{rs}_{r}\{M_{rs}, P_r\}_S - 2B^{rs}_{s}\{M_{rs}, P_s\}_S + 2C_{rs}P_rP_s)\\
&+\sum_{r=1}^{n} C_{rr}P_r^2\end{aligned} \tag{2.9}$$

where the constants A^{ij}_{kl}, B^{ij}_{k} and C^{ij} in (2.9) are given by

$$A^{ij}_{kl} = \tfrac{1}{2}(J^{-1})^p_k \frac{\partial}{\partial x^p}\left((J^{-1})^q_l \frac{\partial}{\partial x^q}\hat{a}^{ij}\right) \tag{2.10a}$$

$$B^{ij}_{u} = (J^{-1})^p_u \frac{\partial}{\partial x^p}\hat{a}^{ij} - 2A^{ij}_{ul}f^l \tag{2.10b}$$

$$C^{ij} = \hat{a}^{ij} - A^{ij}_{kl}f^kf^l - B^{ij}_{k}f^k. \tag{2.10c}$$

Here $(J)^r_s = (\partial f^r/\partial x^s)$ is the Jacobian matrix and

$$\hat{a}^{ij} = a^{rs}\frac{\partial f^i}{\partial x^r}\frac{\partial f^j}{\partial x^s}. \tag{2.11}$$

Proof. Expressing λ in terms of cartesian coordinates gives

$$\lambda = \hat{a}^{lm}P_lP_m \tag{2.12}$$

where

$$\hat{a}^{lm} = a^{ij}\frac{\partial f^l}{\partial x^i}\frac{\partial f^m}{\partial x^j}. \tag{2.13}$$

In these coordinates equation (2.7) becomes

$$\frac{\partial \hat{a}_{ij}}{\partial z^k}+\frac{\partial \hat{a}_{jk}}{\partial z^i}+\frac{\partial \hat{a}_{ki}}{\partial z^j}=0. \tag{2.14}$$

By differentiating equation (2.14) twice it is not difficult to show (e.g. see Katzin and Levine 1965) that

$$\hat{a}^{ij} = A^{ij}_{kl}z^k z^l + B^{ij}_k z^k + C^{ij} \tag{2.15}$$

where the only constraints on the constants in (2.15) are

$$A^{ij}_{kl} = A^{ji}_{kl} = A^{ij}_{lk} \qquad B^{ij}_k = B^{ji}_k \qquad C^{ij} = C^{ji} \tag{2.16a}$$

$$A^{ij}_{kl} + A^{ki}_{jl} + A^{jk}_{il} = 0 \tag{2.16b}$$

$$B^{ij}_k + B^{ki}_j + B^{jk}_i = 0. \tag{2.16c}$$

A simple count shows that there are $D(n) = n(n+1)^2(n+2)/12$ independent quantities in (2.15). Thus the space of second-order constants of the motion is $D(n)$ dimensional.

It is easy to verify (see Kalnins and Miller 1980) that the expressions:

$$\{M_{rs}, M_{tu}\}_S \qquad \{M_{rt}, M_{su}\}_S \qquad 1\leqslant r<s<t<u\leqslant n \tag{2.17a}$$

$$\{M_{rs}, M_{ru}\}_S \qquad \{M_{rs}, M_{su}\}_S \qquad \{M_{ru}, M_{su}\}_S$$

$$\{M_{ru}, P_s\}_S \qquad \{M_{rs}, P_u\}_S \qquad 1\leqslant r<s<u\leqslant n \tag{2.17b}$$

$$M^2_{rs} \qquad \{M_{rs}, P_r\}_S \qquad \{M_{rs}, P_s\}_S \qquad P_rP_s \qquad 1\leqslant r<s\leqslant n \tag{2.17c}$$

$$P^2_r \qquad 1\leqslant r\leqslant n \tag{2.17d}$$

form a basis of linearly independent elements for the enveloping algebra with dimension $2\,{}^nC_4+5\,{}^nC_3+4\,{}^nC_2+{}^nC_1 = D(n)$. (Note that not all of the products Q_lQ_m are linearly independent.) Thus the space of the second-order constants of the motion is just the enveloping algebra of $\mathbb{C}^n$.

