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COMMENTS AND REPLIES

# Comment on 'Conservative discretizations of the Kepler motion'

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**Abstract**
We show that the exact integrator for the classical Kepler motion, recently found by Kozlov (2007 *J. Phys. A: Math. Theor.* **40** 4529–39), can be derived in a simple natural way, using a well-known exact discretization of the harmonic oscillator. We also draw attention to important earlier references, where the exact discretization of the four-dimensional isotropic harmonic oscillator has been applied to the perturbed Kepler problem.

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In recent years several conservative discretizations of the classical Kepler problem have been proposed [1–5]. These numerical integrators preserve all integrals of motion and trajectories but only Kozlov's schemes are of order higher than 2. Kozlov also found the exact integrator by guessing its proper form and summing up some infinite series [4].

In this comment we show that Kozlov's exact integrator can be derived in a simple elementary way. Conservative discretizations of the three-dimensional Kepler motion obtained in [3, 4] consist in applying the midpoint rule (or the discrete gradient method, compare [6]) to the isotropic four-dimensional harmonic oscillator equations:

$$\frac{\mathrm{d}\mathbf{Q}}{\mathrm{d}s} = \frac{1}{4}\mathbf{P}, \qquad \frac{\mathrm{d}\mathbf{P}}{\mathrm{d}s} = 2E\mathbf{Q} \qquad (\mathbf{Q}, \mathbf{P} \in \mathbb{R}^4) \tag{1}$$

where $E = \mathrm{const}$ is the energy integral of the considered Kepler motion. Then, the authors of [3, 4] use the Kustaanheimo–Stiefel (KS) transformation. This classical transformation is given by ([7], see also [4])

$$\mathbf{q} = \begin{pmatrix} Q_1^2 - Q_2^2 - Q_3^2 + Q_4^2 \\ 2Q_1Q_2 - 2Q_3Q_4 \\ 2Q_1Q_3 + 2Q_2Q_4 \end{pmatrix}, \tag{2}$$

$$\mathbf{p} = \frac{1}{2|\mathbf{Q}|^2} \begin{pmatrix} P_1Q_1 - P_2Q_2 - P_3Q_3 + P_4Q_4 \\ P_1Q_2 + P_2Q_1 - P_3Q_4 - P_4Q_3 \\ P_1Q_3 + P_2Q_4 + P_3Q_1 + P_4Q_2 \end{pmatrix}, \tag{3}$$

where $\mathbf{Q}$, $\mathbf{P}$ are subject to the constraint

$$P_1 Q_4 - P_2 Q_3 + P_3 Q_2 - P_4 Q_1 = 0. \tag{4}$$

The KS transformation, together with the Lévi-Cività time transformation

$$\frac{\mathrm{d}t}{\mathrm{d}s} = |\mathbf{q}| \tag{5}$$

maps the four-dimensional harmonic oscillator (1) into the three-dimensional Kepler problem equations:

$$\frac{\mathrm{d}\mathbf{q}}{\mathrm{d}t} = \mathbf{p}, \qquad \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = -\frac{k\mathbf{q}}{|\mathbf{q}|^3} \qquad (\mathbf{q}, \mathbf{p} \in \mathbb{R}^3), \tag{6}$$

where $k = \text{const}$. Using (2), (3) and (4) we can verify the useful identities

$$|\mathbf{q}|^2 = |\mathbf{Q}|^4, \qquad |\mathbf{P}|^2 = 4|\mathbf{p}|^2|\mathbf{Q}|^2, \tag{7}$$

which imply the equivalence of the energy conservation laws:

$$\frac{1}{2}\mathbf{p}^2 - \frac{k}{|\mathbf{q}|} = E \quad \Longleftrightarrow \quad \frac{1}{8}|\mathbf{P}|^2 - E|\mathbf{Q}|^2 = k. \tag{8}$$

The phenomenon of interchanging coupling constants with integrals of motion (like $k \leftrightarrow E$) is quite well known in the theory of integrable systems, see [8] (compare also [9], where more general results can be found).

In order to derive Kozlov's numerical results in a simple straightforward way it is sufficient to note that the KS transformation (used by Kozlov) reduces the Kepler motion to linear ordinary differential equations with constant coefficients (namely to the harmonic oscillator) and for all such equations there exist explicit exact numerical integrators ([10, 11], see also [12]). By the exact discretization of an ordinary differential equation $\dot{x} = f(x)$, where $x(t) \in \mathbb{R}^N$, we mean the one-step numerical scheme of the form $X_{n+1} = \Phi_h(X_n)$, such that $X_n = x(t_n)$, compare [10, 11].

The system (1), equivalent to the four-dimensional harmonic oscillator equation, admits the exact discretization (see, for instance, [12]):

$$\begin{aligned} \frac{\mathbf{Q}_{j+1} - \mathbf{Q}_j}{\delta(h_j)} &= \frac{1}{4}\frac{\mathbf{P}_{j+1} + \mathbf{P}_j}{2}, \\ \frac{\mathbf{P}_{j+1} - \mathbf{P}_j}{\delta(h_j)} &= 2E\frac{\mathbf{Q}_{j+1} + \mathbf{Q}_j}{2}, \end{aligned} \tag{9}$$

where $h_j := s_{j+1} - s_j$ is the (variable) $s$-step, $\mathbf{Q}_j, \mathbf{P}_j$ denote $j$th iteration of the numerical scheme (not to be confused with the coordinates $Q_j$, $P_j$) and

$$\delta(h_j) = \frac{2}{\omega}\tan\frac{\omega h_j}{2}, \qquad \omega^2 = -\frac{1}{2}E. \tag{10}$$

