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Discrete Effects in Classical Mechanics

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By utilizing some results of discrete mechanics, effects related to the discretization of the equations of motion of classical mechanics are analyzed. Some examples of periodic motions are developed and it is shown that the discrete frequencies are different from the continuous one. Numerical calculations involving orbits are presented. A numerical algorithm, suggested by discrete mechanics, is compared with conventional methods of second order.

1. INTRODUCTION

It is known that physical theories are normally formulated within the space-time continuum using differential calculus. In recent years, however, there has been a substantial growth of interest in discrete mechanics, where, in contrast, it is assumed that time and length may be discrete variables. The supposition that space-time has a discrete structure was often proposed as a possible way for the elimination of the infinities inherent in conventional quantum field theory (Toller, 1977). Many authors have developed various methods of introducing quantized space-time into physical theory (Namsrai, 1985). Among these, Lee (1983) has suggested that there exists in nature another fundamental constant, which can be regarded as the average space-time spacing, and has proposed a new formulation of mechanics where time is treated as a discrete dynamical variable.

Lee's discrete formulation of mechanics finds its greatest applications in quantum and relativistic mechanics, but it suffers from some inadequacies in classical mechanics (D'Innocenzo *et al.*, 1984). Nevertheless, it has been shown (D'Innocenzo *et al.*, 1984, 1987) that a simple modification of the form of the discrete action eliminates some difficulties for the harmonic oscillator, producing results which are in agreement with those of other classical discrete models (LaBudde and Greenspan, 1974; Renna, 1987).

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Therefore, starting from Lee's discrete mechanics model and from its modified version, it is possible to examine in a fairly simple way some effects due to discretization. Since the differential equations of continuum theory are replaced, in discrete physics, with difference equations, only numerical solutions are in general available. However, in some cases the algebraic structure of the equations of motion is very simple and the search for solutions sometimes demands only easy operations of an arithmetical or numerical nature. Moreover, through the preservation of the validity of the discrete conservation laws, it is possible to avoid instabilities in numerical calculations. In addition to the physical intuition that can be gained from these studies, there is the possibility not only of comparing different methods of approximation in the solutions of differential equations by the solutions of difference equations, but of suggesting some concrete improvements, too.

We introduce discrete classical equations of motion in Section 2. We use them to resolve, in Section 3, the harmonic oscillator and show that the discrete frequency is different from the continuous frequency. Next, in Section 4, we make some observations about the form of the discrete solutions for the motion of a particle on a circular orbit and subject to the gravitational force. Finally, in Section 5, the numerical calculations for an elliptical motion are presented and a numerical method, suggested by discrete mechanics, is compared with the second-order Taylor approximation.

2. DISCRETE EQUATION OF MOTION

In discrete classical mechanics, the physical quantities and the continuous dynamical variables are replaced by a sequence of discrete values that are functions of the discrete time t_n, and the continuous equations of motion by the proper corresponding discrete equations, so as to obtain the fundamental conservation laws of physics. Of course, the discrete equations must tend to the continuous ones when the discrete time steps $\Delta t_n = t_n - t_{n-1}$ tend to zero. Nevertheless, there is a certain arbitrariness in defining discrete physical quantities. The velocity can be defined, for small time intervals, by approximating the path by straight lines

$$\mathbf{v}_n = \frac{\mathbf{r}_n - \mathbf{r}_{n-1}}{t_n - t_{n-1}} \tag{1}$$

where $\mathbf{r}_n \equiv \mathbf{r}(t_n)$. In each tract of path, the potential $V(\mathbf{r})$ can be defined in an arbitrary point of the tract.

Let us consider a particle of mass m and subject to the potential $V(\mathbf{r})$. Different discrete models deal with different discrete Newton's equations corresponding to $\mathbf{F} = m\mathbf{a}$.

