A Note on Symplectic Algorithm

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Abstract We present the symplectic algorithm in the Lagrangian formalism for the Hamiltonian systems by virtue of the noncommutative differential calculus with respect to the discrete time and the Euler–Lagrange cohomological concepts. We also show that the trapezoidal integrator is symplectic in certain sense.

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1 Introduction
It is well known that the symplectic algorithm[1,2] for the finite dimensional Hamiltonian systems are very powerful and successful in numerical calculations in comparison with other various non-symplectic computational schemes since the symplectic schemes preserve the symplectic structure in certain sense. On the other hand, the Lagrangian formalism is quite useful for the Hamiltonian systems. Since both are important at least in the equal footing, it should not be useless to establish the symplectic algorithms in the Lagrangian formalism. As a matter of fact, the Lagrangian formalism is more or less earlier to be generalized to the infinite dimensional systems such as classical field theory.

In this note we present the symplectic geometry and symplectic algorithm in the Lagrangian formalism in addition to the Hamiltonian one for the finite dimensional Hamiltonian systems with the help of the Euler–Lagrange (EL) cohomological concepts introduced very recently by the authors in Ref. [5].

In the course of numerical calculation, the “time” $t \in R$ is always discretized, usually with equal spacing $h = \Delta t$,

$$t \in R \rightarrow t \in T = \{(t_k, t_{k+1} = t_k + h, \ k \in Z) \}.$$

It is well known that the differences of functions on $T$ with respect to $T$ do not obey the Leibniz law. In order to show that the symplectic structure at different moments $t_k$ is preserved, some well-established differential calculus should be employed. This implies that some noncommutative differential calculus (NCDC) on $T$ and the function space on it should be used even for the well-established symplectic algorithms. In this note we employ this simple NCDC.[3,4] We also show that the trapezoidal integrator is symplectic in certain sense. Finally, we end with some remarks.

2 The Necessary and Sufficient Condition for Symplectic Preserving Law
In this section, we first recall some well-known contents in the Lagrangian formalism for the finite dimensional Hamiltonian systems. We employ the ordinary calculus to show that the symplectic structure is preserved by introducing the EL cohomological concepts such as the EL one-forms, the null EL one-form, the coboundary EL one-form and the EL condition and so forth.[5] It is important to emphasize that the symplectic structure-preserving is in the function space in general rather than in the solution space of the EL equation only. The reason will be explained later.

Let time $t \in R$ be the base manifold, $M = M^n$ the configuration space on $t$,

$$q = [q^1(t), \cdots, q^n(t)]^T$$

the (canonical) coordinates on it, $T$ the transport, $TM$ the tangent bundle of $M$ with coordinates

$$(q, \dot{q}) = ([q^1(t), \cdots, q^n(t)]^T, [\dot{q}^1(t), \cdots, \dot{q}^n(t)]^T),$$

$F(TM)$ the function space on $TM$.

The Lagrangian of the systems under consideration is $L(q^i, \dot{q}^i)$ with the well-known EL equation from the variational principle

$$\frac{\partial L}{\partial q^i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}^i} = 0.$$ (1)

Let us introduce the EL one-form[5]

$$E(q^i, \dot{q}^i) : = \left\{ \frac{\partial L}{\partial \dot{q}^i} - \frac{d}{dt} \frac{\partial L}{\partial q^i} \right\} dq^i.$$ (2)

It is clear that the EL equation is given by the null EL one-form,

$$E(q^i, \dot{q}^i) = 0,$$

which is a special case of the coboundary EL one-forms

$$E(q^i, \dot{q}^i) = d_0(q^i, \dot{q}^i).$$ (3)
where \( \alpha(q^i, \dot{q}^i) \) is an arbitrary function of \((q^i, \dot{q}^i)\) in the function space \( F(TM) \).

