High-Accuracy Numerical Integration of Charged Particle Motion – with Application to Ponderomotive Force

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(Received 30 November 2015 / Accepted 3 January 2016)

A high-accuracy numerical integration algorithm for a charged particle motion is developed. The algorithm is based on the Hamiltonian mechanics and the operator decomposition. The algorithm is made to be time-reversal symmetric, and its order of accuracy can be increased to any order by using a recurrence formula. One of the advantages is that it is an explicit method. An effective way to decompose the time evolution operator is examined; the Poisson tensor is decomposed and non-canonical variables are adopted. The algorithm is extended to a time dependent fields' case by introducing the extended phase space. Numerical tests showing the performance of the algorithm are presented. One is the pure cyclotron motion for a long time period, and the other is a charged particle motion in a rapidly oscillating field.

Keywords: numerical integration, charged particle motion, time reversal symmetry, high accuracy, recurrence formula, time dependent field, ponderomotive force

DOI: 10.1585/pfr.11.1303003

Charged particle motion is an essence of plasma physics. We often need to calculate its orbit very accurately for a long time period, when the plasma is sufficiently collisionless for example. In this letter, we report a new numerical algorithm which enables us to follow a charged particle orbit without accumulating discretizing error.

The algorithm developed here is based on Hamiltonian mechanics, especially an operator decomposition. Also the order of accuracy of the algorithm can be increased to an arbitrary high order by a recurrence formula. These algorithms were developed separately for quantum Monte Carlo simulation [1, 2] and celestial mechanics [3]. As we show below, the straightforward application of the algorithm may not work for a charged particle motion. In this letter, we will extend the algorithm for a charged particle motion, where the Poisson tensor will be decomposed and the non-canonical variables will be used instead of canonical variables as in the previous studies. Some of the related results were already presented in [4]. The same idea was also published in [5], which had been developed independently. We will first review the operator decomposition method and the recurrence formula to increase order of accuracy. Then we will discuss how to decompose the time evolution operator. We will find that a useful algorithm can be developed by decomposing the Poisson tensor rather than the Hamiltonian, although this does not mean the Hamiltonian does not play a role: the Hamiltonian should be expressed in a way that the algorithm is applicable. We will present two numerical tests to show the usefulness and effectiveness of the algorithm.

In the following five paragraphs, the basic idea of the operator decomposition and the recurrence formula of [1–3] is explained briefly. Let us consider a Hamiltonian of the following form: $H[q,p] = H_1[p] + H_2[q]$, where q and p are canonical coordinate and momentum, respectively. For example, a harmonic oscillator has the Hamiltonian of this form $H := \frac{1}{2}(p^2 + q^2)$. Suppose we consider dynamics only by $H_1[q]$. We then obtain evolution equations $\dot{q} = \partial_p H_1[p] = f(p)$ and $\dot{p} = -\partial_q H_1[p] \equiv 0$. Namely, p does not change during this evolution. Note that ∂_p and ∂_q denote partial derivative with respect to p and q, respectively, and the dot $\dot{}$ denotes time derivative. Since p is a constant, we can easily and exactly integrate the evolution equation to obtain $q(t) = f(p)t + q_0$ with q_0 being a constant. Similarly, dynamics only by H_2 gives us the following evolution equations $\dot{q} = \partial_p H_2[q] \equiv 0$ and $\dot{p} = -\partial_q H_2[q] = g(q)$. Therefore, q does not change and we obtain $p(t) = g(q)t + p_0$ with p_0 being a constant.