In Lee's discrete formulation of mechanics the classical action is replaced by

$$A_d = \sum_{n=1}^{N+1} \{\tfrac{1}{2}m\mathbf{v}_n^2 - \tfrac{1}{2}[V(\mathbf{r}_n) + V(\mathbf{r}_{n+1})]\}(t_n - t_{n-1}) \tag{2}$$

where N is the number of intermediate points between the initial and final positions.

By setting

$$\frac{\partial A_d}{\partial \mathbf{r}_n} = 0 \tag{3}$$

and

$$\frac{\partial A_d}{\partial t_n} = 0 \tag{4}$$

one finds the equations

$$m\frac{\mathbf{v}_{n+1} - \mathbf{v}_n}{\frac{1}{2}(t_{n+1} - t_{n-1})} = -\nabla V(\mathbf{r}_n) \tag{5}$$

$$E_n \equiv \tfrac{1}{2}m\mathbf{v}_n^2 + \tfrac{1}{2}[V(\mathbf{r}_n) + V(\mathbf{r}_{n-1})] = E_{n+1} \tag{6}$$

where $\nabla \equiv \partial/\partial \mathbf{r}_n$ is the gradient operator. Equation (5) is the discrete equivalent of Newton's law, while equation (6) represents the law of conservation of energy for discrete mechanics. In continuous mechanics the energy conservation law is a consequence of Newton's equations for conservative systems, while in discrete mechanics these two are independent and are obtained treating both $\mathbf{r}$ and t as dynamical variables.

The system of equations (5) and (6) has simple analytical solutions for the case $V = 0$, which leaves undetermined the time intervals, and for the case $\nabla V = \text{const}$, which yields equal-time spacing, while it is hard to resolve this system for more complicated potentials (except numerically). If we consider, instead of action (2), the following discrete action (D'Innocenzo *et al.*, 1987)

$$A_d = \sum_{n=1}^{N+1} \left[\frac{1}{2}m\mathbf{v}_n^2 - V\left(\frac{\mathbf{r}_n + \mathbf{r}_{n-1}}{2}\right)\right](t_n - t_{n-1}) \tag{7}$$

from (3) and (4) we obtain

$$m\frac{\mathbf{v}_{n+1} - \mathbf{v}_n}{t_{n+1} - t_n} = -\nabla\left[V\left(\frac{\mathbf{r}_n + \mathbf{r}_{n-1}}{2}\right)\frac{t_n - t_{n-1}}{t_{n+1} - t_n} + V\left(\frac{\mathbf{r}_{n+1} + \mathbf{r}_n}{2}\right)\right] \tag{8}$$

$$E_n \equiv \frac{1}{2}m\mathbf{v}_n^2 + V\left(\frac{\mathbf{r}_n + \mathbf{r}_{n-1}}{2}\right) = E_{n+1} \tag{9}$$

This choice is dictated by the fact that equations (8) and (9) leave unchanged the cases $V=0$ and $\nabla V=\text{const}$, but lead to simple analytical solutions with equal time spacings for the oscillator and smoother behavior for other potentials compared to that of equations (5) and (6).

In what follows we consider equal time spacing $\varepsilon = t_n - t_{n-1}$. This is a useful but inessential simplification for the aims of the present work.

3. THE HARMONIC UNIDIMENSIONAL OSCILLATOR

In order to show some typical distinctive feature of the discrete motion, we consider simple problems whose solutions are periodic, such as the harmonic oscillator.

For a unidimensional harmonic oscillator, $V=\frac{1}{2}kx^2$, equations (5) and (6) become

$$x_{n+1} - 2x_n + x_{n-1} = -\omega^2\varepsilon^2 x_n \tag{10}$$

$$E_n = \tfrac{1}{2}mv_n^2 + \tfrac{1}{4}k(x_n^2 + x_{n-1}^2) = E_{n+1} \tag{11}$$

where, as usual, $\omega^2 = k/m$.

