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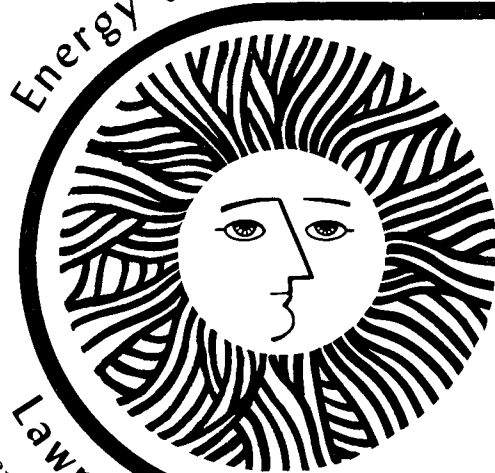
Time Dependent Canonical Transformations And The Symmetry-Equals-Invariant Theorem

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DISCLAIMER

TIME DEPENDENT CANONICAL TRANSFORMATIONS
AND THE SYMMETRY-EQUALS-INVARIANT THEOREM*

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Abstract

Expressions for the remainder function of a time dependent
infinitesimally generated canonical transformation have recently
been found by Dewar, who considered the action of the transformation
operators on Liouville's equation. Here an alternate proof of the
remainder function expression is given, based on the transformations
of particle trajectories. Then, using this expression, a proof of
the symmetry-equals-invariant theorem is given.

I. Introduction

In the canonical transformation theory presented in most texts,[1,2] the generating function $F(q, P, t)$ of mixed variables plays a major role. Knowledge of this function allows one to calculate the new Hamiltonian using the equation:

$$K = H + \frac{\partial F}{\partial t} \quad .$$

(1)

$\frac{\partial F}{\partial t}$ is known as the remainder function of the transformation. Another topic presented in most texts is that of infinitesimal canonical transformations. By successively doing infinitesimal transformations, one can generate a family of canonical transformations. The formula corresponding to Equation (1) was not known for a family of canonical transformations until recently, when Deprit[3] found such an expression in terms of a power series expansion. Then Dewar[4] cast Deprit's theory in operator form, and found an expression for the Hamiltonian by considering the action of these operators on Liouville's equation.

The first part of this paper is devoted to deriving Dewar's result by considering the individual particle trajectories rather than Liouville's equation. In this formulation it is seen that finding the remainder function is a calculus problem. The final result of the transformation theory is then used to prove the symmetry-equals-invariant theorem. This theorem has been discussed previously,[5,6] but its proof can be made more rigorous by using the new transformation theory.

II. Theory of Infinitesimal Canonical Transformations

This section begins with the introduction of notation and the statement of elementary facts concerning canonical transformations. Then the fundamental theorem will be stated and proven.

Following Saletan and Cromer,[1] the set of canonical variables is denoted by the vector z, such that $q_1, \ldots, q_n = z_1, \ldots, z_n$ and $p_1, \ldots, p_n = z_{n+1}, \ldots, z_{2n}$. The matrix γ is defined to contain the Poisson bracket relations:

$$\gamma_{ij} \equiv \{z_i, z_j\} = \begin{array}{l} 1 \text{ for } j = i+n \\ -1 \text{ for } i = j+n \\ 0 \text{ otherwise} \end{array} \tag{2}$$

The matrix γ is seen to be antisymmetric and invertible.

$$\gamma_{ij} = -\gamma_{ji} \tag{3a}$$

$$-\sum_k \gamma_{ik} \gamma_{kj} = \delta_{ij} \tag{3b}$$

It will be necessary to consider time-dependent canonical transformations which depend differentially on a parameter θ. A transformation is canonical if it preserves the Poisson bracket relations:

$$\{Z_m(z, t, \theta), Z_\ell(z, t, \theta)\} \equiv \sum_{ij} \frac{\partial Z_m}{\partial z_i} \gamma_{ij} \frac{\partial Z_\ell}{\partial z_j} = \gamma_{m\ell}. \tag{4}$$

