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Lie Algebras and Canonical Integration

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Summary

In this note we apply Lie algebric methods (see Ref. 1) to the problem of finding generalization of the Runge Kutta method of numerical integration of ordinary partial differential equation to respect the symplectic invariance of Hamiltonian systems. The aim is to rephrase the canonical integration technique of R. Ruth (ref. 2) in a Lie Algebraic language. This allows us to easily derive the conditions for the coefficients of the integration formulas from a purely algebraic problem. Besides claifying the method, this allows us to easily derive higher order formulas.

1. Introduction

Differential equations derived from an Hamiltonian via the Hamilton equations have the property that the solutions of such equations can be represented as a canonical transformation on the initial condition. A general canonical transformation has the property of being symplectic, that is if

$$\vec{q}^{\,fin}(\vec{q}^{\,in},\vec{p}^{\,in},t),\ \vec{p}^{\,fin}(\vec{q}^{\,in},\vec{p}^{\,in},t) \qquad (1\text{-}1)$$

are the final coordinates and momenta as function of the initial coordinates and momenta, the Poisson Bracket is invariant. If we define the Poisson Bracket of two arbitrary functions of $\vec{p}^{\,in}$ and $\vec{q}^{\,in}$ as

$$[f,g] \stackrel{def}{=} \sum_{i=1}^{3} \left[\left(\frac{\partial f}{\partial q_i^{in}}\right)\left(\frac{\partial g}{\partial p_i^{in}}\right) - \left(\frac{\partial f}{\partial p_i^{in}}\right)\left(\frac{\partial g}{\partial q_i^{in}}\right)\right], \qquad (1\text{-}2)$$

then

$$[q_i^{fin},p_j^{fin}] = \delta_{ij} = [q_i^{in},p_j^{in}],$$

$$[p_i^{fin},p_j^{fin}] = 0 = [p_i^{in},p_j^{in}] \qquad (1\text{-}3)$$

$$[q_i^{fin},q_j^{fin}] = 0 = [q_i^{in},q_j^{in}].$$

Equations (1-3) follow from the Hamilton Jacobi equations

$$\frac{\partial}{\partial t} q_i = \frac{\partial H(\vec{q},\vec{p},t)}{\partial p_i} = - [H,q_i] \qquad (1\text{-}4)$$

$$\frac{\partial}{\partial t} p_i = - \frac{\partial H(\vec{q},\vec{p},t)}{\partial q_i} = - [H,p_i]$$

by using the Jacobi property of the P.B.:

$$[f,[g,h]] + [h,[f,g]] + [g,[h,f]] = 0 \qquad (1\text{-}5)$$

The canonical conditions of Eq. (1-3) impose strong restrictions on the functions $\vec{q}^{fin}$ and $\vec{p}^{fin}$. For instance they imply that the Jacobian determinant of the map from the initial to the final condition is exactly one. Ordinary methods to integrate differential equations, when applied to Eqs. (1-4) do not exactly preserve the conditions (1-3). As a result, the Jacobian will not be exactly unity and extraneous damping or amplification of the motion will result in the approximate solutions. This can be a problem if the approximation is applied to problems that require to follow a dynamical system for very long times.

Explicit methods that preserve the canonical conditions (1-3) have been derived by R. Ruth [2]. In the following we will re-derive and generalize his result using Lie Algebraic methods [1].

2. Lie Operators and Lie Transformations

If we define a vector $\vec{z}$, that has as its components coordinates and momenta,

$$\vec{z} = (\vec{q},\vec{p}) = (q_1,q_2,q_3,p_1,p_2,p_3) \tag{2-1}$$

then the Hamilton equation can be written as (summation of repeated indices is assumed)

$$\frac{\partial z_i}{\partial t} = J_{ij} \frac{\partial H}{\partial z_j} . \tag{2-2}$$

J is the 6x6 matrix

$$\begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} , \tag{2-3}$$

where I is the 3x3 identity matrix.