The discrete equation (10) has the solution

$$x_n = A\cos \nu t_n + B\sin \nu t_n \tag{12}$$

where $t_n = n\varepsilon$ and

$$\nu = \frac{1}{\varepsilon}\arcsin\left[\omega\varepsilon\left(1-\frac{\omega^2\varepsilon^2}{4}\right)^{1/2}\right] \tag{13}$$

is the discrete frequency, as one can easily verify by substituting equation (12) into equation (10). The constants A and B depend on the boundary conditions.

For small time intervals ($\varepsilon \to 0$) we have

$$\nu = \omega\left(1+\frac{\omega^2\varepsilon^2}{24}\right) + O(\varepsilon^4) \tag{14}$$

Thus, one sees that this discrete frequency is greater than the continuous frequency ω. As for the energy, one easily sees that, with ν given by (13), the discrete energy E_n as given by (11) is not conserved, namely $E_n \neq E_{n+1}$. The reason is that equation (12) is still the solution of equation (11), but with a frequency ν different from (13). In fact, imposing that $E_n = E_{n+1}$ and substituting (12) into equation (11), we obtain

$$\nu = \frac{1}{\varepsilon}\arcsin\frac{\omega\varepsilon(1+\omega^2\varepsilon^2/4)^{1/2}}{1+\omega^2\varepsilon^2/2} \tag{15}$$

For small time intervals this frequency can be approximated by (we omit in the following terms of order ε^4)

$$\nu \simeq \omega(1 - \tfrac{5}{24}\,\omega^2\varepsilon^2) \tag{16}$$

Thus, the frequency ν of the solution of equation (11) is less than ω, contrary to the frequency of the solution of equation (10).

The numerical results of the motion of this discrete oscillator are compared in Figure 1 with the continuous solution $x = A\cos\omega t + B\sin\omega t$. Circles and crosses represent equation (12) with ν given by (13) and (15), respectively. We have chosen the following numerical values: $A = \omega = 1.57$, $B = 0$, $\varepsilon = 0.25$.

We observe that, with regard to the methods of numerical calculation, equation (10) represents nothing else than the Euler algorithm. Thus, we argue that the Euler algorithm applied to a periodic motion yields a trajectory with a period $\tau = 2\pi/\nu \simeq T(1 - \pi^2\varepsilon^2/6T^2)$ less than the continuous period $T = 2\pi/\omega$.

Equations (10) and (11) are soluble separately, while the system formed by these two has no analytical solutions. These equations descend from equations (5) and (6), that is, from (2). The results are different if instead we use equations (8) and (9), which descend from (7). For the harmonic oscillator, equation (8) becomes

$$x_{n+1} - 2x_n + x_{n-1} = -\frac{\omega^2\varepsilon^2}{4}(x_{n+1} + 2x_n + x_{n-1}) \tag{17}$$

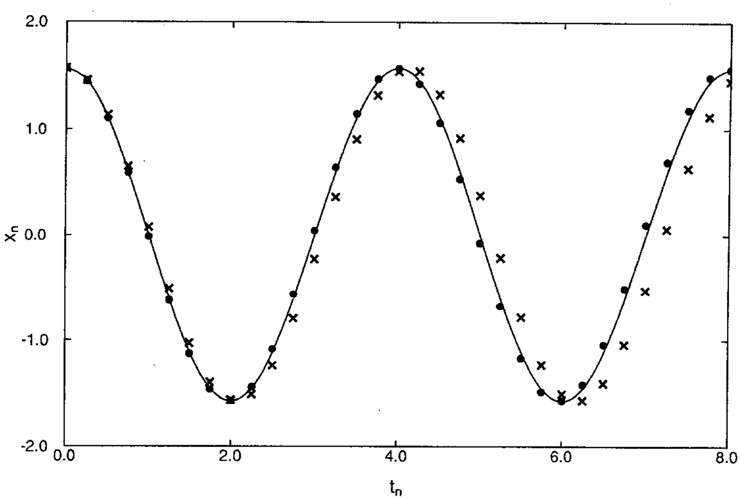

Fig. 1. Discrete coordinates (circles and crosses) for the one-dimensional harmonic oscillator compared with the continuous solution.