From (2.12) and (2.15)

$$A^{ij}_{kl} = \frac{1}{2}\frac{\partial^2 \hat{a}^{ij}}{\partial z^k\,\partial z^l} \tag{2.18a}$$

$$B^{ij}_u = \frac{\partial}{\partial z^u}(\hat{a}^{ij} - A^{ij}_{kl}z^k z^l) \tag{2.18b}$$

$$C^{ij} = \hat{a}^{ij} - A^{ij}_{kl}z^k z^l - B^{ij}_k z^k \tag{2.18c}$$

and equations (2.10a), (2.10b) and (2.10c) in theorem 2.1 follow directly from these expressions.

Since λ is a member of the enveloping algebra

$$\lambda = \sum_{r=1}^{n-3}\sum_{s=r+1}^{n-2}\sum_{t=s+1}^{n-1}\sum_{u=t+1}^{n}(a^{rt}_{su}\{M_{rs}, M_{tu}\}_S + a^{rs}_{tu}\{M_{rt}, M_{su}\}_S)$$
$$+\sum_{r=1}^{n-2}\sum_{s=r+1}^{n-1}\sum_{u=s+1}^{n} + \sum_{r=1}^{n} c_{rr}P^2_r a^{rr}_{su}\{M_{rs}, M_{ru}\}_S + \ldots \tag{2.19}$$

for some constants a^{rt}_{su}, a^{rs}_{tu}, a^{rr}_{su}, c_{rr}, etc.

We can obtain $a^{rt}_{su}, a^{rs}_{tu}, \ldots, c_{rr}$ in terms of A^{ij}_{kl}, B^{ij}_{k}, C^{ij} by substituting $M_{ij} = z^iP_j - z^jP_i$ in (2.19) and differentiating λ. For example, for $r<s<t<u$:

$$a^{rt}_{su} = \frac{\partial^4 \lambda}{\partial z^s\, \partial z^u\, \partial P_r\, \partial P_t} = 4A^{rt}_{su}. \tag{2.20}$$

The other coefficients are obtained in the same way. This completes the proof.

In a similar fashion we can express any first-order constant of the motion as a linear combination of members of the Lie algebra.

3. Determination of the symmetries characterising separable systems for the Helmoltz equation

As before we need only concern ourselves with the case $V=0$ and then (1.1) is the Helmholtz equation:

$$-\frac{\hbar^2}{2m}\Delta\psi = E\psi. \tag{3.1}$$

Already we know that every (multiplicatively) separable coordinate system for (3.1) is an (additively) separable system for the HJ equation (1.3). The work of Kalnins and Miller (1982) implies that for each separable system $\{x^l\}$ there exist n second-order partial differential operators

$$\mathcal{S}_k = \alpha^{ij}_{(k)}(x^l)\frac{\partial^2}{\partial x^i \partial x^j} + \beta^i_{(k)}(x^l)\frac{\partial}{\partial x^i} + \gamma_{(k)}(x^l) \tag{3.2}$$

such that for a separable solution $\psi(x^l)$

$$\mathcal{S}_k\psi = c_k\psi \tag{3.3}$$

where the c_k are the separation constants. (Without loss of generality $\mathcal{S}_1 = \Delta$ and $c_1 = E$.) The work of Kalnins and Miller (1982) implies that in a flat space $\mathbb{C}^n$ these operators can be written in the 'formally' self-adjoint form

$$\mathcal{S}_k = \frac{1}{\sqrt{g}}\frac{\partial}{\partial x^i}\left(\sqrt{g}\, a^{ij}_{(k)}\frac{\partial}{\partial x^j}\right) + h_k(x^l) \tag{3.4}$$

for some functions $h_k(x^l)$, and that the $\mathcal{S}_k$ pairwise commute:

$$[\mathcal{S}_k, \mathcal{S}_l] = 0 \qquad k, l = 1, \ldots, n. \tag{3.5}$$

In particular we will show that

$$\mathcal{S}_k = A^{lm}_{(k)}\{\mathcal{Q}_l, \mathcal{Q}_m\}_{\mathrm{S}}. \tag{3.6}$$

