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AN OUTLINE OF THE GEOMETRICAL THEORY OF THE SEPARATION OF VARIABLES IN THE HAMILTON-JACOBI AND SCHRÖDINGER EQUATIONS

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1. About the definition of separation

A Hamiltonian function H on a symplectic $2n$-dimensional manifold (M, ω) is **separable** if there exists a canonical coordinate system $(\underline{q}, \underline{p}) = (q^i, p_i)$, $\omega = dp_i \wedge dq^i$ such that the H-J equation $H(\underline{q}, \underline{p}) = E$, where $p_i = \partial W / \partial q^i$ has a **complete solution** of the form $W(\underline{q}, \underline{c}) = \sum_i W_i(q^i, \underline{c})$, where $\underline{c} = (c_i)$ are n constant parameters satisfying the **completeness condition**

$$\det \left[\frac{\partial^2 W}{\partial \underline{q} \partial \underline{c}} \right] \neq 0.$$

If we assume this as a basic definition, then the theory of the separation of variables in the Hamilton-Jacobi equation has only two basic theorems:

Theorem 1.1. *The Hamiltonian H is separable in the canonical coordinates $(\underline{q}, \underline{p})$ if and only if the* ***Levi-Civita separability conditions*** *are satisfied (no summation over the indices $i \neq j$; $\partial_i = \partial / \partial q^i$, $\partial^i = \partial / \partial p_i$)* [12]

$$\partial^i \partial^j H \, \partial_i H \, \partial_j H + \partial_i \partial_j H \, \partial^i H \, \partial^j H - \partial^i \partial_j H \, \partial_i H \, \partial^j H - \partial_i \partial^j H \, \partial^i H \, \partial_j H = 0.$$

Theorem 1.2. *Every Hamiltonian is separable.*

Proof. This is aconsequence of the Jacobi theorem. There exists a local canonical transformation $(\underline{q}, \underline{p}) \to (\underline{a}, \underline{b})$ such that $(\underline{a})$ are ignorable: $H = h(\underline{b})$. The Levi-Civita conditions w.r.to $(\underline{a}, \underline{b})$ are obviously satisfied. □

The true problem is in fact to find such a canonical transformation, and this is just done by solving the Hamilton-Jacobi equation, in any manner, by separation or not. As a consequence, if we want an effective theory (with a larger number of theorems) we must specify special classes of

(i) symplectic manifolds,
(ii) canonical coordinates and canonical transformations,
(iii) Hamiltonians.

A convenient choice is the following:

(i) cotangent bundles T^*Q of Riemannian manifolds (Q, g^{ij}),
(ii) canonical fibered coordinates and canonical point transformations,
(iii) natural Hamiltonians, $H = G + V = \frac{1}{2}\, g^{ij} p_i p_j + V$.

In item (iii) we can consider, as a special but fundamental case, the geodesic Hamiltonian $H = G = \frac{1}{2}\, g^{ij} p_i p_j$ and the general natural Hamiltonian with vector potential $H = G{+}A{+}V = \frac{1}{2}\, g^{ij} p_i p_j {+} A^i p_i {+} V$.[5] Coordinates on Q for which the geodesic Hamiltonian G is separable are called **separable**. The separation of G is a necessary condition for the separation of $H = G{+}A{+}V$.

2. Separable webs

In accordance with the choices above it is convenient to think of "equivalence classes" of separable coordinates and consquently, of "coordinate surfaces" and "webs" (families of foliations). Indeed, if the separation occurs in a coordinate system $\underline{q}$, it occurs also in a class of "equivalent" separable coordinate systems, each other related by suitable point-transformations. Indeed, the separation is not a property of a particular coordinate system, but a property of an equivalence class. Hence, what we need at the beginning of our theory is to solve two problems: (i) to give a definition of "equivalent separable coordinates" and (ii) to find "geometrical" (or "intrinsic" or "coordinate-independent") objects representing such an equivalence class. Problem (i) can be solved by the symplectic interpretation of a complete solution of the H-J equation: it is a (local) Lagrangian foliation of T^*Q transversal to the fibers such that the Hamiltonian is constant on each leaf, and it is described by equations $p_i = \partial_i W$. Then we say that two separable systems $\underline{q}$ and $\underline{q}'$ are **equivalent**[1] if the corresponding complete solutions W and W' describe the same foliation (in the intersection of their domains of definition). Problem (ii) can be solved by the analysis of the Levi-Civita separability conditions. In the case of the **orthogonal separation**, where we deal with diagonalized metric tensors, $g^{ij} = 0$ for $i \neq j$, it is clear that an orthogonal separable coordinate system $\underline{q}$ is equivalent to any other coordinate system $\underline{q}'$ which is related to $\underline{q}$ by a rescaling i.e., by a point-transformation whose Jacobian matrix is diagonal. Such a transformation leaves invariant the coordinate hypersurfaces $q^i = \text{const}$. Hence, the notion of equivalence class of orthogonal separable cordinates is replaced by the geometrical and more general notion of **separable orthogonal web**, consisting of n pairwise orthogonal foliations of submanifolds of codimension 1, $(\mathcal{S}^i) = (\mathcal{S}^1, \ldots, \mathcal{S}^n)$, such that any adapted local coordinate system $\underline{q}$ is separable. It can be proved that[3]

