Newton’s graphical method as a canonical transformation

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Abstract

This work shows that, Newton’s Proposition 1 in the Principia, is an exact graphical representation of a canonical transformation, a first-order symplectic integrator generated at a finite time-step by the Hamiltonian. A fundamental characteristic of this canonical transformation is to update the position and velocity vectors sequentially, thereby automatically conserving the phase-volume and the areal velocity due to a central force. As a consequence, the continuous force is naturally replaced by a series of impulses. The convergence of Newton’s Proposition 1 in the limit of $\Delta t \to 0$ can be proved easily and the resulting error term for the linear and the inverse square force can explain why Hooke was able to obtain an elliptical orbit for the former but not the latter.
I. INTRODUCTION

Newton’s Proposition 1, Theorem 1, in Book I of his Principia, has always been admired for its effortless demonstration of Kepler’s area law for any central force. Recently in this Journal, Nauenberg transcribed Newton’s graphical construction into an algebraic algorithm, cited existing algorithms as unaware of their connections to Newton’s Proposition 1 and credited Ref. for explicitly identifying Newton’s Proposition 1 with a particular algorithm. This is very surprising, since Nauenberg himself has correctly identified the algorithm corresponding to Proposition 1 ten years earlier!

It seems clear that even after identifying Newton’s Proposition 1 with an algebraic algorithm, the authors of Ref. and Nauenberg, were unaware of the nature of the algorithm itself. This work further identifies the algorithm as one of two fundamental canonical transformations generated by the Hamiltonian. As such, it automatically obeys Liouville’s theorem in conserving phase-volume and maintains the constancy of the areal velocity due to any central force. Moreover, the algorithm can also be derived as a symplectic integrator, with known error Hamiltonians. These error Hamiltonians can precisely quantify the algorithm’s behavior under different central forces. This then allows us to understand one important incident in the history of mechanics.

In an earlier work, Nauenberg has woven together a compelling account of how Hooke has written to Newton, and told Newton of his idea “of compounding the celestial motions of the planetts of a direct motion by the tangent and an attractive motion toward the central body...” Nauenberg suggested that Newton may have absorbed Hooke’s idea in formulating his Proposition 1. Of course, Newton’s Proposition 1 is mathematically more precise than Hooke’s mere description, and its proof of Kepler’s second law owed nothing to Hooke. But the story continued with Hooke: upon learning of Newton’s graphical construction, he immediately applied it to the case of a linearly increasing central force and obtained an elliptical orbit! However, there is no indication that Hooke was ever successful in obtaining an elliptical orbit for the inverse square force. This work will explain why in Section V.

In the next section we identify the two fundamental canonical transformations 1A and 1B generated by the Hamiltonian of the system. In Section we show that Newton’s Proposition 1 is an exact graphical representation of transformation 1B and that this algorithm should be named after Newton. In Section we resolve questions about convergence and
time-reversibility by showing that 1B can also be derived as a symplectic integrator from Trotter splitting. Moreover, we argue that Newton’s graphical method corresponds to a “n+1/2” 1B algorithm and is completely time-reversible for every position on the trajectory. In Section V, we show that the error Hamiltonian associated with 1B is very different for a linear and an inverse square force, thereby explaining why Hooke can obtain an elliptical orbit for the former, but not the latter. A brief concluding statement is given in Section VI.

II. CANONICAL TRANSFORMATION

(This discussion is adapted from Ref.[9].) A canonical transformation \((q_i, p_i) \rightarrow (Q_i, P_i)\) is a transformation which preserve the form of Hamilton’s equations for both sets of variables.\(^7,8\) Canonical transformations can be derived on the basis of four types of generating functions,\(^7,8\) \(F_1(q_k, Q_k, t), F_2(q_k, P_k, t), F_3(p_k, Q_k, t), F_4(p_k, P_k, t)\). For our purpose, we will only need to use \(F_2\) and \(F_3\) without any explicit time-dependence, given by

\[
p_i = \frac{\partial F_2(q_k, P_k)}{\partial q_i}, \quad Q_i = \frac{\partial F_2(q_k, P_k)}{\partial P_i},
\]