Next, let us consider a formal solution of the Hamiltonian system. The evolution equation can be rewritten in a symplectic form as $\dot{z} = \mathcal{J}\partial_z H[z]$, with $z := (q,p)^{\mathrm{T}}$ and $\mathcal{J} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ being an anti-symmetric tensor, called a Poisson tensor. If we write $\mathcal{J}\partial_z H[z] =: V_H[z]$, we obtain a formal solution as $z(t) = \mathrm{e}^{tV_H} z(0)$ where $z(0)$ is an initial condition. For the Hamiltonian of the separable form $H[z] = H_1[p] + H_2[q]$, we have $\mathcal{J}\partial_z H[z] =: V_{H_1}[z] + V_{H_2}[z]$, where $V_{H_i}[z] := \mathcal{J}\partial_z H_i[z]$ $(i = 1, 2)$. Therefore the formal solution is $z(t) = \mathrm{e}^{t(V_{H_1}+V_{H_2})} z(0)$.

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Suppose we try to advance time by small Δt. Since the operator V_{H_1} and V_{H_2} do not commute, we recognize that

$$\mathrm{e}^{\Delta t(V_{H_1}+V_{H_2})} = \mathrm{e}^{\Delta t V_{H_1}}\mathrm{e}^{\Delta t V_{H_2}} + O(\Delta t^2). \tag{1}$$

The right-hand side, except for the $O(\Delta t^2)$ term, expresses a sequential operation of $\mathrm{e}^{\Delta t V_{H_2}}$ followed by $\mathrm{e}^{\Delta t V_{H_1}}$. The exponential operator $\mathrm{e}^{\Delta t V_{H_2}}$ gives us time evolution only by H_2, which can be easily and exactly integrated as we observed. Similarly, $\mathrm{e}^{\Delta t V_{H_1}}$ gives us time evolution only by H_1. Therefore, the decomposed exponential operators give us an first-order, explicit algorithm. Let us call this sequential operation of decomposed operators as $G_1(\Delta t)$.

Next, we consider an operator decomposition

$$\mathrm{e}^{\Delta t V_H} = \mathrm{e}^{\frac{\Delta t}{2}V_{H_2}}\mathrm{e}^{\Delta t V_{H_1}}\mathrm{e}^{\frac{\Delta t}{2}V_{H_2}} + O(\Delta t^3). \tag{2}$$

Since the error term scales as $O(\Delta t^3)$, this gives us the second-order algorithm $S_2(\Delta t) := \mathrm{e}^{\frac{\Delta t}{2}V_{H_2}}\mathrm{e}^{\Delta t V_{H_1}}\mathrm{e}^{\frac{\Delta t}{2}V_{H_2}}$. We easily verify that $S_2(-\Delta t)S_2(\Delta t) = S_2(\Delta t)S_2(-\Delta t) = 1$; it is time-reversal symmetric.

Finally, let us introduce a recurrence formula to increase the order of accuracy of the algorithm. It was shown that a higher-order time evolution operator can be constructed by multiplying lower-order ones [1]. Here we adopt a recurrence formula of the form

$$S_{2m}(\Delta t) = S_{2m-2}(p_{m1}\Delta t)\cdots S_{2m-2}(p_{mr}\Delta t), \tag{3}$$

where a lower order operator S_{2m-2} is multiplied r times to generate a higher order one S_{2m}, where $m = 2, 3, \cdots$. Each time step of S_{2m-2} is given by $p_{mj}\Delta t$ with $j = 1, \cdots, r$. We can preserve the time-reversal symmetry for odd numbers r without loss of generality. $r = 3$ gives us rather complex time stepping. If we choose $r = 5$, we may use $p_{mj} = k_m$ for $j = 1, 2, 4, 5$ and $p_{m3} = 1 - 4k_m$ with a real $k_m := \frac{1}{4-4^{\frac{1}{2m-1}}}$. The order of accuracy is not affected by the choice of r, however, the numerical factor of the error term may be different with r. Also the numerical stability may depend on r. We have not investigated these aspects. These are our future issues.

