1 Some additional results for the Verlet transformations

1.1 Verlet dynamics as a sequence of canonical transformations

Let us consider the Verlet transformation as a phase space transformation $(q,p) \to (Q,P)$ given by (again one particle in one dimension)

$$
\begin{aligned}
Q &= q + \frac{p}{m}\Delta t + \frac{\Delta t^2}{2m}F(q) \\
P &= p + \frac{\Delta t}{2}F(q) + \frac{\Delta t}{2}F(Q)
\end{aligned} \tag{1}
$$

These transformations are denoted as $Q(q,p)$ and $P(q,p)$. The inverse transformation (that should be denoted as $q(Q,P)$ and $p(Q,P)$) can be obtained by inverting the previous relations or by using the transformation properties of the Verlet update under time reversal:

$$
\begin{aligned}
q &= Q - \frac{P}{m}\Delta t + \frac{\Delta t^2}{2m}F(Q) \\
p &= P - \frac{\Delta t}{2}F(q) - \frac{\Delta t}{2}F(Q)
\end{aligned} \tag{2}
$$

We want to show that this transformation is canonical. For instance, we can show that there exists a generating function $G(q,Q)$ such that

$$
\left(\frac{\partial G}{\partial q}\right)_Q = p \qquad \left(\frac{\partial G}{\partial Q}\right)_q = -P \tag{3}
$$

It is easy to verify that the function

$$
G(q,Q) = -\frac{m}{2\Delta t}(q-Q)^2 + \frac{\Delta t}{2}[U(q) - U(Q)]
$$

provides indeed the required transformation.

1.2 Canonical transformations in classical mechanics

Let us now review a few results on canonical transformations in classical mechanics. A canonical transformation guarantees that the equations of motion can also be written in canonical form when using the new coordinates. In practice, if we define a new Hamiltonian $H_2(Q,P) = H(q(Q,P),p(Q,P))$, we can rewrite the time derivatives of Q and P, defined by

$$
\begin{aligned}
\dot{Q} &= \left(\frac{\partial Q}{\partial q}\right)_p \dot{q} + \left(\frac{\partial Q}{\partial p}\right)_q \dot{p} = \left(\frac{\partial Q}{\partial q}\right)_p \left(\frac{\partial H}{\partial p}\right)_q - \left(\frac{\partial Q}{\partial p}\right)_q \left(\frac{\partial H}{\partial q}\right)_p \\
\dot{P} &= \left(\frac{\partial P}{\partial q}\right)_p \dot{q} + \left(\frac{\partial P}{\partial p}\right)_q \dot{p} = \left(\frac{\partial P}{\partial q}\right)_p \left(\frac{\partial H}{\partial p}\right)_q - \left(\frac{\partial P}{\partial p}\right)_q \left(\frac{\partial H}{\partial q}\right)_p
\end{aligned}
$$

as Hamilton's equations:

$$
\dot{Q} = \left(\frac{\partial H_2}{\partial P}\right)_Q \qquad \dot{P} = -\left(\frac{\partial H_2}{\partial Q}\right)_P
$$

This equivalence implies several relations between partial derivatives of the different coordinates. We do this check in the Appendix. There is also an analogous relations for the Liouvillians. Define

$$iL(q,p) = -\frac{\partial H}{\partial q}\frac{\partial}{\partial p} + \frac{\partial H}{\partial p}\frac{\partial}{\partial q} \qquad iL_2(Q,P) = -\frac{\partial H_2}{\partial Q}\frac{\partial}{\partial P} + \frac{\partial H_2}{\partial P}\frac{\partial}{\partial Q}$$

Then, for any function A of the coordinates and of the momenta, we have (proof in the Appendix)

$$iL(q,p)A[Q(q,p),P(q,p)] = \Big[iL_2(Q,P)A(Q,P)\Big]_{Q=Q(q,p),P=P(q,p)}. \tag{4}$$

In words:

a) [left-hand side] Consider $A(Q,P)$ and then express Q and P in terms of q,p, computing $f(q,p) = A[Q(q,p),P(q,p)]$; then, apply the the differential operator $iL(q,p)$ to $f(q,p)$ obtaining a function $g(q,p)$;

b) [right-hand side] Consider $A(Q,P)$ and apply to it the differential operator $iL_2(Q,P)$, obtaining a function $h(Q,P)$; then express Q and P in terms of q,p, computing $g_2(q,p) = h[Q(q,p),P(q,p)]$;

c) The result (4) implies $g(q,p) = g_2(q,p)$.