Taking the exterior derivative \( d \) of the Lagrangian, we get
\[
dL(q^i, \dot{q}^i) = E(q^i, \dot{q}^i) + \frac{d}{dt} \theta,
\]
where \( \theta \) is the canonical one-form defined by
\[
\theta = \frac{\partial L}{\partial \dot{q}^i} dq^i.
\]
Making use of nilpotency of \( d \),
\[
d^2L(q, \dot{q}) = 0,
\]
it follows that if the EL one-form is closed with respect to \( d \), i.e.,
\[
dE(q^i, \dot{q}^i) = 0,
\]
which is called the EL condition,\(^5\) the symplectic conservation law with respect to \( t \) holds,
\[
\frac{d}{dt} \omega = 0,
\]
where the symplectic structure \( \omega \) is given by
\[
\omega = d\theta = \frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j} dq^i \wedge dq^j + \frac{\partial^2 L}{\partial \dot{q}^i \partial q^j} dq^i \wedge d\dot{q}^j.
\]

It is important to note that although the null EL one-form and the coboundary EL one-forms satisfy the EL condition and they cohomologically trivial, this does not mean that the closed EL one-forms are always exact. As a matter of fact, the equation (8) shows that the EL one-form is not always exact since the canonical one-form is not trivial in general. In addition, it is also important to note that the \( q^i(t) \), \( i = 1, \ldots, n \) in the EL condition are still in the function space in general rather than in the solution space of the equation only. This means that the symplectic two-form \( \omega \) is conserved with respect to \( t \) with the closed EL condition in general rather than in the solution space only.

In order to transfer to the Hamiltonian formalism, we introduce the canonical momenta
\[
p_j = \frac{\partial L}{\partial \dot{q}^j},
\]
and take a Legendre transformation to get the Hamiltonian function
\[
H(q^i, p_j) = p_i \dot{q}^i - L(q^i, \dot{q}^i).
\]
Then the EL equation becomes the canonical equations as follows:
\[
\dot{q}^i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_j = -\frac{\partial H}{\partial q^j}.
\]

It is clear that a pair of the EL one-forms should be introduced now,
\[
E_1(q^i, p_j) = \left( \dot{q}^i - \frac{\partial H}{\partial \dot{q}^i} \right) dp_j,
\]
\[
E_2(q^i, p_j) = -\left( \dot{p}_j + \frac{\partial H}{\partial q^j} \right) dq^j.
\]

In terms of \( z^T = (q^i, \ldots, q^n, p_1, \ldots, p_n) \), the canonical equations and the EL one-form become
\[
\dot{z} = J^{-1} \nabla_z H,
\]
\[
n_{ooa}2E(z) = dz^T (Jz - \nabla_z H).
\]

Now it is straightforward to show that the symplectic structure-preserving law
\[
\frac{d}{dt} \omega = 0,
\]
\[
\omega = dz^T \wedge J dz
\]
holds if and only if the (closed) EL condition is satisfied
\[
dE(z) = 0.
\]

### 3 The Necessary and Sufficient Condition for Discrete Symplectic Preserving Law

Now we consider the symplectic structure-preserving of symplectic algorithm in the Lagrangian formalism. As was mentioned above, in the course of numerical calculation, the “time” \( t \in R \) is discretized with equal spacing \( h = \Delta t \),
\[
t \in R \rightarrow t \in T = \{ t_k, t_{k+1} = t_k + h, \ k \in Z \}. \quad (17)
\]
At the moment \( t_k \), the coordinates of the space \( M_k^n \in M_k^2 = \{ \cdots M_1^n \times \cdots \times M_k^n \cdots \} \) are denoted by \( q^{(k)} \), the symplectic structure by
\[
\omega^{(k)} = dq^{(k)}_t \wedge dq^{(k)}_z,
\]
and \( q^{(k)}_t \) now is the (forward-)difference of \( q^{(k)} \),
\[
\Delta q^{(n)} = \partial q^{(n)} = q^{(k+1)} - q^{(k)}.
\]