In addition to being canonical, the transformations $z(z, t, \theta)$ are required to be invertible, twice differentiable in all arguments simultaneously, and to reduce to the identity when $\theta = 0$:

$$z[z^{-1}(z, t, \theta), t, \theta] = z^{-1}[z(z, t, \theta), t, \theta] = z \tag{5a}$$

$$z(z, t, 0) = z \tag{5b}$$

It will also be necessary to consider functions of the phase space variables z, the time t, and the parameter θ. By transforming the variables, new functions can be formed from old. As an example, the function $f(z, t, \theta)$ can be defined by transforming the function $F(z, t)$ according to:

$$f(z, t, \theta) \equiv F(Z(z, t, \theta), t) \tag{6}$$

To avoid ambiguities in taking derivatives, a very explicit notation must be introduced. The symbol

$$\left.\frac{\partial F}{\partial z_\ell}\right|_{Z(z, t, \theta), t, \theta} \tag{7}$$

means: take the derivative of the function $F(z, t)$ with respect to the variable z_ℓ, then for the variables z, substitute $Z(z, t, \theta)$. When the arguments are not explicitly written, they are assumed to be z. This notation is illustrated by applying the chain rule to equation (6):

$$\frac{\partial f}{\partial t} = \left.\frac{\partial F}{\partial t}\right|_{Z(z, t, \theta), t} + \sum_\ell \left.\frac{\partial F}{\partial z_\ell}\right|_{Z(z, t, \theta), t} \times \frac{\partial Z_\ell}{\partial t} . \tag{8}$$

Finally, one more fact is needed which can be stated in the form of a lemma:

<u>Lemma</u>

Given a differentiable family of invertible canonical mappings $Z(z, t, \theta)$, there exists a function $w(z, t, \theta)$ such that

$$\frac{\partial Z_i}{\partial \theta} = +\left\{w(z, t, \theta), Z_i(z, t, \theta)\right\} . \tag{9}$$

This statement is shown to be true in Reference 1, p. 222. For completeness, a proof is included in Appendix A. Using (9) and (5), it is possible to show that the inverse transformation satisfies the following relation with the same function w:

$$\frac{\partial Z\bar{\ell}^1}{\partial \theta} = -\left\{ w \left(\underset{\sim}{Z}^{-1} (\underset{\sim}{z}, t, \theta), t, \theta \right), Z_\ell^{-1} (\underset{\sim}{z}, t, \theta) \right\} \tag{10}$$

The function $w(\underset{\sim}{z}, t, \theta)$ is here known as the generating function of the transformation $\underset{\sim}{Z}(\underset{\sim}{z}, t, \theta)$. This function is not to be confused with the generating functions of mixed variables used by Goldstein,[2] which are known here as the "mixed generating functions."

Now that the basic properties of canonical transformations have been discussed, it is possible to discuss the problem at hand. First it is assumed that the evolution in time of the variables $\underset{\sim}{z}$ is given by a Hamiltonian $h(\underset{\sim}{z}, t)$. Then it is known (Ref. 1, Ch. VI) that there exists a function K which gives the evolution of the transformed variables according to

$$\dot{Z}_\ell (\underset{\sim}{z}, t, \theta) = \left\{ Z_\ell, K(\underset{\sim}{Z}(\underset{\sim}{z}, t, \theta), t, \theta) \right\} . \tag{11}$$

The objective here is to find the new Hamiltonian K.