Theorem 2.1. *An orthogonal web is separable if and only if there exists a Killing two-tensor* $\mathbf{K}$ *with simple eigenvalues and eigenvectors orhogonal to the leaves of the web. A potential* V *is separable in this web (i.e., the Hamiltonian* $H = G + V$ *is separable) if and only if the one-form* $\mathbf{K}dV$*, the image of* dV *by* $\mathbf{K}$*, is closed,*

$$d(\mathbf{K}dV) = 0. \tag{1}$$

As a corollary we have

Theorem 2.2. *A natural Hamiltonian* $H = G + V$ *is separable if and only if there exists a Killing two-tensor* $\mathbf{K}$ *with pointwise simple eigenvalues and normal (i.e., orthogonally integrable or surface forming) eigenvectors, such that equation* (1) *is satisfied.*

Such a tensor $\mathbf{K}$ has been called **charactreristic tensor** and equation (1) **characteristic equation**.

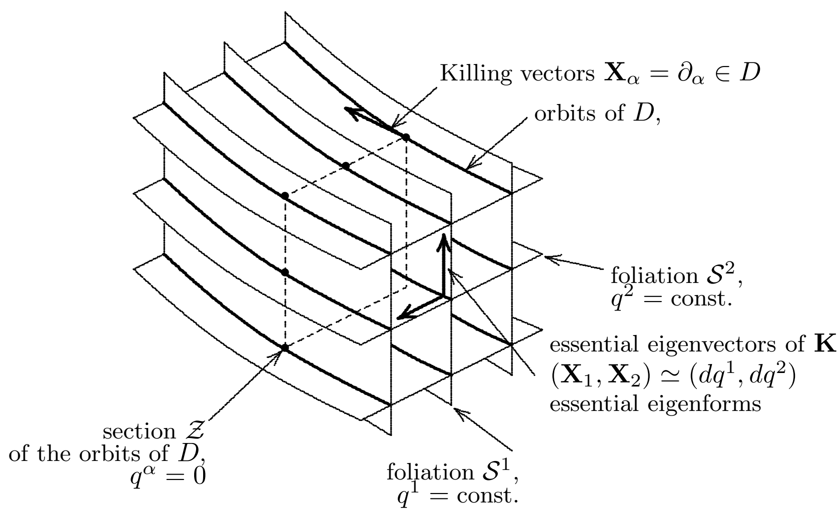
For the **general separation** (also called "non-orthogonal" separation) a basic property is the existence, within an equivalence calss, of **standard coordinates** (q^a, q^α), $a = 1, \ldots, m$, $\alpha = m+1, \ldots, n$, where (q^α) are ignorable and (q^a) are called **essential**, for which the metric tensor assume the **standard form** [1,2,4]

$$[g^{ij}] = \left[\begin{array}{ccc|c} g^{11} & & 0 & \\ & \ddots \; g^{aa} & & 0 \\ 0 & & \ddots \; g^{mm} & \\ \hline & 0 & & g^{\alpha\beta} \end{array}\right]$$

Then it can be proved that an equivalence class of separable coordinates is geometrically represented by a **separable Killing web** $(\mathcal{S}^a, D, \mathbf{K})$ made of the following objects:[4]

$$\begin{aligned} \mathcal{S}^a &= (\mathcal{S}^1, \mathcal{S}^2, \dots, \mathcal{S}^m) = m \text{ orthogonal foliations of hypersurfaces} \\ D &= r\text{-dimensional } (r = m - n) \text{ space of commuting Killing vectors} \\ &\quad \text{tangent to the foliations } \mathcal{S}^a \\ \mathbf{K} &= D\text{-invariant Killing 2-tensor with } m \text{ eigenvectors } (\mathbf{X}_a) \\ &\quad \text{orthogonal to } \mathcal{S}^a \text{ and corresponding to distinct eigenvalues } \lambda^a. \end{aligned}$$