In the case of the constant step $h_j = h$ and $E < 0$, we recognize here the exact integrator found by Kozlov (see formulae (4.11) and (4.14) from [4], taking into account that $\delta(h) = ha(h) = hb(h)$ and $E = -A$). The hyperbolic and parabolic cases (formulae (4.16) and (4.18) from [4]) follow immediately when we take imaginary $\omega$ (i.e. $E > 0$) or $\omega = 0$. The exact numerical scheme (9) preserves the energy integral, i.e.

$$\tfrac{1}{8}|\mathbf{P}_j|^2 - E|\mathbf{Q}_j|^2 = k. \tag{11}$$

Note that the system (9) can be rewritten in the explicit form:

$$\begin{aligned} \mathbf{Q}_{j+1} &= \cos\omega h_j\, \mathbf{Q}_j + \frac{\sin\omega h_j}{4\omega}\, \mathbf{P}_j, \\ \mathbf{P}_{j+1} &= -4\omega\sin\omega h_j\, \mathbf{Q}_j + \cos\omega h_j\, \mathbf{P}_j. \end{aligned} \tag{12}$$

This system is a direct consequence of evaluating the exact solution of (1) at $s = s_j$ and $s = s_j + h_j$, compare [12].

Equation (5) can be solved exactly in different (but more or less equivalent) ways, compare [4, 13, 14]. Here we propose one more approach, reducing this problem to linear ordinary differential equations with constant coefficients. If $\mathbf{Q}$, $\mathbf{P}$ satisfy (1) and $t$ satisfies (5), then we easily check that

$$\frac{\mathrm{d}\mathbf{w}}{\mathrm{d}s} = \Omega\mathbf{w}, \qquad \mathbf{w} = \begin{pmatrix} |\mathbf{Q}|^2 \\ |\mathbf{P}|^2 \\ \mathbf{Q}\cdot\mathbf{P} \\ t \end{pmatrix}, \qquad \Omega = \begin{pmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 4E & 0 \\ 2E & \frac{1}{4} & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \tag{13}$$

In such a case we can proceed in a standard way. The general solution is given by $\mathbf{w}(s) = \exp(s\Omega)\mathbf{w}(0)$. Therefore, the exact discretization, $\mathbf{w}_n = \mathbf{w}(hn)$, satisfies

$$\mathbf{w}_{n+1} = \exp(h\Omega)\mathbf{w}_n, \tag{14}$$

and the problem reduces to the well-known, purely algebraic procedure of computing $\mathrm{e}^{\Omega h}$. In our particular case we observe that $\Omega^4 = 2E\Omega^2$ which simplifies computations. The last row in equation (14) reads

$$t_{j+1} = t_j + \frac{\sin 2h\omega}{4\omega}\left(|\mathbf{Q}_j|^2 - \frac{|\mathbf{P}_j|^2}{16\omega^2}\right) + \frac{h}{2}\left(|\mathbf{Q}_j|^2 + \frac{|\mathbf{P}_j|^2}{16\omega^2}\right) + \frac{\mathbf{Q}_j\cdot\mathbf{P}_j\sin^2 h\omega}{4\omega^2}. \tag{15}$$

One can check by direct computation that discretization (15), although has a simpler form, is identical with formulae (4.11), (4.15) of [4]. Finally, eliminating $|\mathbf{P}_j|^2$ by virtue of (11), we get

$$t_{j+1} = t_j + \frac{hk}{4\omega^2}\left(1 - \frac{\sin 2h\omega}{2h\omega}\right) + \frac{\sin 2h\omega}{2\omega}|\mathbf{Q}_j|^2 + \frac{\mathbf{Q}_j\cdot\mathbf{P}_j\sin^2 h\omega}{4\omega^2}. \tag{16}$$

Another approach (see [13]) consists in computing the integral $\int |\mathbf{Q}(s)|^2\mathrm{d}s$, where $\mathbf{Q}$ is the exact solution of (1). Formula (86) from [13] is identical to (16) (although notation is quite different).

In celestial mechanics the exact discretization of the Kepler motion via the KS transformation appeared as a quite natural step [13–15], although the conservative properties of the exact integrator are not discussed explicitly in these papers. Long ago Stiefel and Bettis, working in the framework of the Gautschi approach [17], applied the exact discretization of the harmonic oscillator to the perturbed Kepler motion [15, 16].

More recently, Mikkola [13] and Breiter [14] proposed new integrators for the perturbed Kepler problem, using the exact solution of the four-dimensional isotropic harmonic oscillator equation and the exact discretization (16) of the time (known to Stumpff even before the KS transform was invented, compare [13]). In particular, the numerical scheme (12) can be found in [13], p 162, and in [14], p 234. Breiter follows [18] using an additional constant in the definition of the KS transformation (in fact scaling both $\mathbf{q}$ and $\mathbf{p}$). The freedom of choosing this parameter can be used to fix the value of $\omega$ (e.g. $\omega = 1$) which may have numerical advantages [14].

These important results of celestial mechanics are not mentioned in [4] and, in general, they seem to be rather unknown in the field of geometric numerical integration [19]. It is worthwhile to mention that the exact discretization of the harmonic oscillator equation has been recently used to construct new geometric integrators of high accuracy ('locally exact discrete gradient schemes') [12, 20]. We plan to apply this scheme to the perturbed Kepler problem using the Kustaanheimo–Stiefel map.

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