Substitution of equation (12) into equation (17) leads to

$$\nu = \frac{1}{\varepsilon} \arcsin \frac{\omega\varepsilon}{1+\omega^2\varepsilon^2/4} \tag{18}$$

i.e., for small time intervals,

$$\nu \simeq \omega(1 - \tfrac{1}{12}\omega^2\varepsilon^2) \tag{19}$$

Again ν is different from ω, but this time the discrete energy (9) is conserved, as one can easily verify by substituting (12) with ν given by (18) into

$$\frac{1}{2} m v_n^2 + \frac{1}{2} k \left(\frac{x_n + x_{n-1}}{2}\right)^2 = \frac{1}{2} m v_{n+1}^2 + \frac{1}{2} k \left(\frac{x_{n+1} + x_n}{2}\right)^2 \tag{20}$$

We observe that in this case, as can be seen from (17), the force at x_n is weighted through the neighboring points x_{n+1} and x_{n-1} with twice the weight for x_n.

Thus, by choosing the action (7), one can see that the discrete harmonic oscillator has discrete solutions given by (12), i.e., analogous to the continuous solutions, but with a frequency ν less than the continuous frequency ω.

4. DISCRETE CIRCULAR ORBITS

We now take up a problem with two degrees of freedom: a particle on a circular orbit. Let $\mathbf{r}$ be the radius vector from some given origin of a particle on a circular orbit and subject to the force

$$\mathbf{F} = -c \frac{\mathbf{r}}{r^3} \tag{21}$$

Since the potential energy is $V(\mathbf{r}) = -c/|\mathbf{r}|$, equation (5) leads to

$$\frac{\mathbf{v}_{n+1} - \mathbf{v}_n}{\varepsilon} = -\frac{c}{m} \frac{\mathbf{r}_n}{r_n^3} \tag{22}$$

while equation (6) leads to

$$\frac{1}{2} m \mathbf{v}_n^2 - \frac{c}{2}\left(\frac{1}{r_n} + \frac{1}{r_{n-1}}\right) = \frac{1}{2} m \mathbf{v}_{n+1}^2 - \frac{c}{2}\left(\frac{1}{r_{n+1}} + \frac{1}{r_n}\right) \tag{23}$$

where $\mathbf{v}_n$ is again given by (1).

Since $r_n = r_{n+1} = R$, the discrete energy (23) is conserved (see Figure 2) and applying the procedures of the previous section, we have that the solution of equations (22) and (23) is

$$\mathbf{r}_n = R(\cos \nu t_n \hat{x} + \sin \nu t_n \hat{y}) \tag{24}$$

where ν is given by (13) with $\omega^2 = c/mR^3$.

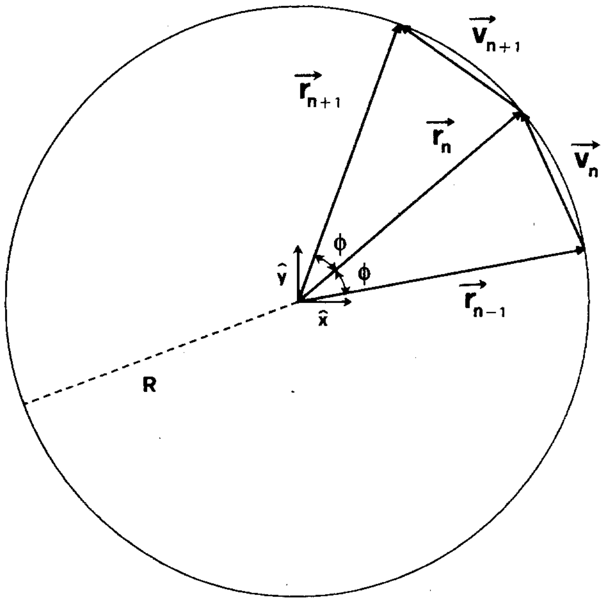

Fig. 2. Discrete circular motion with $\phi = \nu\varepsilon$ and $\varepsilon = 1$. The vectors $\mathbf{r}_n$ are given by (24), apart from an arbitrary phase.