Now the EL equation becomes the difference discrete Euler–Lagrange (DEL) equation which can be derived from the difference discrete variational principle,\(^5\)
\[
\frac{\partial L^{(k)}}{\partial q^{(k+1)}} = \frac{\partial L^{(k)}}{\partial q^{(k)}} = 0.
\]
Now we consider the difference discrete symplectic structure and its preserving property. Taking the exterior derivative $d$ on $T^*(M^n_{TD})$, we get
\[
d L_D^{(k)} = \frac{\partial L_D^{(k)}}{\partial q^{i(k)}} dq^{i(k)} + \frac{\partial L_D^{(k)}}{\partial q^{j(k)}} dq^{j(k)}.
\]
By means of the modified Leibniz law with respect to $\Delta_t$ and introducing the DEL one-form,
\[
E_D^{(k)}(q^{i(k)}, q^{j(k)}) := \left\{ \frac{\partial L_D^{(k)}}{\partial q^{i(k)}} - \Delta_t \left( \frac{\partial L_D^{(k-1)}}{\partial q^{i(k-1)}} \right) \right\} dq^{i(k)},
\]
we have
\[
d L_D^{(k)} = E_D^{(k)} + \Delta_t \theta_D^{(k)},
\]
where $\theta_D^{(k)}$ is the discrete canonical one-form,
\[
\theta_D^{(k)} = \frac{\partial L_D^{(k-1)}}{\partial q^{i(k-1)}} dq^{i(k)},
\]
then there exists the following discrete symplectic two-form on $T^*(M^n_{TD})$,
\[
\omega_D^{(k)} = d \theta_D^{(k)} = \frac{\partial^2 L_D^{(k-1)}}{\partial q^{i(k-1)} \partial q^{j(k-1)}} dq^{i(k-1)} \wedge dq^{j(k-1)} + \frac{\partial^2 L_D^{(k-1)}}{\partial q^{i(k-1)} \partial q^{j(k-1)}} dq^{j}(k-1) \wedge dq^{i(k)}.
\]
It is easy to see that the null DEL one-form $E_D^{(k)} = 0$ gives rise to the DEL equation and it is a special case of the coboundary DEL one-forms
\[
E_D^{(k)} = d \alpha_D^{(k)}(q^{i(k)}, q^{j(k)}),
\]
where $\alpha_D^{(k)}(q^{i(k)}, q^{j(k)})$ is an arbitrary function of $(q^{i(k)}, q^{j(k)})$.

Finally, due to the nilpotency of $d$ on $T^*(M^n_{TD})$ it is easy to prove from Eq. (22) that iff the DEL one-form satisfies what is called the DEL condition
\[
d E_D^{(k)} = 0,
\]
i.e., the DEL one-form is closed, the discrete (difference) symplectic structure-preserving law holds,
\[
\Delta_t \omega_D^{(k)} = 0.
\]

Similar to the continuous case, the closed DEL one-forms are not always exact and this difference discrete symplectic structure-preserving law is held in function space in general rather than in solution space only.

Let us consider the following DEL equation
\[
q^{(k)} - 2q^{(k+1)} + q^{(k+2)} = -h^2 \frac{\partial L}{\partial q}(q^{(k+1)}).
\]
Introducing the DEL one-form$^5$
\[
E_D^{(k+1)} := d(q^{T(k+1)}) \left\{ q^{(k)} - 2q^{(k+1)} + q^{(k+2)} - h^2 \frac{\partial L}{\partial q}(q^{(k+1)}) \right\},
\]
the null DEL one-form is corresponding to the DEL equation and the DEL condition directly gives rise to
\[
d q^{T(k+2)} \wedge dq^{(k+1)} = dq^{T(k+1)} \wedge dq^{(k)}.
\]
It follows that
\[
\Delta_t \omega^{(k)} = \frac{1}{h} [dq^{T(k+1)} \wedge dq^{(k+1)} - dq^{T(k)} \wedge dq^{(k)}] = 0.
\]
This means that the (forward-)difference scheme is symplectic. It can be proved that the scheme with respect to the (backward-)difference of $q^{(n)}$,
\[
\Delta_t q^{(k)} = q^{(k)} - q^{(k-1)}
\]

\[\text{(31)}\]
is also symplectic as well.