The eigenvectors $\mathbf{X}_a$ and the eigenvalues λ^a are called **essential**. It is remarkable the fact that, under these conditions, D is normal i.e., the distribution orthogonal to D is completely integrable; this means that there exists a foliation of m-dimensional manifolds orthogonal to the orbits of D. Any coordinate system (q^a, q^α) such that (i) equation $q^a =$ const. describes (locally) the foliation $\mathcal{S}^a$, and (ii) (∂_α) form a basis of D and equations $q^\alpha = 0$ describe a submanifold $\mathcal{Z}$ orthogonal to D, is a standard separable coordinate system. The following picture illustrates the case $m = 2$.



A separable Killing web is fully represented by a pair $(D, \mathbf{K})$, which has been called **characteristic Killing pair**,[4] where D is a r-dimensional space of commuting Killing vectors and $\mathbf{K}$ is a D-invariant Killing 2-tensor with $m = n - r$ normal eigenvectors corresponding to distinct eigenvalues. Then a geometrical characterization of the general separation for a natural Hamiltonian is given by the following [4]

Theorem 2.3. *The Hamiltonian $H = G + V$ is separable if and only if there exists a characteristic Killing pair $(D, \mathbf{K})$ such that*

$$DV = 0, \qquad d(\mathbf{K}dV) = 0$$

3. First integrals

The separation is related to the existence of a complete system of first integrals in involution. Thus, separable Hamiltonian systems form a special class of integrable system.

Definition 3.1. A **Killing-Stäckel algebra** on a Riemannian manifold Q_n is an n-dimensional space $\mathcal{K}$ of Killing 2-tensors with n common and normal eigenvectors.

It follows that the elements of a KS-algebra commute as linear operators

$$\mathbf{K}_1\mathbf{K}_2 - \mathbf{K}_2\mathbf{K}_1 = 0, \qquad \forall\, \mathbf{K}_1, \mathbf{K}_2 \in \mathcal{K}, \tag{2}$$

and are in involution,

$$\{P(\mathbf{K}_1), P(\mathbf{K}_2)\} = 0, \qquad \forall\, \mathbf{K}_1, \mathbf{K}_2 \in \mathcal{K}. \tag{3}$$

Here we use the notation $P_{\mathbf{K}} = P(\mathbf{K}) = K^{ij} p_i p_j$. This second property follows from the so-called **Killing-Eisenhart equations**[9,6]

$$\partial_i \lambda^j = (\lambda^i - \lambda^j)\partial_i \ln g^{jj} \tag{4}$$

which characterize the Killing tensors diagonalized in orthogonal coordinates. It is a remarkable fact (firstly pointed out by Kalnins and Miller[10]) that, conversely,

Theorem 3.1. *An n-dimensional space $\mathcal{K}$ of Killing tensors is a KS-algebra if and only if its elements commute and are in involution (equatons* (2) *and* (3) *hold).*[6]

The analysis of the Killing-Eisenhart equations (4) shows that

Theorem 3.2. *Any KS-algebra contains the metric tensor $\mathbf{G} = (g^{ij})$ and it is uniquely determined by a **characteristic Killing tensor** $\mathbf{K}$ i.e., by a Killing tensor with simple eigenvalues and normal eigenvectors.*[6]

Theorem 3.3. *If the characteristic equation $d(\mathbf{K}dV) = 0$ is satisfied by a characteristic Killing tensor $\mathbf{K}$, then it is satisfied by all elements of the KS-algebra $\mathcal{K}$ generated by $\mathbf{K}$, and the functions*

$$H_{\mathbf{K}} = \tfrac{1}{2}\, P_{\mathbf{K}} + V_{\mathbf{K}}, \qquad dV_{\mathbf{K}} = \mathbf{K}\, dV, \qquad \forall\, \mathbf{K} \in \mathcal{K}, \tag{5}$$

form an n-dimensional space $\mathcal{H}(\mathcal{K}, V)$ of quadratic first integrals in involution.[6]

For the general separation we have similar definitions and results: the space of quadratic first integrals, whose dimension is m, is implemented by the r-dimensional space of linear first integrals $P_{\mathbf{X}} = X^i p_i$ associated with the Killing vectors $\mathbf{X} \in D$.[6]