We remark that (24) does not represent the general, discrete solution of (22) and (23), because we have "forced" the particle to be on a circular trajectory. The general solution, with the appropriate boundary conditions, can be obtained only numerically. However, the circular orbit case is interesting since we can derive the frequencies of the solutions of the discrete equations of motion.

Similar results are obtained for equations (8) and (9), which now read

$$\frac{\mathbf{v}_{n+1}-\mathbf{v}_n}{\varepsilon} = -2\frac{c}{m}\left[\frac{\mathbf{r}_n+\mathbf{r}_{n-1}}{|\mathbf{r}_n+\mathbf{r}_{n-1}|^3}+\frac{\mathbf{r}_{n+1}+\mathbf{r}_n}{|\mathbf{r}_{n+1}+\mathbf{r}_n|^3}\right] \tag{25}$$

$$\frac{1}{2}m\mathbf{v}_n^2-\frac{2c}{|\mathbf{r}_n+\mathbf{r}_{n-1}|}=\frac{1}{2}m\mathbf{v}_{n+1}^2-\frac{2c}{|\mathbf{r}_{n+1}+\mathbf{r}_n|} \tag{26}$$

Solutions of (25) and (26) are still given (for circular orbits) by (24), but with ν given approximately by

$$\nu \simeq \omega(1+\tfrac{5}{48}\omega^2\varepsilon^2) \tag{27}$$

This result can be obtained by observing that, with $\omega^2 = c/mR^3$, any component of (25), as for example the x component, becomes (Figure 2)

$$x_{n+1}-2x_n+x_{n-1} = -\frac{\omega^2\varepsilon^2}{4\cos^3(\varphi/2)}(x_{n+1}+2x_n+x_{n-1}) \tag{28}$$

which differs from (17) only in the presence of $\cos^3(\varphi/2)$, $\varphi = \nu\varepsilon$, in the denominator of the right member.

If the solution is given by the x component of (24), equation (28) leads to

$$1 - \cos \nu\varepsilon = \frac{\omega^2 \varepsilon^2}{4 \cos^3(\varphi/2)} (1 + \cos \nu\varepsilon) \tag{29}$$

Taking as first approximation ν given by (18), we have

$$\cos^3 \frac{\varphi}{2} \equiv \cos^3 \frac{\nu\varepsilon}{2} = \left(1 + \frac{\omega^2 \varepsilon^2}{4}\right)^{-3/2} \tag{30}$$

and substituting this value into (29), we obtain (27). Alternatively, we could also look for a frequency $\nu \simeq \omega(1 + \alpha\omega^2\varepsilon^2)$ and substitute this directly into (29) in order to obtain $\alpha = 5/48$.

Let us now consider the two-dimensional analogue of the linear oscillator. Let a mass m be acted on by a force

$$\mathbf{F} = -k_1 x\hat{x} - k_2 y\hat{y} \tag{31}$$

If $k_1 = k_2$, the trajectory can be a circle. It is straightforward to see that, in this case, the discrete equations which descend from (5) and (6) still have the solution (24) with frequency ν given by (13), while the discrete equations which descend from (8) and (9) have the solution (24), but with the frequency ν given by (18). Thus, in both the formulations of discrete mechanics which correspond to the choice (2) or to the choice (7) of the discrete action the two-dimensional harmonic oscillator has solutions with time intervals of constant length.