4 On the Symplectic Schemes

We now show some well-known symplectic schemes in the Lagrangian formalism for the Hamiltonian systems.

4.1 The Euler Mid-point Scheme for Separable Hamiltonian Systems

The well-known Euler mid-point scheme for the separable Hamiltonian systems is as follows:

\[ q^{(n+1)} - q^{(n)} = \frac{h}{2}(p^{(n+1)} + p^{(n)}), \quad p^{(n+1)} - p^{(n)} = -hV\left(\frac{q^{(n+1)} + q^{(n)}}{2}\right), \quad (32) \]

from which it follows that

\[ (p^{(n+1)} - p^{(n)}) + (p^{(n)} - p^{(n-1)}) = -hV\left(\frac{q^{(n+1)} + q^{(n)}}{2}\right) - hV\left(\frac{q^{(n)} + q^{(n-1)}}{2}\right), \quad (33) \]

\[ \frac{2}{h}(q^{(n+1)} - q^{(n)} - q^{(n)} + q^{(n-1)}) = -hV\left(\frac{q^{(n+1)} + q^{(n)}}{2}\right) - hV\left(\frac{q^{(n)} + q^{(n-1)}}{2}\right). \quad (34) \]

Now it is easy to get the Euler mid-point scheme in the Lagrangian formalism,

\[ q^{(n+1)} - 2q^{(n)} + q^{(n-1)} = -\frac{h^2}{2}\left[V\left(\frac{q^{(n+1)} + q^{(n)}}{2}\right) + V\left(\frac{q^{(n)} + q^{(n-1)}}{2}\right)\right]. \quad (35) \]

In order to show that it is symplectic, we first introduce the DEL one-form as follows:

\[ E_D^{(n)} = dq^{T(n)}\left\{q^{(n+1)} - 2q^{(n)} + q^{(n-1)} + \frac{h^2}{2}\left[V\left(\frac{q^{(n+1)} + q^{(n)}}{2}\right) + V\left(\frac{q^{(n)} + q^{(n-1)}}{2}\right)\right]\right\}. \quad (36) \]

Then the DEL condition gives rise to

\[ dq^{(n+1)} \wedge dq^{T(n)} + dq^{(n-1)} \wedge dq^{T(n)} = -\frac{h^2}{4}V_{qq}^{(n+1/2)} dq^{(n+1)} \wedge dq^{T(n)} + \frac{h^2}{4}V_{qq}^{(n-1/2)} dq^{(n-1)} \wedge dq^{T(n)}, \quad (37) \]

where

\[ V^{(n+1/2)} = V\left(\frac{q^{(n+1)} + q^{(n)}}{2}\right). \]

That is

\[ \left(1 + \frac{h^2}{4}V_{qq}^{(n+1/2)}\right) dq^{T(n)} \wedge dq^{(n+1)} = \left(1 + \frac{h^2}{4}V_{qq}^{(n-1/2)}\right) dq^{T(n)} \wedge dq^{(n-1)}. \quad (38) \]

Now it is easy to prove that

\[ dp^{T(n+1)} \wedge dq^{(n+1)} = \left(1 + \frac{h^2}{4}V_{qq}^{(n+1/2)}\right) dq^{T(n+1)} \wedge dq^{(n)}. \quad (39) \]

Therefore, the Euler mid-point scheme is symplectic.