The Poisson Bracket of two functions of z can be written as

$$[f,g] = \frac{\partial f}{\partial z_i} J_{ij} \frac{\partial g}{\partial z_j} \tag{2-4}$$

and Eq. (2-2) can be written as

$$\frac{\partial z_i}{\partial t} = - [H,z_i] \tag{2-5}$$

The canonical conditions of Eq. (1-3) can be rewritten as

$$[z_i^{fin}, z_j^{fin}] = J_{ij} = [z_i^{in}, z_j^{in}] \qquad (2\text{-}6)$$

A Lie operator :f:, where f is a general function of z is defined by its action on a function g:

$$:f:g \equiv [f,g] \qquad (2\text{-}7)$$

Products of Lie operators are defined as

$$(:f::h:)\, g \equiv :f:(:h:g) = [f,[h,g]].$$

Note that the product of two Lie operators is generally <u>not</u> a Lie operator. There may not be a function t such that

$$:t:g = [t,g] = [f,[h,g]] \text{ for all } g.$$

The commutator of two Lie operators, however is a Lie operator

$$(:f::h: - :h::f:)\, g = [f,[h,g]] - [h,[f,g]]$$

$$= [[f,h],g] = :[f,g]:\, g, \text{ for all } g\text{'s}.$$

In the next to last step the Jacobi identity (1-5) has been used. The identity

$$:f::g: - :g::f: = :[f,g]: \qquad (2\text{-}8)$$

shows that the commutator of two Lie operators is a Lie operator.

Powers of a Lie operator :f: are defined as

$$:f:^0 g = g$$

$$:f:^1 g = [f,g] \tag{2-9}$$

$$\vdots$$

$$:f:^n g = [f,(:f:^{n-1} g)]$$

The exponential of a Lie operator :f: is defined as a power series

$$\exp(:f:) \overset{def}{=} \sum_{m=0}^{\infty} :f:^m/m! \tag{2-10}$$

Since (2-9) shows that each power of :f: when applied to a function g(z) gives a function of z, exp(:f:) will also, if the series converges. The operator exp(:f:) is called the Lie transformation associated with the function f. Lie transformations form a group, that is given f any g, then an h exists such that

$$e^{:f:} e^{:g:} = e^{:h:} \tag{2-11}$$

This follows from Eq. (2-8) using the CBH theorem. Every Lie transformation has an inverse

$$\exp(:-f:)\ \exp(:f:) = 1. \tag{2-12}$$

An important relationship relates Lie transformations and Lie operators:

$$\exp(:f:)\ :g:\ \exp(-:f:) = :(\exp(:f:)g) \tag{2-13}$$

Eq. (2-13) can be derived using Eq. (2-8), by expanding the two exponentials using Eq. (2-10).

Lie transformations have the important property that they preserve Poisson Brackets, that is for all f, h, and g.

$$[(e^{:f:}g),\ (e^{:f:}h)] = e^{:f:}[g,h] \tag{2-14}$$

Eq. (2-14) is easily derived in "colonized" form:

$$:[(e^{:f:}g),\ (e^{:f:}h)]:$$

$$= :(e^{:f:}g):\ :(e^{:f:}h): - :(e^{:f:}h):\ :(e^{:f:}g):$$

$$= e^{:f:}\ :g:\ e^{-:f:}\ e^{:f:}\ :h:\ e^{:-f:} - e^{:f:}\ :h:\ e^{-:f:}\ e^{:f:}\ :g:\ e^{-:f:}$$

$$= e^{:f:}\ (:g::h: - :h::g:)\ e^{-:f:}$$

$$= e^{:f:}\ (:[g,h]:)\ e^{-:f:} = :(e^{:f:}[g,h]):$$

In this derivation use has been made first of Eq. (2-8), then (2-13), (2-12), then (2-8) again and finally of Eq. (2-13) a second time.

When applied to z Eq. (2-14) has the important result that for all :f: the transformation $e^{:f:}$ is canonical, that is if

$$z_i^{fin} = e^{:f:}\, z_i, \tag{2-15}$$

then

$$[z_i^{fin}, z_j^{fin}] = e^{:f:}[z_i, z_j] = e^{:f:}J_{ij} = J_{ij} \tag{2-16}$$

In the last step we have used the fact, that since J_{ij} is a constant, all Poisson Brackets are zero and ony the identity survives in the series of Eq. (2-10).

Having shown that a Lie transformation is a canonical transformation, the problem of finding an explicit approximation to equation (2-5) is reduced to approximately the evolution form initial to final condition with a sequence of Lie transformations. If the Hamiltonian $H(\vec{z})$ is time independent Eq. (2-5) can be written as

$$\dot{z}_i(t) = -\ :H:z_i(t),$$

with the solution

$$z_i(t) = e^{-t:H:}z_i. \tag{2-17}$$

If H(z,t) is time dependent a formal, but useless solution of Eq. (2-5) is

$$z_i(t) = T\ e^{-\int_o^t\ :H(t'):dt'}\ z_i, \tag{2-18}$$

where T denotes a time ordering of the exponential from left to right with increasing time.