Consider the standard expression for computing the time derivative of the function $Z_\ell (\underset{\sim}{z}, t, \theta)$:

$$\dot{Z}_\ell (\underset{\sim}{z}, t, \theta) = \frac{\partial Z_\ell}{\partial t} + \left\{ Z_\ell, h \right\} . \tag{12}$$

Suppose a function $r(\underset{\sim}{z}, t, \theta)$ can be found such that the partial derivative of Z_ℓ with respect to time can be written in the form:

$$\frac{\partial Z_\ell}{\partial t} = \left\{ Z_\ell, r \right\} . \tag{13}$$

Then equation (12) becomes

$$\dot{Z}_\ell = \{Z_\ell, k\} \ , \tag{14a}$$

where

$$k = h + r \ . \tag{14b}$$

Thus the function K which is in (11) is given by:

$$K(\underset{\sim}{z}, t, \theta) = k(\underset{\sim}{Z}^{-1}(\underset{\sim}{z}, t, \theta), t, \theta) \ . \tag{15}$$

Now it is seen that to complete the transformation theory, the function $r(\underset{\sim}{z}, t, \theta)$ which satisfies (13) must be found. The function r is found by differentiating (9) with respect to time.

$$\frac{\partial}{\partial \theta} \left(\frac{\partial Z_i}{\partial t} \right) = \{\frac{\partial w}{\partial t}, Z_i\} + \{w, \frac{\partial Z_i}{\partial t}\} \tag{16}$$

Equation (16) is a differential equation in θ for the function $\frac{\partial Z_i}{\partial t}$. This equation, together with a boundary condition, uniquely specifies $\frac{\partial Z_i}{\partial t}$. The appropriate boundary condition follows from (5b):

$$\frac{\partial Z_i}{\partial t}\bigg|_{\underset{\sim}{z}, t, 0} = 0 \ . \tag{17}$$

I now assert that the following set of formulas gives a solution to (16) and (17):

$$\frac{\partial Z_i}{\partial t} = \{Z_i, r\} \tag{18}$$

$$r(\underset{\sim}{z}, t, \theta) = R(\underset{\sim}{Z}(\underset{\sim}{z}, t, \theta), t, \theta) \tag{19a}$$

$$R(\underset{\sim}{z}, t, \theta) = - \int_0^\theta d\theta' \ \frac{\partial w}{\partial t}\bigg|_{\underset{\sim}{Z}^{-1}(\underset{\sim}{z}, t, \theta'), t, \theta'} \tag{19b}$$

Proving this assertion completes the task of finding K.

To prove that (18) is a solution, it must first be noted that when θ is zero, R vanishes. Using (19a) and (18), this implies that (17) is

satisfied. To prove that (16) is satisfied by (18) and (19), I will calculate both sides of equation (16) using (18) and (19), and show them to be equal.

Using (18), the left hand side of equation (16) can be put in the form:

$$\text{L.H.S.} = \left\{\frac{\partial Z_i}{\partial \theta}, r\right\} + \left\{Z_i, \frac{\partial r}{\partial \theta}\right\} . \tag{20}$$

Rewriting the second term using (19a) and the chain rule gives:

$$\text{L.H.S.} = \left\{\frac{\partial Z_i}{\partial \theta}, r\right\} + \left\{Z_i, \frac{\partial R}{\partial \theta}\Big|_{Z(\zeta,t,\theta),t,\theta}\right\}$$

$$+ \sum_\ell \left\{Z_i, \frac{\partial R}{\partial z_\ell}\Big|_{Z(\zeta,t,\theta),t,\theta} \times \frac{\partial Z_\ell}{\partial \theta}\right\} . \tag{21}$$

Then using (9) on the first and third terms, equation (21) becomes:

$$\text{L.H.S.} = \left\{\{w,Z_i\}, r\right\} + \left\{Z_i, \frac{\partial R}{\partial \theta}\Big|_{Z(\zeta,t,\theta),t,\theta}\right\}$$

$$+ \sum_\ell \left\{Z_i, \frac{\partial R}{\partial z_\ell}\Big|_{Z(\zeta,t,\theta),t,\theta} \times \{w,Z_\ell\}\right\}. \tag{22}$$