4.2 The Euler Mid-point Scheme for Generic Hamiltonian Systems

For the general Hamiltonian \( H \), the similar preserved symplectic form can also be given. Let us start with

\[ q^{(n+1)} - q^{(n)} = \hbar H_p\left(\frac{p^{(n+1)} + p^{(n)}}{2}, \frac{q^{(n+1)} + q^{(n)}}{2}\right), \]

\[ p^{(n+1)} - p^{(n)} = -\hbar H_q\left(\frac{p^{(n+1)} + p^{(n)}}{2}, \frac{q^{(n+1)} + q^{(n)}}{2}\right). \quad (40) \]

Introduce a pair of DEL one-forms

\[ E_D^{(n)}(q) = dq^{T(n)}\left\{q^{(n+1)} - q^{(n)} - \hbar H_p\left(\frac{p^{(n+1)} + p^{(n)}}{2}, \frac{q^{(n+1)} + q^{(n)}}{2}\right)\right\}, \]

\[ E_D^{(n)}(p) = dp^{T(n)}\left\{p^{(n+1)} - p^{(n)} + \hbar H_q\left(\frac{p^{(n+1)} + p^{(n)}}{2}, \frac{q^{(n+1)} + q^{(n)}}{2}\right)\right\}. \quad (41) \]

The DEL conditions for the pair of the DEL one-forms now read

\[ d\left(E_D^{(n)}(q) + E_D^{(n)}(p)\right) = 0. \quad (42) \]
From these conditions it follows that

\[
(dq^{(n)})^T \wedge \left[ \frac{1}{2} h (n+1/2) + 2 \left( 1 + \frac{1}{2} h (n-1/2) \right) \right] dq^{(n+1)}
= (dq^{(n-1)})^T \wedge \left[ \frac{1}{2} h (n-1/2) + 2 \left( 1 + \frac{1}{2} h (n-1/2) \right) \right] dq^{(n)}.
\]

This shows that the following two-form in \((dq^{(k)})\) is preserved,

\[
(dq^{(n-1)})^T \wedge \left[ \frac{1}{2} h (n+1/2) \right] dq^{(n+1)}
= (dq^{(n-1)})^T \wedge \left[ \frac{1}{2} h (n-1/2) \right] dq^{(n)}.
\]

It can be shown that it is nothing but the preserved symplectic structure,

\[
2(dq^{(n+1)})^T \wedge dq^{(n+1)} = -(dq^{(n)})^T \wedge \left[ \frac{1}{2} h (n+1/2) \right]
+ 2 \left( 1 + \frac{1}{2} h (n+1/2) \right) \left( 1 - \frac{1}{2} h (n+1/2) \right) dq^{(n+1)}.
\]

In terms of \(z^T = (q^T, p^T)\), the mid-point scheme can be expressed as

\[
\Delta \Delta z^{(k)} = J^{-1} \nabla z H D^{(k)} \left( \frac{1}{2} (z^{(k+1)} + z^{(k)}) \right).
\]

The DEL one-form for the scheme at \(t_k\) now becomes

\[
E_{D1}^{(k)} = \frac{1}{2} \partial \left( (z^{(k+1)} + z^{(k)}) \right)^T \left\{ J \Delta z^{(k)} - \nabla z H D^{(k)} \left( \frac{1}{2} (z^{(k+1)} + z^{(k)}) \right) \right\}.
\]

It is now straightforward to show that the symplectic structure-preserving law

\[
\Delta_t (d z^{(k)} T \wedge J d z^{(k)}) = 0
\]
holds if and only if the DEL form is closed.

### 4.3 The High Order Symplectic Schemes

Similarly, it can be checked that the high order symplectic schemes preserve also some two-forms in \(dq^{(k)}\) which are in fact the symplectic structures. Let us consider two examples for this point.

The first one is proposed by Feng et al. in terms of generating function.\(^6\) The scheme is as follows:

\[
z^{(n+1)} = z^{(n)} + h J^{-1} \nabla z H \left( \frac{1}{2} \left( z^{(n+1)} + z^{(n)} \right) \right) - \frac{h^3}{24} J^{-1} \nabla z \left( (\nabla z H)^T J H_{zz} J \nabla z H \right) \left( \frac{1}{2} \left( z^{(n+1)} + z^{(n)} \right) \right).
\]

In this case \(\mathcal{H}\) can be introduced as

\[
\mathcal{H} = H - \frac{h^2}{24} (\nabla z H)^T J H_{zz} J \nabla z H.
\]