In general Eq. (2-17) is not useful if an explicit canonical approximation is desired, because if one truncates the exponential to a finite order, the transformation is not exactly canonical. There are however Lie transformations that can be explicitly computed. These are the Lie transformations $e^{:f:}$ where f is only a function of $\vec{p}$ or $\vec{q}$.

If $K(\vec{p})$ is only a function of $\vec{p}$, then the actin of $e^{-:K(p):}$ on $\vec{p}$ and $\vec{q}$ is as follows

$$\vec{p}^f = e^{-:K(p):}\,\vec{p} = \vec{p} - [K(p),\vec{p}] + \cdots = \vec{p}$$

$$\vec{q}^f = e^{-:K(\vec{p}):}\,q = \vec{q} - [K(p),\vec{q}] + \frac{[K(p),[K(p),\vec{q}]]}{2} + \cdots$$

$$= \vec{q} + \frac{\vec{\partial}}{\partial p} K \qquad (2\text{-}19)$$

All higher order terms are zero because the commutator of two functions of $\vec{p}$ only is zero. In the same way one can show that if V(q) is a function of $\vec{q}$ only then

$$\vec{p}^f = e^{-:V(q):}\,\vec{p} = \vec{p} - \frac{\vec{\partial}}{\partial q} V(q)$$

$$\vec{q}^f = e^{-:V(q):}\,\vec{q} = \vec{q} \qquad (2\text{-}20)$$

3. Time Independent Hamiltonians

We will now show how to use Eq. (2-19) and (2-20) to derive explicit integration formulas in case the Hamiltonian H has the form

$$H(\vec{p},\vec{q}) = K(\vec{p}) + V(\vec{q}) \tag{3-1}$$

To start with we will assume that V is time independent, we will discuss the case V is dependent on t later, and show it does not add any essential difficulty.

If we have the coordinate and momenta z_i at the time t and we want the coordinates and momenta z_j^h at time t + h, the formal expression for z_i^h can be obtained from Eq. (2-17):

$$z_i^h = e^{-h:K(p): - h:V(p):} z_i \tag{3-2}$$

Note that Eq. (3-2) cannot be explicitly evaluated. However, if h is small one could try the Trotter formula:

$$e^{-h:K(p): - h:V(q):} = e^{-h:V(q):} e^{-h:K(p):} + O(h^2) \tag{3-3}$$

If one neglects the term of order h^2 and higher on the LHS of Eq. (3-3) one gets an approximation good only to first order in h, however since the product of two canonical transformations is a canonical transformation the symplectic condition will be preserved to all orders in h.

The approximation (3-3) to the exponential of H gives the following scheme for computing p_i^h, q_i^h in tems of p_i, q_i. First $e^{-h:V(q):}$ is applied on q,p giving

$$q_i^1 = q_i, \; p_i^1 = p_i - h \frac{\partial V(q)}{\partial q_i} \tag{3-4}$$

Then $e^{-h:K(p):}$ is applied giving

$$q_i^h = q_i^l + h \frac{\partial K(p^l)}{\partial p_i} \qquad p_i^h = p^l \tag{3-5}$$

Maybe at this point a digression is necessary to explain why the canonical transformation corresponding to the Lie transformation on the left is applied first. If the final condition is given as a product of Lie transformations

$$\vec{z}^f = \mathcal{A}_1 \mathcal{A}_2 \mathcal{A}_3 \mathcal{A}_4 \ldots \mathcal{A}_n \vec{z} \, , \tag{3-6}$$

and the action of $\mathcal{A}_i$ on z is given by the canonical transformation $\vec{C}_i(\vec{z})$

$$\mathcal{A}_i \vec{z} = \vec{C}_i(\vec{z}) \, , \tag{3-7}$$

then the action of the Lie transformation in Eq. (3-6) is as follows:

$$z^f = \mathcal{A}_1 \ldots \mathcal{A}_{N-1} \vec{C}_N(\vec{z})$$

$$= \mathcal{A}_1 \ldots \mathcal{A}_{N-2} \vec{C}_N(\vec{C}_{N-1}(\vec{z}))$$

$$\vdots$$

$$= \vec{C}_N (\cdots \vec{C}_2(\vec{C}_1(\vec{z})) \cdots).$$

Since functions "operate" from the inside of the parentheses to the outside, one sees that the canonical transformations corresponding to the product of Lie transformation in Eq. (3-7) act from the left to the right, C_1 acting first and C_N acting last.