Recognizing the chain rule in the following form,

$$\sum_\ell \frac{\partial R}{\partial z_\ell}\Big|_{Z_\ell(\zeta,t,\theta),t,\theta} \times \{w,Z_\ell\} = \{w, R(Z(\zeta,t,\theta),t,\theta)\} , \tag{23}$$

and inserting (19b) into the second term of (22) results in:

$$\text{L.H.S.} = \left\{\{w,Z_i\}, r\right\} + \left\{\frac{\partial w}{\partial t}, Z_i\right\} + \left\{Z_i, \{w,r\}\right\} . \tag{24}$$

Jacobi's identity allows equation (24) to be written in its final form.

$$\text{L.H.S.} = \left\{\frac{\partial w}{\partial t}, Z_i\right\} + \left\{w, \{Z_i, r\}\right\} \tag{25}$$

This expression is seen to equal the right hand side of (16) upon using (18), proving the assertion.

The results of this section show the existence of a formula giving the new Hamiltonian in terms of the infinitesimal generating function w. Combining (14b), (15), and (19), the final result is:

$$K(\underset{\sim}{z},t,\theta) = h(\underset{\sim}{Z}^{-1}(\underset{\sim}{z},t,\theta), t) - \int_0^\theta d\theta' \left.\frac{\partial w}{\partial t}\right|_{\underset{\sim}{Z}^{-1}(\underset{\sim}{z},t,\theta'), t,\theta'} \tag{26}$$

To connect these results to Dewar's,[4] operators corresponding to the transformation are defined by:

$$\left(T(\theta)f\right)(\underset{\sim}{z},t,\theta) = f\left(\underset{\sim}{Z}(\underset{\sim}{z},t,\theta), t,\theta\right) \tag{27}$$

Then equation (26) becomes

$$K = T^{-1}(\theta)h - \int_0^\theta d\theta' \, T^{-1}(\theta') \frac{\partial w}{\partial t}(\theta') \tag{28}$$

Though this equation appears to differ from Dewar's equation (27),[4] it is only because of differences in conventions.

As Dewar points out, by expanding w in a power series in θ, Deprit's perturbation theory can be derived. Since the operator T is also a power series, this way of doing perturbation theory involves multiplying series. I would like to point out that in practical calculation, (28) is more convenient than Dewar's formula since there is one less operator series to multiply.

III.   The Symmetry-Equals-Invariant Theorem

Now I would like to consider the application of (26) to the symmetry-equals-invariant theorem.   In its time dependent form, this theorem was partially discussed by Whittaker.[6]   Recently, Anderson gave a more complete discussion.[5]   Here I would like to show that the proof of this theorem need not be based on expansions; in fact, its proof for a finite composition of infinitesimal transformations becomes straightforward using (26).

First, definitions for the terms used must be given.   A family of canonical transformations is said to be a symmetry, if the new Hamiltonian K is identical in form to the old Hamiltonian h up to the addition of an arbitrary function of t and θ alone.

$$K(\underset{\sim}{z},t,\theta) = h(\underset{\sim}{z},t) + f(t,\theta) \tag{29}$$

An invariant of the motion $g(\underset{\sim}{z},t)$ is any function whose total time derivative is zero.

$$\dot{g} \equiv \frac{\partial g}{\partial t} + \{g,h\} = 0 \tag{30}$$

With these definitions, the following theorem is proven.

The Symmetry-Equals-Invariant Theorem

Given a family of canonical transformations which is a symmetry of the Hamiltonian h, one can construct an invariant of the motion g. Conversely, the canonical transformation generated by any invariant g is a symmetry of the Hamiltonian.