(1)

and

\[
q_i = -\frac{\partial F_3(p_k, Q_k)}{\partial p_i}, \quad P_i = -\frac{\partial F_3(p_k, Q_k)}{\partial Q_i}.
\]

(2)

In (1), the first equation is an implicit equation for finding \(P_i\) in terms of \(q_i\) and \(p_i\). The second, is an explicit equation for determining \(Q_i\) in terms of \(q_i\) and the updated \(P_i\). This can be viewed naturally as a sequence of two transformations: first to \(P_i\) then \(Q_i\). As shown in Ref.[9], this sequential updating of \(P_i\) and \(Q_i\) automatically guarantees Liouville’s theorem,\(^7,8\) the preservation of phase-volume, so that the determinant of the Jacobian of transformation is one. Similarly for \(F_3\), but now first transform to \(Q_i\) then \(P_i\). This sequential updating of \(Q_i\) and \(P_i\) is a hallmark of canonical transformations and naturally leads to the replacement of a continuous force by a series of impulses.

Among canonical transformations, the most important one is when \(Q_i = q_i(t)\) and \(P_i = p_i(t)\), which solves the dynamics of the system. For an arbitrary \(t\), the required transformation is generally unknown. However, when \(t\) is infinitesimally small, \(t \rightarrow \Delta t\), it is well known that the Hamiltonian is the infinitesimal generator of time evolution.\(^7,8\) Less well known is the fact that even when \(\Delta t\) is finite, the resulting transformation generated by the
Hamiltonian remains canonical, and gives an excellent approximate trajectory. Let’s take
\[ F_2(q_i, P_i) = \sum_{i=1}^{n} q_i P_i + \Delta t H(q_i, P_i) \]  
(3)

where
\[ H(q_i, p_i) = \sum_{i=1}^{n} \frac{p_i^2}{2m} + V(q_i) \]
is the usual separable Hamiltonian. For this generating function (3), \( \Delta t \) is simply an arbitrary parameter, need not be small. The transformation equations (1) then give,
\[ P_i = p_i - \Delta t \frac{\partial V(q_i)}{\partial q_i}, \quad Q_i = q_i + \Delta t \frac{P_i}{m} \]
(4)

If one regards \( q_i = q_i(t), p_i = p_i(t) \) and \( Q_i = q_i(t + \Delta t), P_i = p_i(t + \Delta t) \) then the above is precisely the algorithm that Cromer’s student rediscovered accidentally \(^4\). For uniformity, we will following Ref\(^9\) in referring to this as algorithm 1A. Similarly, taking
\[ F_3(p_i, Q_i) = -\sum_{i=1}^{n} p_i Q_i + \Delta t H(Q_i, p_i) \]
(5)

and applying (2) gives the other canonical algorithm
\[ Q_i = q_i + \Delta t \frac{P_i}{m}, \quad P_i = p_i - \Delta t \frac{\partial V(Q_i)}{\partial Q_i} \]
(6)

This algorithm has no name, but was listed by Stanley \(^10\), as the second LPA algorithm. We will refer to this algorithm as 1B. Among the many elementary algorithms studied, such as those by Stanley \(^10\), only these two, and their variants, were later found to be explicit, self-starting and symplectic. For the ease of comparison, we will define \( r_n = q(n \Delta t), v_n = p(n \Delta t)/m, a(r) = F(r)/m = -\nabla V(r)/m \). The above two algorithms can then be succinctly given in modern notations as 1A:
\[ \begin{align*}
v_{n+1} &= v_n + \Delta t a(r_n) \\
r_{n+1} &= r_n + \Delta t v_{n+1}
\end{align*} \]
(7)

and 1B:
\[ \begin{align*}
r_{n+1} &= r_n + \Delta t v_n \\
v_{n+1} &= v_n + \Delta t a(r_{n+1})
\end{align*} \]
(8)