A better approximation than Eq. (3-3) is the following

$$e^{-h(:K:+:V:)} = e^{-\frac{h}{2}:K:} e^{-h:V:} e^{-\frac{h}{2}:K:} + O(h^3) \qquad (3\text{-}9)$$

Eq. (3-3) gives rise to the following scheme

$$p_i^1 = p_i \quad , \quad q_i^1 = q_i + \frac{h}{2}\frac{\partial K(p)}{\partial p_i}$$

$$p_i^h = p_i^1 - h\frac{\partial V(q^1)}{\partial q_i} \quad , \quad q^h = q_i^1 + \frac{h}{2}\frac{\partial K(p^h)}{\partial p_i} \qquad (3\text{-}10)$$

Equations (3-10) correspond to the second order scheme given in Ref. 2.

Let's now suppose we can find coefficients c_1, c_2, c_3 and d_1, d_2, d_3 such that

$$e^{-h:K:-h:V:} = e^{-c_1h:V:} e^{-d_1h:K:} e^{-c_2h:V:} e^{-d_2h:K:} e^{-c_3h:V:} e^{-d_3h:K:} + O(h^4) \qquad (3\text{-}11)$$

From Eq. (3-11) one derives the third order scheme of Ref. 2.

$$p_i^1 = p_i - c_1h\frac{\partial V(q)}{\partial q_i} \quad , \quad q_i^1 = q_i + d_1h\frac{\partial K(p^1)}{\partial p_i}$$

$$p_i^2 = p_i^1 - c_2h\frac{\partial V(q^1)}{\partial q_i} , \quad q^2 = q_i^1 + d_2h\frac{\partial K(p^2)}{\partial p_i} \qquad (3\text{-}12)$$

$$p_i^h = p^2 - c_3h\frac{\partial V(q^2)}{\partial q_i} , \quad q_i^h = q_i^2 + d_3h\frac{\partial K(p^h)}{\partial p_i}$$

The coefficients c_1, c_2, c_3 and d_1, d_2, d_3 can be obtained from Eq. (3-11) that can be put in the form

$$e^{h(A+B)} = e^{c_1 hA} e^{d_1 hB} e^{c_2 hA} e^{d_2 hB} e^{c_3 hA} e^{d_3 hB} + O(h^4) \qquad (3\text{-}13)$$

where A,B are arbitrary operators. Equations for the c's and d's can be obtained by expanding (3-13) to third order in h.

The first order equation is

$$hA + hB = c_1 hA = d_1 hB + c_2 hA + d_2 hB + c_3 hA + d_3 hB$$

from which one can deduce, since A and B are arbitrary that

$$1 = c_1 + c_2 + c_3 \qquad 1 = d_1 + d_2 + d_3$$

The second order equations are dropping the powers of h and collecting independent terms

$$\frac{A^2}{2} = \frac{c_1^2 A^2}{2} + \frac{c_2^2}{2} A^2 + \frac{c_3^2}{2} A^2 + c_1 c_2 A^2 + c_1 c_3 A^2 + c_2 c_3 A^2$$

this is not an independent equation since is the square of

$$\frac{1}{2} = \frac{1}{2} (c_1 + c_2 + c_3)^2$$

The equation in B^2 is also automatically satisfied. The equations for term AB is

$$\frac{AB}{2} = (c_1 d_1 + c_1 d_2 + c_1 d_3 + c_2 d_2 + c_2 d_3 + c_3 d_3)\ AB$$

or

$$\frac{1}{2} = c_1 + c_2 (d_2 + d_3) + c_3 d_3$$

The equation for BA is

$$\frac{BA}{2} = (d_1 c_2 + d_1 c_3 + d_2 c_3)\ AB$$

$$\frac{1}{2} = c_2 d_1 + c_3 (d_1 + d_2)$$

Only one of the two past equations is independent.