Then the fourth-order symplectic scheme can be rewritten as

\[
z^{(n+1)} = z^{(n)} + h J^{-1} \nabla z \mathcal{H} \left( \frac{1}{2} \left( z^{(n+1)} + z^{(n)} \right) \right).
\]

Introducing an associated DEL form,

\[
E_{D2}^{(k)} = \frac{1}{2} \partial \left( (z^{(k+1)} + z^{(k)}) \right)^T \left\{ J \Delta z^{(k)} - \nabla z \mathcal{H}^{(k)} \left( \frac{1}{2} \left( z^{(k+1)} + z^{(k)} \right) \right) \right\},
\]

it is easy to see that \(E_{D1}\) and \(E_{D2}\) differ an exact form,

\[
E_{D1}^{(k)} - E_{D2}^{(k)} = \frac{h^2}{24} \partial \alpha, \quad \alpha = (\nabla z H)^T J H_{zz} J \nabla z H.
\]

The second one is a symplectic Runge–Kutta (RK) scheme. First, the stage vector is taken symplectic RK.
method is nothing but the mid-point scheme. Second, the stage two and order-four RK method is as follows:

\[ y^{(n+1)} = y^{(n)} + \frac{h}{2}(f(Y_1) + f(Y_2)), \]
\[ Y_1 = y^{(n)} + h\left[\frac{1}{4}f(Y_1) + \left(\frac{1}{4} + \frac{1}{2\sqrt{3}}\right)f(Y_2)\right], \]
\[ Y_2 = y^{(n)} + h\left[\left(\frac{1}{4} - \frac{1}{2\sqrt{3}}\right)f(Y_1) + \frac{1}{4}f(Y_2)\right]. \]

(53)

It can be expressed in terms of Hamiltonian \( H \) as

\[ q^{(n+1)} = q^{(n)} + \frac{h}{2}[H_p(P_1, Q_1) + H_p(P_2, Q_2)], \]
\[ p^{(n+1)} = p^{(n)} - \frac{h}{2}[H_q(P_1, Q_1) + H_q(P_2, Q_2)], \]

(54)

where

\[ Q_1 = q^{(n)} + h\left[\frac{1}{4}H_p(P_1, Q_1) + \left(\frac{1}{4} + \frac{1}{2\sqrt{3}}\right)H_p(P_2, Q_2)\right], \]
\[ P_1 = p^{(n)} - h\left[\frac{1}{4}H_q(P_1, Q_1) + \left(\frac{1}{4} + \frac{1}{2\sqrt{3}}\right)H_q(P_2, Q_2)\right], \]
\[ Q_2 = q^{(n)} + h\left[\left(\frac{1}{4} - \frac{1}{2\sqrt{3}}\right)H_p(P_1, Q_1) + \frac{1}{4}H_p(P_2, Q_2)\right], \]
\[ P_2 = p^{(n)} - h\left[\left(\frac{1}{4} - \frac{1}{2\sqrt{3}}\right)H_q(P_1, Q_1) + \frac{1}{4}H_q(P_2, Q_2)\right]. \]

(55)

Introducing a pair of the DEL one-forms

\[ E_D^{(n)}(q) : = dp^{(n)}\left\{q^{(n+1)} - q^{(n)} - \frac{h}{2}(H_p(P_1, Q_1) + H_p(P_2, Q_2))\right\}, \]
\[ E_D^{(n)}(p) : = dq^{(n)}\left\{p^{(n+1)} - p^{(n)} + \frac{h}{2}(H_q(P_1, Q_1) + H_q(P_2, Q_2))\right\}, \]

(56)

then the DEL conditions, i.e., their closed condition

\[ d(E_D^{(n)}(q) + E_D^{(n)}(p)) = 0, \]

(57)

gives rise to the symplectic preserving property

\[ dp^{(n+1)} \wedge dq^{(n+1)} = dp^{(n)} \wedge dq^{(n)}. \]

(58)

It can also be shown that \( \omega^{(n+1)} = dp^{(n+1)} \wedge dq^{(n+1)} \) may be expressed as \( dp^{(n+1)} \wedge dq^{(n)} \) with some coefficients.