4. The separation of the Schrödinger equation

On the space of smooth (real or complex-valued) functions ψ on Q we consider the following second-order linear differential operators,

$$
\begin{aligned}
&\Delta\psi = g^{ij}\,\nabla_i\nabla_j\,\psi = \delta\nabla\psi \quad \text{(Laplacian operator)}\\
&\Delta_{\mathbf{K}}\psi = \nabla_i(K^{ij}\nabla_j\psi) = \delta(\mathbf{K}\nabla\psi) \quad \text{(pseudo-Laplacian operator)}\\
&\widehat{P}_{\mathbf{K}}\psi = -\,\hbar^2\,\Delta_{\mathbf{K}}\psi = -\,\nabla_i(K^{ij}\nabla_j\psi)\\
&\widehat{H}_{\mathbf{K}}\psi = \tfrac{1}{2}\,\widehat{P}_{\mathbf{K}}\psi + V_{\mathbf{K}}\cdot\psi = -\,\tfrac{\hbar^2}{2}\,\Delta_{\mathbf{K}}\psi + V_{\mathbf{K}}\cdot\psi.\\
&\widehat{H}\psi = \widehat{H}_{\mathbf{G}}\psi = -\,\tfrac{\hbar^2}{2}\,\Delta\psi + V\cdot\psi \quad \text{(Schrödinger operator).}
\end{aligned}
$$

Notation: ∇ is the gradient operator, $\nabla\psi = (g^{ij}\partial_j\psi)$; ∇_i is the covariant derivative w.r.to the Levi-Civita connection; δ is the divergence (or co-differential) operator on vector fields or on skew-symmetric contravariant tensors, $\delta\mathbf{A} = (\nabla_i A^{ij\cdots k})$; on functions $\delta f = 0$; it follows that $\delta^2 = 0$.
A general definition of separation of variables for partial differential equations of any order is due to Kalnins and Miller.[11] This theory has been revisited and implemented by two definitions[6] of **separation** for the Shrödinger equation

$$\widehat{H}\psi = E\psi.$$

Definition 4.1. The Schrödinger equation is **freely separable** if it admits a **complete separated solution** of the form

$$\psi(\underline{q},\underline{c}) = \prod_{i=1}^{n}\psi_i(q^i,\underline{c})$$

depending on $2n$ parameters $\underline{c} = (c_I)$ satisfying the **completeness condition**

$$\det\left[\frac{\partial u_i}{\partial c_I}\;\middle|\;\frac{\partial v_i}{\partial c_I}\right] \neq 0, \qquad u_i = \frac{\psi_i'}{\psi_i}, \quad v_i = \frac{\psi_i''}{\psi_i}.$$

Theorem 4.1. *The Schrödinger equation is freely separable if and only if there exists a characteristic Killing tensor* $\mathbf{K}$ *(with simple eigenvalues and normal eigenvectors) such that* $d(\mathbf{K}dV) = 0$ *and* $\mathbf{KR} = \mathbf{RK}$*, where* $\mathbf{R}$ *is the Ricci tensor.*[6]

The commutation condition $\mathbf{KR} = \mathbf{RK}$ is called **Robertson condition**. In other words, the Schrödinger equation is freely separable if and only if the corresponding HJ-equation is orthogonally separable and the Robertson condition, whose coordinate expression is[8] $R_{ij} = 0$ for $i \neq j$, is satisfied.

It is known that the multiplicative separation of the Schrödinger equation is related to the existence of symmetry operators.[13] The commutation relations between the second-order operators associated with the orthogonal separation are considered in the following theorem:[7]

Theorem 4.2. *If $\mathcal{K}$ is a KS-algebra and V is a separable potential, then the following five conditions are equivalent*

$$\begin{aligned}
&\big[\widehat{H}_{\mathbf{K}}, \widehat{H}\big] = 0, \quad \forall\, \mathbf{K} \in \mathcal{K} \\
&\delta(\mathbf{KR} - \mathbf{RK}) = 0, \quad \forall\, \mathbf{K} \in \mathcal{K} \qquad (^{*}) \\
&\partial_i R_{ij} - \Gamma_i\, R_{ij} = 0, \qquad i \neq j, \;\; i\ n.s. \qquad (^{**}) \\
&\big[\widehat{H}_{\mathbf{K}_1}, \widehat{H}_{\mathbf{K}_2}\big] = 0, \quad \forall\, \mathbf{K}_1, \mathbf{K}_2, \in \mathcal{K} \\
&\delta(\mathbf{K}_1\mathbf{R}\mathbf{K}_2 - \mathbf{K}_2\mathbf{R}\mathbf{K}_1) = 0, \quad \forall\, \mathbf{K}_1, \mathbf{K}_2, \in \mathcal{K}
\end{aligned} \tag{6}$$

where $H_{\mathbf{K}}$ are the first integrals in involution defined in (5)*, R_{ij} are the components of $\mathbf{R}$ in any orthogonal separable coordinate system and Γ_i are the contracted Christoffel symbols, $\Gamma_i = g^{hj}\,\Gamma_{hj,i}$.*[7]