Note the sequential updating nature of these two algorithms. In 1A, the updated \( v_{n+1} \) is immediately used to compute \( r_{n+1} \). In 1B, the updated \( r_{n+1} \) is immediately used to
compute $v_{n+1}$. Because of this, not only is phase volume preserved, angular momentum is also automatically conserved for a central force $a(r) = f(r)\mathbf{r}$ at each time step. For example, for algorithm 1B

$$r_{n+1} \times v_{n+1} = r_{n+1} \times (v_n + \Delta t a(r_{n+1})) = r_{n+1} \times v_n = r_n \times v_n. \quad (10)$$

Similarly for algorithm 1A, just substitute in the last updated variable first in the $r \times v$ computation. In 1994, Nauenberg\textsuperscript{6} has already identified Newton’s proposition 1, as used by Hooke, as algorithm 1B. (See Eq.(1) and (2) in Ref.\textsuperscript{6}. He also showed that it conserves angular momentum as in (10).

Other well known algorithms are simply variants of these two. For example, if one changes the label $n$ in $v_n$ to $v_{n-\frac{1}{2}}$ in 1A, and to $v_{n+\frac{1}{2}}$ in 1B, then one has the leap-frog algorithm. Also, by doing a “one and half” 1B from $r_{n-1}$ one gets

$$r_n = r_{n-1} + \Delta t v_{n-1}$$
$$v_n = v_{n-1} + \Delta t a(r_n)$$
$$r_{n+1} = r_n + \Delta t v_n$$

$$= r_n + \Delta t v_{n-1} + \Delta t^2 a(r_n)$$
$$= r_n + r_n - r_{n-1} + \Delta t^2 a(r_n). \quad (11)$$

While (11) is the result of the “one and half” 1B algorithm, eliminating the intermediate velocity $v_{n-1}$ gives (12), which is the Verlet\textsuperscript{3} algorithm. This velocity elimination fundamentally changes algorithm. The “one and half” 1B algorithm is completely time-reversible for every position. Starting with (11), change $\Delta t \rightarrow -\Delta t$ and iterate the algorithm again, one backtracks step-by-step back to $r_{n-1}$:

$$\tilde{r}_{n+1} = r_{n+1} - \Delta t v_n = r_n$$
$$\tilde{v}_{n+1} = v_n - \Delta t a(r_n) = v_{n-1}$$
$$\tilde{r}_{n+2} = r_n - \Delta t v_{n-1} = r_{n-1}. \quad (12)$$

In the Verlet form (12), the algorithm is time-reversible only between $r_{n+1}$ and $r_{n-1}$, but not between every successive position! By eliminating $v_{n-1}$, the algorithm is no longer self-starting, and requires two starting positions $r_0$ and $r_1$. All even positions would time reverse
back to \( r_0 \) and all odd positions time reverse back to \( r_1 \), as if two trajectories are running in parallel. If Verlet’s \( r_1 \) coincide with 1B’s \( r_1 \), then both will yield the same trajectory. If Verlet’s \( r_1 \) is very different from that of 1B, then very different trajectories can result. Thus Verlet is not the same as 1B.

By identical manipulations, one can also derive Verlet from “half and one” 1A algorithm, again going \( r_{n-1} \) to \( r_{n+1} \). Thus both 1A and 1B can give rises to Verlet, and from Verlet, one can infer either 1A or 1B as the underlying algorithm.