5 The Trapezoidal Integrator

It is well known that this scheme is good enough in comparison with other well-known symplectic schemes. But for the long time, it is not clear why it is so satisfactory.

We will show that this scheme is symplectic, but the preserved symplectic structure is not simply \( \omega = dp^T \wedge dq \). Of course, the preserved symplectic structure should be canonically transformed to the one in the simple form with different canonical coordinates and momenta in principle.

The scheme is given by

\[ q^{(n+1)} - q^{(n)} = \frac{h}{2}[H_p^{(n+1)}(p^{(n+1)}, q^{(n+1)}) + H_p^{(n)}(p^{(n)}, q^{(n)})], \]
\[ p^{(n+1)} - p^{(n)} = -\frac{h}{2}[H_q^{(n+1)}(p^{(n+1)}, q^{(n+1)}) + H_q^{(n)}(p^{(n)}, q^{(n)})]. \]

(59)

5.1 For Separable Hamiltonian Systems

Let us now first consider the case of separable Hamiltonian systems. For example, \( H = \frac{1}{2}p^T \Sigma q \). In this case,
We get
\[ q^{(n+1)} - q^{(n)} = \frac{\hbar}{2}(p^{(n+1)} + p^{(n)}), \quad p^{(n+1)} - p^{(n)} = -\frac{\hbar}{2}[V^{(n+1)}(q^{(n+1)}) + V^{(n)}(q^{(n)})]. \]  
(60)

As what have been done before, let us introduce a pair of the EL one-forms,
\[ E_D^{(n)}(q) := dp^{(n)}\left\{ q^{(n+1)} - q^{(n)} - \frac{\hbar}{2}(p^{(n+1)} + p^{(n)}) \right\}, \]
\[ E_D^{(n)}(p) := dq^{(n)}\left\{ p^{(n+1)} - p^{(n)} + \frac{\hbar}{2}[V^{(n+1)}(q^{(n+1)}) - V^{(n)}(q^{(n)})] \right\}. \]  
(61)

Then by some straightforward but more or less tedious calculations, it follows from the DEL condition, i.e. their closed property, that
\[
\frac{2}{\hbar}(dq^{(n)})^T \left( 1 + \frac{\hbar^2}{4} V^{(n)}(q) \right) \wedge (dq^{(n+1)} + dp^{(n-1)}) = -\frac{\hbar}{2}(dq^{(n)})^T \left( 1 + \frac{\hbar^2}{4} V^{(n)}(q) \right) \wedge (V^{(n+1)}(q) dq^{(n+1)} + V^{(n-1)} dq^{(n-1)}).
\]
(62)

We get
\[
(dq^{(n)})^T \left( 1 + \frac{\hbar^2}{4} V^{(n+1)}(q) \right) \wedge \left( 1 + \frac{\hbar^2}{4} V^{(n)}(q) \right) dq^{(n+1)} = -(dq^{(n)})^T \left( 1 + \frac{\hbar^2}{4} V^{(n)}(q) \right) \wedge \left( 1 + \frac{\hbar^2}{4} V^{(n-1)}(q) \right) dq^{(n+1)}.
\]
(63)

This means that the following symplectic structure is preserved
\[
(dq^{(n+1)})^T \left( 1 + \frac{\hbar^2}{4} V^{(n+1)}(q) \right) \wedge \left( 1 + \frac{\hbar^2}{4} V^{(n)}(q) \right) dq^{(n)}.
\]  
(64)

That is
\[
(dp^{(n+1)})^T \wedge \left( 1 + \frac{\hbar^2}{4} V^{(n+1)}(q) \right) dq^{(n+1)} = (dp^{(n)})^T \wedge \left( 1 + \frac{\hbar^2}{4} V^{(n)}(q) \right) dq^{(n)}.
\]  
(65)

It is straightforward to show that this two-form is closed and non-degenerate so that it is the preserved symplectic structure for this scheme.