5. NUMERICAL CALCULATIONS

Discrete mechanics can be used to improve the standard elementary numerical methods. With regard to this point, Stanley (1984) has shown that the more efficient second-order numerical method for resolving differential equations is the *second-order Taylor approximation* (STA)

$$\begin{aligned} x_{n+1} &= x_n + v_n \Delta t + \tfrac{1}{2} a_n \Delta t^2 \\ v_{n+1} &= v_n + \tfrac{1}{2}(a_{n+1} + a_n)\Delta t \end{aligned} \tag{32}$$

which appears particularly convenient when used with a variable step Δt.

The STA method can be improved by using some results of discrete mechanics. As an example, we choose

$$\begin{aligned} v_{n+1} &= v_n + a_n^d \Delta t \\ x_{n+1} &= x_n + \tfrac{1}{2}(v_{n+1} + v_n)\Delta t \end{aligned} \tag{33}$$

where a_n^d is the discrete acceleration, which depends upon the particular model of discrete mechanics chosen.

In a previous paper (Renna, 1987) we have proposed a model of discrete mechanics founded on a correspondence between analytical and discrete Hamilton equations and on the definition of a proper discrete gradient, thus retaining in a natural way symmetries and conservation laws. In particular, the discrete energy coincides with the continuous energy at the discrete physical point of the phase space. If the potential energy of a particle of mass m is $V(\mathbf{r}) = -c/|\mathbf{r}|$, it has been demonstrated that the discrete equations of motion become

$$\frac{\mathbf{r}_{n+1} - \mathbf{r}_n}{\varepsilon} = \frac{\mathbf{v}_{n+1} + \mathbf{v}_n}{2} \tag{34}$$

$$\frac{\mathbf{v}_{n+1} - \mathbf{v}_n}{\varepsilon} = -\frac{c}{m} \frac{\mathbf{r}_{n+1} + \mathbf{r}_n}{r_{n+1} r_n (r_{n+1} + r_n)} \tag{35}$$

These results are in agreement with the model of discrete mechanics of Greenspan (1974). The discrete acceleration which we have used in the subsequent numerical calculations is just taken from (35). The accuracy of the numerical results is tested by comparing them with the analytical solutions of continuous mechanics.

Implicit formulas such as (33) must be initialized using an explicit method, such as, for example, the Euler method, but they can usefully be utilized for minimizing the local error. In fact, an implicit method, although it requires to be resolved recursively in most instances, maintains stability, that is, ensures that errors in the approximate solution do not grow exponentially.

Following Stanley, we have performed numerical calculations of a highly eccentric orbit. We have compared STA with the discrete algorithm (33) and with the same (33) iterated once. In Table I we report the relative errors in y and in the energy E at the minor axis and in the period T, with a fixed time step. Calculations are achieved with $c/m = GM = 1$, for an orbit with eccentricity $e = 0.9933$ and initial conditions $x_0 = -0.002$ and $y_0 = v_{x0} = 0$. In Table II the errors pertinent to the same methods but with a variable time step, proportional to r, are reported.

The results show that the discrete method (33) gives a better accuracy than STA both with a fixed and with a variable step; moreover, they suggest that (33) can be suitably iterated in order to reduce the errors.

By using a variable step $\Delta t \propto r^{3/2}$, we have continued the calculation of the motion for 300 orbits. The last, 300th orbit is shown in Figure 3, where the continuous curve represents the analytical solution of continuous mechanics, while the dashed and dotted curves represent the orbits calculated with STA and with the discrete approximation, respectively. In the inset of Figure 3 enlarged parts of trajectories are shown. We can see that

Table I. Relative Errors for an Orbit Calculation with Fixed Time Step

Δt	$\Delta y/y$ (%)	$\Delta E/E$ (%)	$\Delta T/T$ (%)
4.0×10^{-6}	3.86[a]	7.43	12.29
	0.60[b]	0.36	0.57
	0.42[c]	$<10^{-3}$	$<10^{-3}$
2.0×10^{-6}	0.98[a]	1.86	2.85
	0.13[b]	0.05	0.07
	0.11[c]	$<10^{-4}$	$<10^{-4}$
1.0×10^{-6}	0.24[a]	0.46	0.70
	0.03[b]	$<10^{-2}$	$<10^{-2}$
	0.03[c]	$<10^{-5}$	$<10^{5}$

[a] STA.
[b] Discrete approximation.
[c] Iterated discrete approximation.