III. NEWTON’S GRAPHIC CONSTRUCTION

When one examine the diagram of Newton’s Proposition 1 (see Fig.1), one is immediately struck by its ingenious construction. The area sweep out by each point of the orbit is guaranteed to be equal, when the impulse for determine that point is computed at the radial direction of the preceding point. Also, starting at an initial position \( r_0 \), every successive position \( B, C, D, E, F \) on the orbit receives an impulse, except \( B \). Let \( A, B, C, D, \) etc., be denoted by \( r_0, r_1, r_2, r_3 \) etc., and write out the first few iterations of algorithm 1B.\(^9\)

\[
\begin{align*}
  r_1 &= r_0 + \Delta t v_0, & v_1 &= v_0 + \Delta t a(r_1) \\
  r_2 &= r_1 + \Delta t v_1, & v_2 &= v_1 + \Delta t a(r_2) \\
      &= r_0 + 2\Delta t v_0 + \Delta t^2 a(r_1) \\
  r_3 &= r_2 + \Delta t v_2, & v_3 &= v_2 + \Delta t a(r_3) \\
      &= r_2 + \Delta t v_1 + \Delta t^2 a(r_2)
\end{align*}
\]

We can refer to position vectors above and Newton’s diagram simultaneously by the dual notation \( r_0(A), r_1(B) \), etc.. Comparing the diagram with the above positions, one sees that starting at the initial position \( r_0(A) \), \( r_1(B) \) is just a distance \( \Delta t v_0 \) away with no impulse. This is just the Newton’s First Law. At \( r_1(B) \), its continuing “tangential” velocity \( v_0 \) (in the direction of BC) is “compounded” by the central impulse at the radial direction (BV) of \( r_1(B) \), giving rise to \( v_1 \) as stated in \([13]\). This is then Newton’s Second Law. Now one repeats Newton’s First Law and arrived at \( r_2(C) \) from \( r_1(B) \). This is the path ABC in Newton’s diagram. By expanding out \( r_2(C) \) in \([14]\), one sees that it can also be viewed as arriving from \( r_0(A) \) after \( 2\Delta t v_0 \) plus an impulse displacement of \( \Delta t^2 a(r_1) \) computed at the radial direction of the preceding position \( r_1(B) \). This is the path AcC in Newton’s diagram.
FIG. 1: Left: Newton’s Proposition 1 diagram taken from Ref.[11]. Right: trajectories generated by algorithms 1A and 1B for a constant central force.

One then repeat the Second Law to obtain $v_2$, then the First Law to get $r_3(D)$, etc. Thus positions $A$, $B$, $C$, $D$, etc., on Newton’s diagram, exactly match positions $r_0$, $r_1$, $r_2$, $r_3$, etc., generated by algorithm 1B. In Fig.1 the first few numerical positions of 1B with a constant central force is compared to Newton’s diagram for Proposition 1. The numerical positions clearly resemble those in Newton’s carefully constructed diagram. Newton’s Proposition 1 is therefore an exact pictorial representation of algorithm 1B and 1B should be named after Newton because it is simply the repeated applications of his First and Second laws.

We show also in Fig.1, the trajectory generated by algorithm 1A using the same initial condition as 1B. It clearly does not match Newton’s diagram. Algorithm 1A corresponds to applying Newton’s first two laws in the reversed order, producing a trajectory starting with velocity $v_1$.

IV. SYMPLECTIC INTEGRATORS AND TIME REVERSIBILITY

There have been continued debates over whether Newton’s graphical method, which uses a series of impulses $\Delta t a(r_n)$, can converges to the continuum limit. All such discussions are mute because not only is Newton’s graphical method a canonical transformation, it can also be rigorously derived as a symplectic integrator from the Baker-Campbell-Hausdorff
(BCH) formula
\[ e^{\Delta t T} e^{\Delta t V} = e^{\Delta t(T+V)} + \frac{1}{2} \Delta t^2 [T,V] + \cdots, \]
where \( T \) and \( V \) are classical Lie operators:
\[ T = v \cdot \frac{\partial}{\partial r} \quad V = a(r) \cdot \frac{\partial}{\partial v}. \]  \hspace{1cm} (16)

See Refs.\[9,13–15\] for details. The effect of \( e^{\Delta t T} e^{\Delta t V} \) on any function \( W(r,v) \) is
\[ e^{\Delta t T} e^{\Delta t V} W(r,v) = e^{\Delta t T} W(r,v + \Delta t a(r)) = W(r + \Delta t v, v + \Delta t a(r + \Delta t v)), \]
which is precisely equivalent to updating \( r' = r + \Delta t v \) then \( v' = v + \Delta t a(r') \), corresponding to algorithm 1B. (Note that the operators act from right to left, but the resulting algorithm is equivalent to operators acting sequentially from left to right.) Similarly, the action of \( e^{\Delta t V} e^{\Delta t T} \) reproduces algorithm 1A.