Now, let us consider the charged particle case. The Hamiltonian of a charged particle in an electromagnetic field is given by $H[z] = (\boldsymbol{p} - e\boldsymbol{A}(\boldsymbol{q}))^2/2m + e\phi(\boldsymbol{q})$, where $\boldsymbol{q} = (q^1, q^2, q^3)^{\mathrm{T}}$ and $\boldsymbol{p} = (p_1, p_2, p_3)^{\mathrm{T}}$ are canonical coordinates and momenta, respectively, and $\boldsymbol{z} = (q^1, q^2, q^3, p_1, p_2, p_3)^{\mathrm{T}}$. The mass and the charge are denoted by m and e, respectively, $\boldsymbol{A}$ and ϕ are vector and scalar potentials, respectively. Note that a static electromagnetic field is assumed. This Hamiltonian includes $\boldsymbol{p}\cdot\boldsymbol{A}(\boldsymbol{q})$. Then the resultant evolution equation does not have a form which can be easily and exactly integrated in general. Therefore, we need to devise a method.

One simple way may be to introduce non-canonical variables $\boldsymbol{x}$ and $\boldsymbol{v}$, where $\boldsymbol{x}$ is the same as $\boldsymbol{q}$ and $\boldsymbol{v}$ is the velocity. Then the Hamiltonian can be written in a summation of two terms, where one depends only on $\boldsymbol{v}$ and the other only on $\boldsymbol{x}$. Then we may apply the operator decomposition to obtain a useful algorithm [4]. However, in the present paper, let us re-examine under what conditions we can easily and exactly integrate the evolution equation by the operator decomposition. We need to examine two aspects: one is how to choose appropriate variables, and the other is how to decompose the operator. Suppose we transform $\boldsymbol{z}$ to a set of new variables $\boldsymbol{z}' = \boldsymbol{z}'(\boldsymbol{z})$, and we obtain a resultant evolution equation as $\dot{\boldsymbol{z}}' = \mathcal{J}'\partial_{z'}H'[\boldsymbol{z}']$. The Poisson tensor $\mathcal{J}' = (J'_{\alpha\beta})$ with $\alpha, \beta = 1, \cdots, 6$ is a 6×6, anti-symmetric tensor. For αth component of this evolution equation, the right-hand side is $\sum_{\beta=1}^{6} J'_{\alpha\beta}\partial_{z'_\beta}H'[\boldsymbol{z}']$. If this is a constant, the evolution equation can be integrated easily and exactly. In order to realize it, we firstly decompose $\mathcal{J}'$, not the Hamiltonian as in the previous studies, as $\mathcal{J}' = \sum_{\alpha=1}^{6}\mathcal{J}'_\alpha$, where the αth row of $\mathcal{J}'_\alpha$ is the same as $\mathcal{J}'$ and the other rows are set to be zero. Then the formal solution of the evolution equation becomes $\boldsymbol{z}'(t) = \mathrm{e}^{t\sum_{\alpha=1}^{6}\mathcal{J}'_\alpha\partial_{z'}H'[\boldsymbol{z}']}\boldsymbol{z}'(0)$. Considering a small time step Δt, the first-order approximation to the exponential operator is $\mathrm{e}^{\Delta t\sum_{\alpha=1}^{6}\mathcal{J}'_\alpha\partial_{z'}H'[\boldsymbol{z}']} = \prod_{\alpha=1}^{6}\mathrm{e}^{\Delta t\mathcal{J}'_\alpha\partial_{z'}H'[\boldsymbol{z}']} + O(\Delta t^2)$. For the decomposed $\mathcal{J}'_\alpha$ described above, the time evolution by an exponential operator $\mathrm{e}^{\Delta t\mathcal{J}'_\alpha\partial_{z'}H'[\boldsymbol{z}']}$ does not change variables z'_β with $\beta\neq\alpha$. Therefore, if $\sum_{\beta=1}^{6}J'_{\alpha\beta}\partial_{z'_\beta}H'[\boldsymbol{z}']$ does not depend on z'_α, z'_α can be easily and exactly time advanced by the operator $\mathrm{e}^{\Delta t\mathcal{J}'_\alpha\partial_{z'}H'[\boldsymbol{z}']}$. The sequential operations of $\mathrm{e}^{\Delta t\mathcal{J}'_\alpha\partial_{z'}H'[\boldsymbol{z}']}$ with $\alpha = 1, \cdots, 6$ enables us the easy and exact time integration of z'_α with $\alpha = 1, \cdots, 6$, respectively. Note that this is a sufficient condition for our purpose. We may recognize that the condition cannot be met by using the canonical variables for a charged particle motion.