Proof

To prove the first statement, we assume that we know the symmetry $\underset{\sim}{z}(\underset{\sim}{z},t,\theta)$, and we have constructed the generating function $w(\underset{\sim}{z},t,\theta)$ as

in Appendix A. Using the symmetry property (29) in equation (26) gives

$$h(\zeta,t) + f(t,\theta) = h\left(Z^{-1}(\zeta,t,\theta), t\right) - \int_0^\theta d\theta' \left.\frac{\partial w}{\partial t}\right|_{Z^{-1}(\zeta,t,\theta'),t,\theta'} . \quad (31)$$

Differentiating (31) with respect to θ results in

$$\frac{\partial f}{\partial \theta} = \sum_\ell \left.\frac{\partial h}{\partial z_\ell}\right|_{Z^{-1}(\zeta,t,\theta),t} \times \frac{\partial Z_\ell^{-1}}{\partial \theta} + \left.\frac{\partial w}{\partial t}\right|_{Z^{-1}(\zeta,t,\theta),t,\theta} . \quad (32)$$

Now using equation (10) and transforming ζ, (32) becomes

$$\frac{\partial w}{\partial t} + \{w,h\} + \frac{\partial f}{\partial \theta} = 0 . \quad (33)$$

The function $g(\zeta,t,\theta) = w(\zeta,t,\theta) - \int^t dt' \frac{\partial f}{\partial \theta}(t',\theta)$, is seen to be

an invariant of the motion for all θ.

To prove the second statement, I assume a function $g(\zeta,t)$ is known

which is an invariant. Then, the transformation $Z(\zeta,t,\theta)$ is determined by

integrating (9), using

$$w(\zeta,t,\theta) = g(\zeta,t) . \quad (34)$$

To prove this transformation is a symmetry, differentiate (26) with

respect to θ.

$$\frac{\partial K}{\partial \theta} = \sum_\ell \left.\frac{\partial h}{\partial z_\ell}\right|_{Z^{-1}(\zeta,t,\theta),t} \times \frac{\partial Z_\ell^{-1}}{\partial \theta} - \left.\frac{\partial g}{\partial t}\right|_{Z^{-1}(\zeta,t,\theta),t} \quad (35)$$

Using (10), this becomes

$$\frac{\partial K}{\partial \theta} = - \left.\left(\{g,h\} + \frac{\partial g}{\partial t}\right)\right|_{Z^{-1}(\zeta,t,\theta),t} , \quad (36)$$

but since g is an invariant:

$$\frac{\partial K}{\partial \theta} = 0 . \quad (37)$$

This of course tells us that

$$K(\underset{\sim}{z},t,\theta) = K(\underset{\sim}{z},t,0) = h(\underset{\sim}{z},t) \ , \tag{40}$$

proving the theorem.

IV. Conclusions

It has been shown that Dewar's formula for the remainder function for a succession of infinitesimal transformations can be proven by consideration of particle trajectories rather than Liouville's equation. In the process, an equation has been derived which is simpler to use when doing perturbation theory. Finally, this equation has been used to give a rigorous proof of the symmetry-equals-invariant theorem.

V. Acknowledgements

Appendix A: Proof of the Lemma

Lemma

Given a differentiable family of invertible mappings $\zeta(z,t,\theta)$, there exists a function $w(z,t,\theta)$ such that

$$\frac{\partial Z_k}{\partial \theta} = \{w, Z_k\} \tag{A1}$$

Proof

The lemma will be proven by construction. Consider first the vector $\underset{\sim}{V}(z,t,\theta)$ given by

$$V_k(z,t,\theta) = \sum_\ell \gamma_{\ell k} \left. \frac{\partial Z_\ell}{\partial \theta} \right|_{\zeta^{-1}(z,t,\theta), t, \theta} \tag{A2}$$

Suppose $\underset{\sim}{V}$ can be shown to be the gradient of a potential, i.e.

$$V_k = -\frac{\partial W}{\partial z_k} \tag{A3}$$

Then w is given by

$$w(z,t,\theta) = W\left(\zeta(z,t,\theta), t, \theta\right) . \tag{A4}$$

This can be seen by inserting (A2) into (A3), multiplying the result by γ_{km}, summing over k and using (3b) to get

$$\left. \frac{\partial Z_m}{\partial \theta} \right|_{\zeta^{-1}(z,t,\theta)\ t,\theta} = \sum_k \frac{\partial W}{\partial z_k} \gamma_{km} = \{W, z_m\} \tag{A5}$$

Upon transforming z, this becomes

$$\frac{\partial Z_m}{\partial \theta} = \left\{W\left(\zeta(z,t,\theta), t,\theta\right), Z_m(z,t,\theta)\right\} . \tag{A6}$$

So it is seen that once the potential W has been found, the lemma has been proven.