In the limit of \( \Delta t \to 0 \) the convergence of Newton’s algorithm is guaranteed by BCH:
\[ e^{\Delta t T} e^{\Delta t V} \to e^{\Delta t(T+V)} + O(\Delta t^2), \]
where the exact trajectory is given by \( r(t+\Delta t) = e^{\Delta t(T+V)} r(t) \) and \( v(t+\Delta t) = e^{\Delta t(T+V)} v(t) \). This is the standard Trotter\[10\] splitting. There is therefore no question about the convergence, which one can easily verify numerically, the only question is whether this convergence is efficient, which we will discuss in the next section.

From this operator form of 1B, it is well-known that it is not time-reversible, since
\[ e^{\Delta t T} e^{\Delta t V} e^{-\Delta t T} e^{-\Delta t V} \neq 1. \]
(Recall that operators act sequentially from left to right.) However, as we have shown in Section II, the “one and half” 1B, corresponding to \( e^{\Delta t T} e^{\Delta t V} e^{\Delta t T} \) is time-reversible,
\[ e^{\Delta t T} e^{\Delta t V} e^{-\Delta t T} e^{-\Delta t V} e^{-\Delta t T} = 1. \]
It is obvious then that every left-right symmetric operator form as above will yield a time-reversible algorithm\[12\] However, recall also that the very similar Verlet algorithm, by eliminating the intermediate velocity, is only time-reversible for every other position.

In a recent publication, Nauenberg\[11\] first transcribed Newton’s graphical construction in the Verlet form and claimed time-reversibility for Newton’s Proposition 1. (From the Verlet
form, he then inferred algorithm 1A, in contrasted to his earlier deduction of 1B. This work supports his earlier identification.) Nauenberg’s time-reversibility discussion in Ref. 11 is the time reversibility of the Verlet algorithm, the reversibility of every other position on the trajectory, but not every position on the trajectory.

As discussed in Section 11, Newton’s Proposition 1 corresponds to algorithm 1B. If that were completely the case, then as shown above, Newton’s Proposition 1 would not be time-reversible. However, it is clear that Newton’s intention was to compute positions only and would have stopped after the last computation of the position. This interpretation would imply that his graphic method is a “n + 1/2” 1B algorithm, corresponding to,

\[(e^{\Delta t T} e^{\Delta t V})^n e^{\Delta t T},\]

in which only the position but not the velocity is updated at the final step. In this case, the above sequence of operators is left-right symmetric and Newton’s method would be completely time-reversible for every position of the trajectory.

V. THE ERROR HAMILTONIAN

By identifying Newton’s proposition 1 as the symplectic algorithm 1B, one then knows everything about this algorithm, and hence Newton’s graphical construction. For example, the trajectory generated by the algorithm is exact for the approximate Hamiltonian

\[H_A = H + \Delta t H_1 + \Delta t^2 H_2 + \cdots\]

where \(H\) is the original Hamiltonian one is seeking to solve. In the limit of \(\Delta t \rightarrow 0\), only the first-order error Hamiltonian \(H_1\) matters. For algorithm 1B, this is well known to be

\[H_1 = -\frac{1}{2} \mathbf{v} \cdot \mathbf{a}(\mathbf{r}).\]