1.3 Verlet evolution

Now, let us go back to the Verlet dynamics. As we have discussed, one time step can be seen as the result of the application of the unitary operator

$$U_s(\Delta t,q,p) = \exp[iL_p(q,p)\Delta t/2]\ \exp[iL_q(q,p)\Delta t]\ \exp[iL_p(q,p)\Delta t/2]$$

In the next lesson we will prove that $U_s(\Delta t,q,p)$ can be written as a Hamiltonian evolution with respect to a new Hamiltonian $\tilde{H}$, i.e.

$$U_s(\Delta t,q,p) = \exp[i\tilde{L}(q,p)\Delta t] \qquad i\tilde{L}(q,p) = -\frac{\partial \tilde{H}}{\partial q}\frac{\partial}{\partial p} + \frac{\partial \tilde{H}}{\partial p}\frac{\partial}{\partial q}.$$

We are now ready to understand what is happening when we perform more than one step. We wish therefore to compute

$$q(2\Delta t) = U_s(\Delta t,q,p)U_s(\Delta t,q,p)q,$$

which gives us the evolution of the position after two time steps, if we identify (at the end, after applying the differential operators) q with q_0 and p with p_0. The result for the application of one evolution operator $U_s(\Delta t,q,p)$ has already been computed, so that we have

$$q(2\Delta t) = U_s(\Delta t,q,p)\left[q + \frac{p}{m}\Delta t + \frac{\Delta t^2}{2m}F(q)\right]. \tag{5}$$

At this point we could start applying the remaining $U_s(\Delta t,q,p)$. Thus, we could imagine of working as follows. We first write

$$q(2\Delta t) = \exp[iL_p(q,p)\Delta t/2]\ \exp[iL_q(q,p)\Delta t]\ \exp[iL_p(q,p)\Delta t/2]\ \left[q + \frac{\Delta t}{m}p + \frac{\Delta t^2}{2m}F(q)\right].$$

Then we apply again each operator. If we consider the first one, we obtain

$$q(2\Delta t) = \exp[iL_p(q,p)\Delta t/2]\, \exp[iL_q(q,p)\Delta t] \left[q + \frac{\Delta t}{m}\left(p + \frac{\Delta t}{2}F(q)\right) + \frac{\Delta t^2}{2m}F(q)\right].$$

Then, one should shift the q's, and then again p. It is clear that formulae become quite rapidly too complex to be of any use. The way out is relation (4). In our case, there is an additional simplification, due to the fact the Hamiltonian $\tilde{H}$ is invariant under the evolution, i.e. $\tilde{H}[Q(q,p), P(q,p)] = \tilde{H}(q,p)$, which implies $H_2 = \tilde{H}$. In terms of the evolution operators, the relation becomes

$$U_s(\Delta t, q, p) A[Q(q,p), P(q,p)] = \Big[U_s(\Delta t, Q, P) A(Q,P) \Big]_{Q=Q(q,p), P=P(q,p)}. \tag{6}$$

To apply this relation to our example set $A(Q,P) = Q$, so that Eq. (5) can be rewritten as

$$\begin{aligned} q(2\Delta t) &= [U_s(\Delta t, q, p) Q(q,p)] \\ &= [U_s(\Delta t, Q, P) Q]_{Q=q(\Delta t), P=p(\Delta t)} = \left[Q + \frac{\Delta t}{2m} P + \frac{1}{2m}\Delta t^2 F(Q) \right]_{Q=q(\Delta t), P=p(\Delta t)}. \end{aligned} \tag{7}$$

In other words: $q(2\Delta t)$ is obtained by repeating the Verlet single-step update using $q(\Delta t)$ and $p(\Delta t)$ as starting values. Of course, the argument generalizes to the momentum and to any time $n\Delta t$. At this point we have completely verified the equivalence between the symplectic approach and the standard Verlet algorithm.