Just consider

$$\mathcal{T}_k = \mathcal{S}_k - A^{lm}_{(k)}\{\mathcal{Q}_l, \mathcal{Q}_m\}_{\mathrm{S}} \tag{3.7}$$

which is a first-order partial differential operator since by virtue of (3.4) the second-order derivative terms in (3.7) vanish.

Clearly $[\Delta, \mathcal{T}_k] = 0$ and so

$$\mathcal{S}_k = A^{lm}_{(k)}\{\mathcal{Q}_l, \mathcal{Q}_m\}_{\mathrm{S}} + \mathcal{T}_k \tag{3.8}$$

where $\mathcal{T}_k$ is a first-order (Lie) symmetry operator. However, $\mathcal{S}_k$ is not in self-adjoint form unless $\mathcal{T}_k = d_k$ (a constant). Without loss of generality we can take $d_k = 0$ since it only corresponds to a trivial eigenvalue shift. Thus we have verified the simple quantisation rule for obtaining the symmetry operators for separation of the Helmholtz equation from the λ_k for the HJ equation.

4. Applications

We have chosen to frame our results in $\mathbb{C}^n$ since the many resulting real forms can be easily treated in a unified manner. For example, to treat the Klein-Gordon equation for a free particle of spin 0:

$$\Box\psi = \left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\psi = \frac{mc^2}{\hbar^2}\psi \tag{4.1}$$

one simply makes the identifications $z^1 \to x$, $z^2 \to y$, $z^3 \to z$, $z^4 \to \mathrm{i}ct$, $V = 0$, $E = \frac{1}{2}c^2$ in equation (1.1). Also in Reid (1986) (or see Kalnins 1986) it is shown how the time-dependent Schrödinger equation in n spatial dimensions

$$\frac{-\hbar^2}{2m}\Delta\psi + V\psi = \mathrm{i}\hbar\frac{\partial\psi}{\partial t} \tag{4.2}$$

can be obtained from the constant potential Klein-Gordon equation in $n+2$ dimensions by a simple symmetry reduction. Thus the symmetry characterisations for the time-dependent Schrödinger equation can be obtained simply from our formula. Indeed it was from the results generated by the program SEPCAL.V for (4.2), for $n = 1, \ldots, 5$, that the author was able to conjecture the form of the symmetry operators in n dimensions (see Reid (1986) for a proof of the conjecture).

In the following we outline a little of the theory of separation of variables on a Riemannian space applying it to a simple example to illustrate the use of our algorithm.

For example if $\{x^i\}$ is an orthogonal coordinate system it is known that the corresponding HJ equation

$$H = \sum_{i=1}^{n} g^{ii}p_i^2 = E \qquad E \neq 0 \tag{4.3}$$

is separable iff the g^{ii} have Stäckel form. That is, there is a matrix $(\Phi_{ij}(x^i))$ in which the ith row has entries depending on x^i alone, such that $g^{ii} = \Phi^{i1}/\Phi$ $(\Phi = \det(\Phi_{ij}))$. The constants of the motion describing this system can be readily expressed in terms of the Stäckel matrix:

$$\lambda_m = \sum_{i=1}^{n}\frac{\Phi^{im}}{\Phi}p_i^2 \qquad \lambda_1 = H = E. \tag{4.4}$$

Thus given the coordinate transformations and the Stäckel matrix it is possible to find λ_m in terms of the enveloping algebra by using the methods of § 2.