Using the following relation
\[
(dp^{(n+1)})^T = \left( 1 + \frac{\hbar^2}{4} V^{(n+1)}(q) \right) dq^{(n+1)} - \left( 1 + \frac{\hbar^2}{4} V^{(n)}(q) \right) dq^{(n)},
\]  
(66)

one will get this two-form to be the same as Eq. (64).

For the general separable Hamiltonian \( H = T(p) + V(q) \) we can get the preserved symplectic structure for the scheme as follows:
\[
\omega^{(n+1)} = (dp^{(n+1)})^T \wedge \left( 1 + \frac{\hbar^2}{4} T^{(n+1)}(p) V^{(n+1)}(q) \right) dq^{(n+1)}.
\]  
(67)

It is also closed and non-degenerate.

5.2 The Trapezoidal Scheme for General Hamiltonian Systems

For the general system with non-separable Hamiltonian, the trapezoidal scheme gives
\[
q^{(n+1)} - q^{(n)} = \frac{\hbar}{2}(H_p^{(n+1)} + H_p^{(n)}), \quad p^{(n+1)} - p^{(n)} = -\frac{\hbar}{2}(H_q^{(n+1)} + H_q^{(n)}).
\]  
(68)

Similar to the separable Hamiltonian case, let us introduce a pair of DEL one-forms,
\[ E_D^{(n)}(q) := dp^{(n)}\left\{ q^{(n+1)} - q^{(n)} - \frac{\hbar}{2}(H_p^{(n+1)} + H_p^{(n)}) \right\}, \]
\[ E_D^{(n)}(p) := dq^{(n)}\left\{ p^{(n+1)} - p^{(n)} + \frac{\hbar}{2}(H_q^{(n+1)} + H_q^{(n)}) \right\}. \]  
(69)

Similarly, by some straightforward but tedious calculations, the DEL condition for the pair of DEL one-forms gives rise to the following symplectic two-form and its preserving property,
\[
\omega_D^{(n+1)} = \omega_D^{(n)},
\]  
(70)

where
\[
\omega_D^{(n)} = (dp^{(n)})^T \left( 1 + \frac{\hbar^2}{4} H_p^{(n)} H_q^{(n)} - \frac{\hbar^2}{4} H_p^{(n+1)} H_q^{(n+1)} - \frac{\hbar^2}{4} H_p^{(n)} H_q^{(n)} \right) \wedge dq^{(n)} - \frac{\hbar^2}{4}(dq^{(n)})^T H_p^{(n)} H_q^{(n+1)} \wedge dq^{(n)}. \]  
(71)
If we introduce new variables
\begin{align*}
\tilde{p}^{(n)} &= p^{(n)} - \frac{h}{2} H_q^{(n)}, \\
\tilde{q}^{(n)} &= q^{(n)} + \frac{h}{2} H_p^{(n)},
\end{align*}
(72)
it follows that
\begin{equation}
\omega^{(n)}_D = d\tilde{p}^{(n)} \wedge d\tilde{q}^{(n)}.
\end{equation}
(73)
This is another expression for the preserved symplectic structure in the trapezoidal scheme.

6 Some Remarks

i) In order to show whether a scheme for a given Hamiltonian system is symplectic preserving, the first issue in our approach to be considered is to release the scheme from the solution space to the function space. Otherwise, it is difficult to make precise sense for the differential calculation in the solution space. One of the roles played by the EL cohomological concepts is just to release the schemes from the solution space to the function space.

ii) The EL cohomology and its discrete counterpart introduced in Ref. [5] and used here are not trivial for the finite dimensional Hamiltonian systems. It has been shown that the symplectic preserving property is closely linked to the cohomology. Namely, it is equivalent to the closed condition of the EL one-forms. Of course, it is needed to further study the content and meaning of the EL cohomology.

iii) It should be mentioned that all issues studied in this note can be generalized to the case of difference discrete phase space for the separable Hamiltonian systems.[3,4]

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