Remark 4.1. The potential V is involved only in the first and fourth commutation relation. Condition $(^{*}) \Leftrightarrow (^{**})$ has been called **pre-Robertson condition**. It is implied by the Robertson condition. Hence, if the Schrödinger equation is freely separable, then the second-order operators $\widehat{H}_{\mathbf{K}}$ associated with the first integrals in involution $H_{\mathbf{K}}$ commute. The converse is not true in general. It is true if $\mathbf{R} = \kappa\mathbf{G}$ (Einstein spaces).

Definition 4.2. A **reduced separated solution** of the Schrödinger equation is a solution of the form

$$\psi(\underline{q}, \underline{c}) = \prod_{a=1}^{m} \psi_a(q^a, \underline{c}) \;\;\cdot \prod_{\alpha=m+1}^{n} \psi_\alpha(q^\alpha)$$

where $\psi_\alpha = \exp(\kappa_\alpha\, q^\alpha)$, being κ_α constant parameters, and where all the remaining factors depend on further $2m$ parameters $\underline{c} = (c_A)$ $(A = 1, \ldots, 2m)$ satisfying the **completeness condition**

$$\det\left[\frac{\partial u_a}{\partial c_A} \;\middle|\; \frac{\partial v_a}{\partial c_A}\right] \neq 0, \qquad u_a = \frac{\psi_a'}{\psi_a}, \quad v_a = \frac{\psi_a''}{\psi_a} \quad (a = 1, \ldots, m).$$

When such a solution exists we say that the Schrödinger equation is **reductively separable** in the coordinates (q^a, q^α). The coordinates (q^α) and (q^a) are called **constrained** and **free** coordinates respectively.

Theorem 4.3. *The Schrödinger equation is reductively separable if and only if there exists a characteristic Killing pair $(D, \mathbf{K})$ such that: (i) the potential V is D-invariant, $DV = 0$; (ii) the characteristic equation is* *satisfied,* $d(\mathbf{K}dV = 0$*; (iii) the spaces orthogonal to* D *are invariant under the Ricci tensor* $\mathbf{R}$*, interpreted as a linear operator, and the restrictions to these spaces of* $\mathbf{R}$ *and* $\mathbf{K}$ *commute or equivalently, (iii') the essential eigenvectors are eigenvectors of the Ricci tensor* $\mathbf{R}$ *(i.e., "Ricci principal directions").*

This means that the reduced separation always occurs in standard separable coordinates (q^a, q^α) (possibly non-orthogonal) for the HJ-equation; the additional condition (iii), or (iii'), is equivalent to $R_{ab} = 0$ for $a \neq b$.

Theorem 4.4. *If* $(D, \mathcal{K})$ *is a separable Killing algebra and* V *is a separable potential, then the following five conditions are equivalent*

$$\begin{aligned}
&\big[\widehat{H}_{\mathbf{K}}, \widehat{H}\big] = 0, \quad \forall\, \mathbf{K} \in \mathcal{K} \\
&\delta(\mathbf{KR} - \mathbf{RK}) = 0, \quad \forall\, \mathbf{K} \in \mathcal{K} \\
&\partial_a R_{ab} - \Gamma_a\, R_{ab} = 0, \qquad a \neq b, \quad i\ n.s. \\
&\big[\widehat{H}_{\mathbf{K}_1}, \widehat{H}_{\mathbf{K}_2}\big] = 0, \quad \forall\, \mathbf{K}_1, \mathbf{K}_2, \in \mathcal{K} \\
&\delta(\mathbf{K}_1\mathbf{R}\mathbf{K}_2 - \mathbf{K}_2\mathbf{R}\mathbf{K}_1) = 0, \quad \forall\, \mathbf{K}_1, \mathbf{K}_2, \in \mathcal{K}
\end{aligned} \tag{7}$$

where $H_{\mathbf{K}}$ *are the quadratic first integrals defined in* (5)*,* R_{ab} *are the covariant components of the Ricci tensor corresponding to the essential separable coordinates* (q^a) *and* $\Gamma_a = g^{ij}\,\Gamma_{ij,a}$*.*[7]

Conditions (7) are similar to (6). A remark similar to Remark 4.1 holds.

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