To find the potential W, first the symmetry of the partial derivatives of $\underset{\sim}{V}$ must be shown:

$$\frac{\partial V_k}{\partial z_\ell} \overset{?}{=} \frac{\partial V_\ell}{\partial z_k} \quad . \tag{A7}$$

Once this is proven, W is found by integrating $\underset{\sim}{V}$:

$$W = - \int^{\underset{\sim}{z}} \sum_\ell V_\ell(\underset{\sim}{z}',t,\theta)dz'_\ell \quad . \tag{A8}$$

To prove the symmetry (A7), the partial derivative must be calculated. This is done by differentiation of (A2).

$$\frac{\partial V_k}{\partial z_\ell} = \sum_m \gamma_{km} \sum_r \left. \frac{\partial^2 Z_m}{\partial\theta\partial z_r}\right|_{\underset{\sim}{Z}^{-1}(\underset{\sim}{z},t,\theta),\, t,\theta} \times \frac{\partial Z_r^{-1}}{\partial z_\ell} \tag{A9}$$

Digressing for a moment, it is noted that (3b) and (4) can be combined to give:

$$\delta_{j\ell} = \sum_r \frac{\partial Z_j}{\partial z_r} \left(-\sum_{ip} \gamma_{\ell i} \frac{\partial Z_i}{\partial z_p} \gamma_{pr}\right) \tag{A10}$$

Also, differentiating (5a) and transforming $\underset{\sim}{z}$ gives

$$\delta_{j\ell} = \sum_r \frac{\partial Z_j}{\partial z_r} \cdot \left. \frac{\partial Z_r^{-1}}{\partial z_\ell}\right|_{\underset{\sim}{Z}(\underset{\sim}{z},t,\theta)\, t,\theta} \quad . \tag{A11}$$

At this point the fact that the matrix $\dfrac{\partial Z_j}{\partial z_r}$ is invertible, since the transformation $\underset{\sim}{Z}(\underset{\sim}{z},t,\theta)$ is invertible, is used to imply, from (A10) and (A11), the following relationship.

$$\left. \frac{\partial Z_r^{-1}}{\partial z_\ell}\right|_{\underset{\sim}{Z}(\underset{\sim}{z},\theta),\, t,\theta} = -\sum_{ip} \gamma_{\ell i} \frac{\partial Z_i}{\partial z_p} \gamma_{pr} \tag{A12}$$

Transforming ζ in (A12) and inserting the result into (A9) gives the final form for the partial derivative:

$$\frac{\partial V_k}{\partial z_\ell} = \left(\sum_{mrip} -\gamma_{km} \frac{\partial^2 Z_m}{\partial\theta\partial z_r} \gamma_{rp} \frac{\partial Z_i}{\partial z_p} \cdot \gamma_{i\ell} \right)\Big|_{\zeta^{-1}(\zeta,t,\theta),\,t,\theta} \qquad (A13)$$

To prove that the right-hand side of (A13) is symmetric in k and ℓ, equation (4) is differentiated with respect to θ.

$$\sum_{rp} \frac{\partial^2 Z_m}{\partial\theta\partial z_r} \gamma_{rp} \frac{\partial Z_i}{\partial z_p} = - \sum_{rp} \frac{\partial Z_m}{\partial z_r} \gamma_{rp} \frac{\partial^2 Z_i}{\partial\theta\partial z_p} \qquad (A14)$$

Upon inserting this relation into (A13) and using the antisymmetry property of the γ matrix, the symmetry (A7) is seen to be true, proving the lemma.

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