Adding them together one obtains

$$1 = c_1 + c_2 (d_1 + d_2 + d_3 + c_3 (d_1 + d_2 + d_3)$$

$$1 = c_1 + c_2 + c_3.$$

The third order terms A^3 and B^3 are automatically correct. The coefficient B^2A is

$$\frac{B^2 A}{6} = \frac{d_1^2 B^2}{2} c_2 A + \frac{(d_1 + d_2)^2 B^2}{2} c_3 A$$

The coefficient of A^2B is

$$\frac{A^2 B}{6} = \frac{c_1^2 A^2}{2} d_1 B + \frac{(c_1 + c_2)^2 A^2}{2} d_2 B + \frac{(c_1 + c_2 + c_3)^2 A}{2} d_3 B$$

The coefficient of AB^2 is

$$\frac{AB^2}{6} = c_1 A \frac{(d_1 + d_2 + d_3)^2}{2} B^2 + c_2 A \frac{(d_2 + d_3)^2}{2} B^2 + c_3 A \frac{d_3^2}{2} B^2$$

$$\frac{BA^2}{6} = d_1B \frac{(c_2 + c_3)^2}{2} A^2 + d_2B \frac{c_3^2}{2} A$$

and finally,

$$\frac{ABA}{6} = c_1A\ d_1B\ c_2A + c_1A\ d_1B\ c_3A + c_1A\ d_2B\ c_3A + c_2A\ d_2B\ c_3A$$

$$\frac{BAB}{6} = d_1B\ c_2A\ d_2B + d_1B\ c_2A\ d_3B + d_1B\ c_3A\ d_3B + d_2B\ c_3A\ d_3B.$$

Of the last six equations, only 2 are independent.

The number of conditions on the coefficients c_i and d_i required to satisfy eq. 3-11 and the higher order analogs can be computed by using the Campbell-Baker-Hausdorf theorem to bring together the exponents of eq. 3-11 into a single coefficient. Setting to zero the coefficient of the commutators up to the desired order (and to the coefficients of A and B).

To third order five equation are necessary corresponding to the coefficients of A, B, $[A,B]$, $[A,[A,B]]$, $[B,[B,A]]$.

The five equations can be obtained by expanding eq 3-11 and ~~setting~~ identifying the coefficients of

A, B, ~~[A,[A,B]], [B,[A,B]]~~,

BA, B^2A, A^2B.

The resulting equations are

$$c_1 + c_2 + c_3 = 1 \quad , \quad d_1 + d_2 + d_3 = 1 \qquad (A, B)$$

$$c_2 d_1 + c_3 (d_1 + d_2) = 1/2 \qquad (BA)$$

(5-1

$$c_2 d_1^2 + c_3 (d_1 + d_2)^2 = 1/3 \qquad (B^2A)$$

$$d_1 c_1^2 + d_2 (c_1 + c_2)^2 + d_3 (c_1 + c_2 + c_3)^2 \qquad (A^2B)$$

These equations are seen to be equivalent to eq (30) of ref. 2.

To the next order we have

$$e^{tc_1 A} e^{td_1 B} e^{tc_2 A} e^{td_2 B} e^{tc_3 A} e^{td_3 B} e^{tc_4 A} e^{td_4 A} =$$

$$= e^{t(A+B)} + O(t^5) \qquad (3-15)$$

The extra equation requaried above the equivalent of eq (3-12) are determined by setting to zero the coefficients of the three commutators. $[A,[A,[A,B]]]$, $[B,[B,[B,A]]]$ and $[A,[B,[A,B]]]$.

Eight eqations are thus obtained that entirely constrain the coefficients of eq (3-13)

The three extara equations are obtained by identifying the coefficients of B^3A, A^3B, and AB^2A

The resulting equations are:

$$c_1 + c_2 + c_3 + c_4 = 1$$

$$d_1 + d_2 + d_3 + d_4 = 1$$

$$c_2 d_1 + c_3 (d_1 + d_2) + c_4 (d_1 + d_2 + d_3) = \frac{1}{2}$$

$$c_2 d_1^2 + c_3 (d_1 + d_2)^2 + c_4 (d_1 + d_2 + d_3)^2 = \frac{1}{3}$$

$$c_1^2 d_1 + (c_1 + c_2)^2 d_2 + (c_1 + c_2 + c_3)^2 d_3 + d_4 = \frac{1}{3}$$

$$c_2 d_1^3 + c_3 (d_1 + d_2)^3 + c_4 (d_1 + d_2 + d_3)^3 = \frac{1}{4} \qquad (3\text{-}14)$$

$$c_1^3 d_1 + (c_1 + c_2)^3 d_2 + (c_1 + c_2 + c_3)^3 d_3 + d_4 = \frac{1}{4}$$

$$c_1 c_2 d_1^2 + c_1 c_3 (d_1 + d_2)^2 + c_1 c_4 (d_1 + d_2 + d_3)^2$$

$$+ c_2 c_3 d_2^2 + c_2 c_4 (d_2 + d_3)^2 + c_3 c_4 d_3^2 = \frac{1}{12}$$

This is a formidable system of equations to be solved for the c_i's, d_i's.