Therefore in solving the linear central force problem with \(\mathbf{a}(\mathbf{r}) = -\mathbf{r}\), the algorithm is governed by the approximate Hamiltonian

\[H_A = \frac{1}{2} (\mathbf{v}^2 + \mathbf{r}^2 + \Delta t \mathbf{v} \cdot \mathbf{r}),\]

with a first order error Hamiltonian less singular than the original Hamiltonian and only results in minor distortions. It turns out, this first-order approximate Hamiltonian is exactly
conserved by algorithm 1B. (This was noted by Larsen\textsuperscript{[13]} for algorithm 1A, with a minus $\Delta t$ term, in 1983.) Therefore the resulting trajectory of Newton’s algorithm, as long as $|\Delta t| < 2$, is always a closed ellipse, even if it is not the correct elliptical orbit of the original Hamiltonian! See the Appendix for details. This is the reason why Hooke, when using Newton’s graphical method, can claim that a linear force produces an elliptical orbit\textsuperscript{[6]}

By contrast, for the inverse-square central force, the approximate Hamiltonian is

$$H_A = \frac{1}{2} v^2 - \frac{1}{r} + \frac{\Delta t}{2} \frac{v \cdot r}{r^3}.$$

This first-order error Hamiltonian is more singular than the original Hamiltonian (near the force center) and will cause the orbit to precess\textsuperscript{[10]} (and therefore not close), with limited stability, unless $\Delta t$ is extremely small. Thus Hooke, when applying Newton’s graphical method to an inverse-square force, with a fairly large $\Delta t$, would not have been able to produce a closed ellipse of moderate eccentricity\textsuperscript{[6]}. For the same reason, despite being the cornerstone of the \textit{Principia}, Proposition 1 was never used, even by Newton, to prove an elliptical orbit from an inverse-square force.

VI. CONCLUSIONS

In this work, we have shown that knowledge of canonical transformations and symplectic integrators, not only help us to appreciate the prophetic nature of Newton’s proposition 1, which anticipated symplectic integrators centuries earlier, but also help us to understand the historical success and failure of Hooke’s effort to determine central force orbits using Newton’s graphical method.

APPENDIX

The approximate Hamiltonian (17) can be rewritten as

$$H_A = \frac{1}{2} \left( v' \cdot v' + (1 - \frac{\Delta t^2}{4}) r^2 \right),$$

with $v' = v + \Delta t r/2$. Therefore as long $|\Delta t| < 2$, it is a harmonic oscillator with angular frequene $\omega = \sqrt{1 - \Delta t^2/4}$ and trajectory

$$r(t) = r_0 \cos(\omega t) + \frac{v_0}{\omega} \sin(\omega t)$$

(18)
FIG. 2: For a linear central force, Newton’s proposition 1 always produces an ellipse, regardless of the time step size used. The symbols are the outputs of Newton’s algorithm, the solid lines are the predicted orbits (18) of the algorithm. The three time-step sizes used are those of (19).

where \( v'_0 = v_0 + \Delta t r_0/2 \). While (18) gives the correct trajectory of the algorithm, the algorithm’s approximate angular frequency is \( \omega \) given above, but is given by

\[
\omega_A = \cos^{-1}(1 - \Delta t^2/2).
\]

One can therefore choose \( \Delta t \) so that \( T = 2\pi/\omega_A \) is an integer. For \( T = 6, 12, 24 \), one requires

\[
\Delta t = 1, \sqrt{2 - \sqrt{3}} \approx 0.51764, \sqrt{2 - \sqrt{2 + \sqrt{3}}} \approx 0.26105, \quad (19)
\]

respectively. In Fig. 2 we compare the output of Newton’s algorithm at these three time steps with the analytical orbit of (18). For the linear central force case, Newton’s algorithm always produces positions which are exactly on an ellipse, as long as \( |\Delta t| < 2 \). (At \( |\Delta t| = 2 \)
the orbit collapses into a line.) At a large $\Delta t$, as in the case of $\Delta t = 1$, these ellipses are far from the correct orbit, as illustrated in Fig.2.

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