The results we have obtained can be understood quite intuitively. As we have discussed, the Verlet evolution is associated to a Liouvillian $\tilde{L}$ and a conserved Hamiltonian $\tilde{H}$. At least in principle, one can consider the Hamiltonian equations of motion

$$\dot{q} = -\frac{\partial \tilde{H}}{\partial p} \qquad \dot{p} = \frac{\partial \tilde{H}}{\partial q}$$

and the solution $q_H(t)$, $p_H(t)$ that corresponds to the initial conditions $q_H(0) = q_0$ and $p_H(0) = p_0$. By definition, the Verlet values $q(n\Delta t)$ and $p(n\Delta t)$ satisfy

$$q(n\Delta t) = q_H(n\Delta t) \qquad p(n\Delta t) = p_H(n\Delta t).$$

Relation (6) is nothing by the (trivial) observation that we can compute $q(2\Delta t)$ in two different, but equivalent ways:

a) we can solve the Hamilton equations of motion with starting condition $q_H(0) = q_0$ and $p_H(0) = p_0$:

$$q_H(2\Delta t) = \left[e^{i\tilde{L}(q,p)\Delta t} e^{i\tilde{L}(q,p)\Delta t} q \right]_{q=q_0, p=p_0}$$

b) alternatively, we can can use the Hamilton equations of motion with starting condition $q_H(0) = q_0$ and $p_H(0) = p_0$ to compute $Q = q_H(\Delta t)$, $P = p_H(\Delta t)$; then, we can solve the Hamilton equations of motion using a new set of boundary conditions at time $t = \Delta t$: $q_H(\Delta t) = Q$, $p_H(\Delta t) = P$:

$$Q = \left[e^{i\tilde{L}(q,p)\Delta t} q \right]_{q=q_0, p=p_0} \qquad P = \left[e^{i\tilde{L}(q,p)\Delta t} p \right]_{q=q_0, p=p_0}$$

$$q_H(2\Delta t) = \left[e^{i\tilde{L}(q,p)\Delta t} q \right]_{q=Q, p=P} \qquad p_H(2\Delta t) = \left[e^{i\tilde{L}(q,p)\Delta t} p \right]_{q=Q, p=P}.$$

2 Appendix: Differential relations

a) We verify that

$$\left(\frac{\partial Q}{\partial p}\right)_q = -\left(\frac{\partial q}{\partial P}\right)_Q$$

Indeed, we have

$$\left(\frac{\partial Q}{\partial p}\right)_q = \frac{\Delta t}{m} \qquad \left(\frac{\partial q}{\partial P}\right)_Q = -\frac{\Delta t}{m}$$

b) We verify that

$$\left(\frac{\partial Q}{\partial q}\right)_p = \left(\frac{\partial p}{\partial P}\right)_Q$$

Indeed, we have

$$\left(\frac{\partial Q}{\partial q}\right)_p = 1 + \frac{\Delta t^2}{2m}\frac{\partial F(q)}{\partial q}$$

$$\left(\frac{\partial p}{\partial P}\right)_Q = 1 - \frac{\Delta t}{2}\frac{\partial F(q)}{\partial q}\left(\frac{\partial q}{\partial P}\right)_Q = 1 + \frac{\Delta t^2}{2m}\frac{\partial F(q)}{\partial q}$$

c) We verify that

$$\left(\frac{\partial P}{\partial p}\right)_q = \left(\frac{\partial q}{\partial Q}\right)_P$$