Example. Consider parabolic coordinates in two dimensions with coordinate transformations defined by

$$z^1 = \tfrac{1}{2}[(x^1)^2 - (x^2)^2] \qquad z^2 = x^1x^2. \tag{4.5}$$

The Stäckel matrix for this separable system is

$$(\Phi_{ij}) = \begin{pmatrix} (x^1)^2 & -1 \\ (x^2)^2 & 1 \end{pmatrix}. \tag{4.6}$$

Thus

$$\lambda_2 = \sum_{i=1}^{2} \frac{\Phi^{i2}}{\Phi} p_i^2 = \frac{-(x^2)^2 p_1^2 + (x^1)^2 p_2^2}{(x^1)^2 + (x^2)^2} \tag{4.7}$$

where $p_i = \partial W/\partial x^i$. If we carry out the step given in (2.12) the reader can verify that:

$$\lambda_2 = ((x^1)^2 - (x^2)^2) P_2^2 - 2x^1 x^2 P_1 P_2 \qquad P_i = \partial W/\partial z^i. \tag{4.8}$$

In this situation formula (2.9) yields

$$\lambda_2 = A_{22}^{11} M_{12}^2 + 2B_1^{12}\{M_{12}, P_1\}_S - 2B_2^{12}\{M_{12}, P_2\}_S + 2C_{12}\{P_1, P_2\}_S + C_{11}P_1^2 + C_{22}P_2^2. \tag{4.9}$$

Using (2.10)

$$A_{11}^{22} = B_1^{12} = C_{12} = C_{11} = C_{22} = 0 \qquad B_2^{12} = -1. \tag{4.10}$$

Thus

$$\lambda_2 = 2\{M_{12}, P_2\}_S. \tag{4.11}$$

To obtain the corresponding operators for the Helmholtz equation we use the correspondence (2.4)

$$\lambda_2 = 2\{M_{12}, P_2\}_S \to \mathcal{S}_2 = 2\{\mathcal{M}_{12}, \mathcal{P}_2\}_S. \tag{4.12}$$

All of the steps illustrated by this simple example have been automated in the symbolic program SEPCAL.V. The result could have been easily obtained by inspection or by an orbit analysis as in Miller (1977). The formula is most useful in higher dimensions where such methods soon become impractical to apply.

Apart from the constants of the motion many other quantities associated with separation of variables have explicit formulae: the Helmholtz equation, the separation equations for both the Hamilton-Jacobi and Helmholtz equations and also the metric. These formulae are all amenable to symbolic programming and have been incorporated in the program SEPCAL.V. We also note that there are many subsections of the program whose operation does not depend on the space being flat. For example, the subsections involving manipulations with Stäckel matrices and the production of the separation equations can be used for performing calculations in non-flat spaces.

Considerable attention has been devoted by investigators such as Kalnins and Miller to classifying separable systems and providing their algebraic characterisations in terms of commuting sets of operators (see, e.g., Miller *et al* 1981). Miller (1977) has used such algebraic characterisations and the methods of Lie theory to determine overlap coefficients between different separable bases and to find generating functions and integral representations for the separated eigensolutions. Miller (1977) has also demonstrated the utility of this group-theoretic approach in providing simple and well-motivated derivations of special function identities, both old and new.

Deriving the algebraic characterisations, even in low dimensions is an arduous task. The program has already proved useful in spaces of low dimension for checking and correcting previously obtained results and generating the associated miscellaneous details of separation. In Reid (1984) a special class of separable coordinate systems in $\mathbb{C}_5$ is presented and all the miscellany of separation; separation equations, operators, etc, are generated as an example of the use of the program SEPCAL.V. A subclass of these systems was the subject of an article by Kalnins and Reid (1982). The systems presented in Reid (1984) also contain as a four-dimensional subcase the previously uncalculated operators for the coordinate system (3.20) of Kalnins and Miller (1979). Kalnins (1986 private communication) has recently used the program to calculate the operators for the coordinate system (3.21) of Kalnins and Miller (1979), another system whose operators had defied computation by hand. In future the program should prove valuable in extending the above work to higher dimensions.

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