4 Time dependent Hamiltonians

Use 8 coordinates

$$q_1, p_1, q_2, p_2, q_3, p_3, \tau, p_\tau \qquad (4\text{-}1)$$

$$H = K(\vec{p}) + V(\vec{q}, \tau) + p_\tau$$

using the ~~hamilton~~ ~~Jacoby~~ Hamilton equation, we have

$$\dot{\vec{q}} = \frac{\vec{\partial} K(\vec{p})}{\partial \vec{p}}\,;$$

$$\dot{\vec{p}} = -\frac{\vec{\partial} V(\vec{q}, \tau)}{\partial \vec{q}}$$

$$\dot{\tau} = 1 \qquad \dot{p}_\tau = -\frac{\partial V(\vec{q}, \tau)}{\partial \tau}$$

The first thee equation slow that using equation 4-1 with initial condition $\tau=0$ is equivalent to integrating the equation di Hamilton with the time dependent Hamiltonian ~~(except for the value of p_τ which does not affect the~~

$$H = K(\vec{p}) + V(\vec{q}, t) . \qquad (4-2)$$

If we use the expression

$$e^{-t(\hat{V}+H)} = e^{-tc_1 K} e^{-td_1 V} \cdots e^{-tc_N K} e^{-td_N V} + O(t^m);$$

for the 8-dimensional Hamiltonian (4-1) we get the result

$$e^{-t:(K+V):} = e^{-c_1 t:K:} e^{-d_1 t:p_\tau:} e^{-d_1 t:V(q,\tau):} e^{-c_2 t:K:} e^{-d_2 t:p_\tau:} e^{-d_2 t:V(q,\tau):} \cdots + O(t^n) \quad (4-3)$$

by insertin the identity

$$e^{+\sum_{j=1}^{i} d_j t:p_\tau:} e^{-\sum_{j=1}^{i} d_j t:p_\tau:} = 1$$

after each $e^{-d_i t:V(q,\tau):}$

and appling the equation

$$e^{-ct:p_\tau:} :V(q,\tau): e^{ct:p_\tau:} = :V(q,\tau+c):,$$

repeatedly eq (4-3) is shown to

equivalent to

$$e^{-t:V+\hat{K}:} = e^{-c_1 t:V(p,\tau):}\, e^{-d_1 t:K:} \cdots$$

$$\cdots e^{-c_i t:V(p,\tau+\sum_{j=1}^{i-1} d_j t):}\, e^{-d_i t:K:} \cdots$$

$$\cdots e^{-c_n t:V(p,\tau+\sum_{j=1}^{n-1} d_j t):}\, e^{-d_n t:K:}\, e^{-t R_\tau} \qquad [h-4]$$

One sees that this is equivalent to (starting with $t=0$)

$$\vec{p}_1 = \vec{p}_0 - c_1 t \frac{\vec{\partial} V(\vec{q}_0, 0)}{\partial \vec{q}_0} \; ; \quad \vec{q}_1 = \vec{q}_0 + d_1 t \frac{\vec{\partial} K(\vec{p}_1)}{\partial \vec{p}_1} \; ;$$

$$\vdots$$

$$\vec{p}_i = \vec{p}_{i-1} - c_i t \frac{\vec{\partial} V(\vec{q}_{i-1}, \sum_{j=1}^{i-1} d_j t)}{\partial \vec{q}_{i-1}} \; ; \quad \vec{q}_i = \vec{q}_{i-1} + d_i t \frac{\vec{\partial} K(\vec{p}_i)}{\partial \vec{q}_i} \; ;$$

$$\vdots$$

$$\vec{p}_n = \vec{p}_{n-1} - c_n t \frac{\vec{\partial} V(\vec{q}_{n-1}, \sum_{j=1}^{n-1} d_n t)}{\partial \vec{q}_{n-1}} \; ; \quad \vec{q}_n = \vec{q}_{n-1} + d_n t \frac{\vec{\partial} K(\vec{p}_n)}{\partial \vec{p}_n} \; ,$$

$$\tau = 0 + t \qquad [h-5]$$

Eqs (h-5) are a generalization of eq (29) in ref. 2 .

Using the fourth order formulas of (3-13), with eq's (4-5) it is possible to derive a fourth order scheme for the time dependent Hamiltonian (4-2).

The eight ~~four~~ coefficien $c_1, \ldots c_4, d_1 \ldots d_4$ must satisfy eqs. (3-14).

5 Solution of the equations for the coefficients -

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