Indeed, we have

$$\left(\frac{\partial P}{\partial p}\right)_q = 1 + \frac{\Delta t}{2}\frac{\partial F(Q)}{\partial Q}\left(\frac{\partial Q}{\partial p}\right)_q = 1 + \frac{\Delta t^2}{2m}\frac{\partial F(Q)}{\partial Q}$$

$$\left(\frac{\partial q}{\partial Q}\right)_P = 1 + \frac{\Delta t^2}{2m}\frac{\partial F(Q)}{\partial Q}$$

d) We verify that

$$\left(\frac{\partial P}{\partial q}\right)_p = -\left(\frac{\partial p}{\partial Q}\right)_P$$

Indeed, we have

$$\left(\frac{\partial P}{\partial q}\right)_p = \frac{\Delta t}{2}\frac{\partial F(q)}{\partial q} + \frac{\Delta t}{2}\frac{\partial F(Q)}{\partial Q}\left(\frac{\partial Q}{\partial q}\right)_p = \frac{\Delta t}{2}\frac{\partial F(q)}{\partial q} + \frac{\Delta t}{2}\frac{\partial F(Q)}{\partial Q} + \frac{\Delta t^3}{4m}\frac{\partial F(q)}{\partial q}\frac{\partial F(Q)}{\partial Q}$$

$$\left(\frac{\partial p}{\partial Q}\right)_P = -\frac{\Delta t}{2}\frac{\partial F(Q)}{\partial Q} - \frac{\Delta t}{2}\frac{\partial F(q)}{\partial q}\left(\frac{\partial q}{\partial Q}\right)_P = -\frac{\Delta t}{2}\frac{\partial F(q)}{\partial q} - \frac{\Delta t}{2}\frac{\partial F(Q)}{\partial Q} - \frac{\Delta t^3}{4m}\frac{\partial F(q)}{\partial q}\frac{\partial F(Q)}{\partial Q}$$

We will now use these relations to prove the relation (4).

$$\begin{aligned} iL(q,p)A[Q(q,p),P(q,p)] &= \left(-\frac{\partial H}{\partial q}\frac{\partial}{\partial p} + \frac{\partial H}{\partial p}\frac{\partial}{\partial q}\right)A[Q(q,p),P(q,p)] \\ &= -\frac{\partial H}{\partial q}\left[\left(\frac{\partial A}{\partial Q}\right)_P\left(\frac{\partial Q}{\partial p}\right)_q + \left(\frac{\partial A}{\partial P}\right)_Q\left(\frac{\partial P}{\partial p}\right)_q\right] \\ &\quad +\frac{\partial H}{\partial p}\left[\left(\frac{\partial A}{\partial Q}\right)_P\left(\frac{\partial Q}{\partial q}\right)_p + \left(\frac{\partial A}{\partial P}\right)_Q\left(\frac{\partial P}{\partial q}\right)_p\right] \end{aligned}$$

Now, using the previous relations we can replace the derivates of Q and P with respect to q, p with the derivatives of q, p with respect to Q, P, so that

$$
\begin{aligned}
iL(q,p)A[Q(q,p),P(q,p)] &= -\left[\frac{\partial H}{\partial q}\left(\frac{\partial q}{\partial Q}\right)_P + \frac{\partial H}{\partial p}\left(\frac{\partial p}{\partial Q}\right)_P\right]\left(\frac{\partial A}{\partial P}\right)_Q \\
&\quad + \left[\frac{\partial H}{\partial q}\left(\frac{\partial q}{\partial P}\right)_Q + \frac{\partial H}{\partial p}\left(\frac{\partial p}{\partial P}\right)_Q\right]\left(\frac{\partial A}{\partial Q}\right)_P \\
&= -\frac{\partial H_2}{\partial Q}\left(\frac{\partial A}{\partial P}\right)_Q + \frac{\partial H_2}{\partial P}\left(\frac{\partial A}{\partial Q}\right)_P \\
&= iL_2(Q,P)A(Q,P)\Big|_{Q=Q(q,p),P=P(q,p)}
\end{aligned}
$$