Table II. Relative Errors for an Orbit Calculation with Variable Time Step

Iterations per orbit (in thousands)	$\Delta y/y$ (%)	$\Delta E/E$ (%)	$\Delta T/T$ (%)
3.5	0.63[a]	1.25	1.91
	0.20[b]	0.08	0.12
	0.16[c]	$<10^{-4}$	$<10^{-4}$
6.9	0.15[a]	0.31	0.47
	0.04[b]	0.01	0.01
	0.04[c]	$<10^{-6}$	$<10^{-5}$
13.8	0.05[a]	0.09	0.12
	0.01[b]	$<10^{-3}$	$<10^{-3}$
	0.01[c]	$<10^{-7}$	$<10^{-5}$

[a] STA.
[b] Discrete approximation.
[c] Iterated discrete approximation.

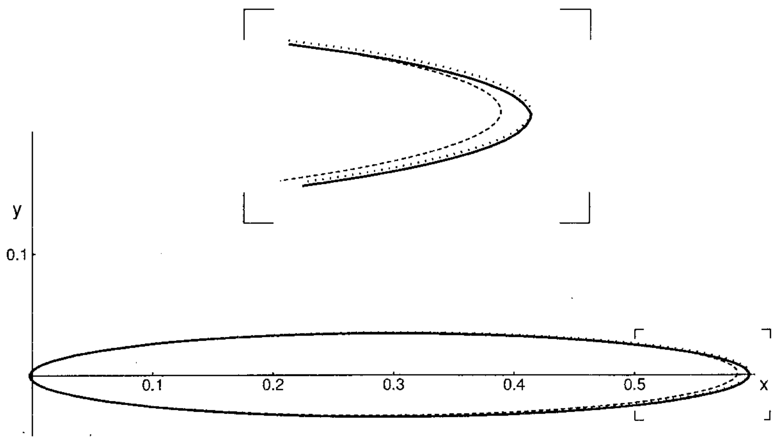

Fig. 3. The calculation of the 300th elliptical orbit of high eccentricity ($e=0.9933$). The theoretical orbit is shown by a solid line. The results of the second-order Taylor approximation are shown as a dashed line, the discrete results as a dotted line.

the discrete formulas permit us to reproduce sufficiently well the exact trajectory. The mean relative errors of this final orbit are $\langle \Delta E/E \rangle = 0.06\%$ and $\langle \Delta y/y \rangle = 2.55\%$. The "retard indicator" $(t_{300} - 300T)/T = -0.59$ shows an advance of more than half a period.

The mean relative errors of the 300th orbit calculated with STA are $\langle \Delta E/E \rangle = 1.54\%$, $\langle \Delta y/y \rangle = 3.77\%$, while one has $(t_{300} - 300T)/T = -4.38$.

The calculations have been performed with about 5300 iterations per orbit for the approximation (33) and with only about 2700 iterations for the STA. The reason, however, is that the errors in STA grow if one increases further the number of iterations.

6. CONCLUSIONS

We have shown, with some useful examples, that in the framework of discrete mechanics it is possible, in a simple way, to bring out indications on the effects of discretization in some interesting problems of classical mechanics. The most evident effect regards the difference between the discrete and the continuous frequencies. The calculated discrete solutions are strictly related to the exact continuous solutions and conserve the discrete energy and total linear and angular momentum. Hence, discrete mechanics can be particularly useful in numerical calculations, as we have shown by analyzing the motion of a particle subject to a gravitational force.

The extension of the numerical equations that we have obtained to more complicated (many-body) systems is straightforward, thus allowing the studies of phenomena of greater complexity.

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