Now, let us consider what variables we should adopt. A simple choice may be the non-canonical variables $\boldsymbol{x} = (x, y, z)^{\mathrm{T}}$ and $\boldsymbol{v} = (v_x, v_y, v_z)^{\mathrm{T}}$. Then the Hamiltonian is rewritten as $H'[\boldsymbol{z}'] = \frac{m}{2}\boldsymbol{v}^2 + e\phi(\boldsymbol{x})$, and the Poisson tensor $\mathcal{J}$ transforms to

$$\mathcal{J}' := \frac{1}{m}\left(\begin{array}{c|cc} \mathsf{0} & \multicolumn{2}{c}{\mathsf{1}} \\ \hline & 0 & \frac{e}{m}B_z \quad -\frac{e}{m}B_y \\ -\mathsf{1} & -\frac{e}{m}B_z & 0 \quad \frac{e}{m}B_x \\ & \frac{e}{m}B_y & -\frac{e}{m}B_x \quad 0 \end{array}\right),$$

where $\mathsf{0}$ and $\mathsf{1}$ denote 3×3 zero and unit matrices, respectively. We can confirm that $\partial_{z'_\alpha}\left(\sum_{\beta=1}^{6}J'_{\alpha\beta}\partial_{z'_\beta}H[\boldsymbol{z}']\right) = 0$. Therefore, the operator decomposition and the use of the non-canonical variables enables us the easy and exact integration of the evolution equation. The time-reversal symmetric and the higher-order algorithm can be obtained as in the canonical variable case.

As a final part of the theoretical development, we

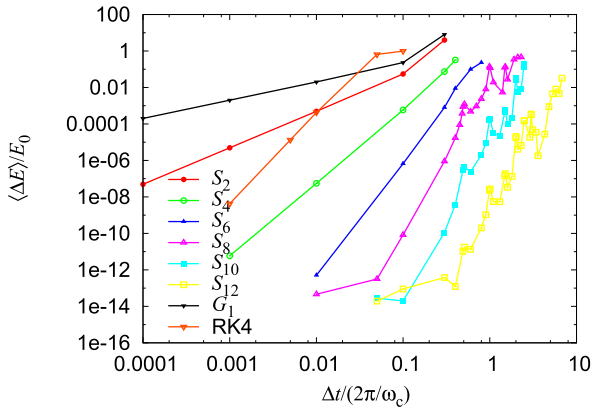

Fig. 1 A measure of relative energy change $\langle \Delta E \rangle / E_0$ during 10^4 cyclotron period is plotted by changing Δt for various algorithms. G_1 is first order and is not time-reversal symmetric. S_{2m} is $2m$th order and is time-reversal symmetric. RK4 denotes 4th-order Runge-Kutta method.

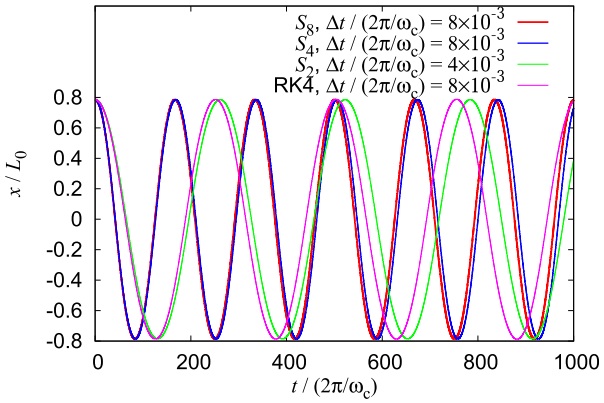

Fig. 2 Time evolution of the particle position $x(t)$ is plotted for several orders of accuracy. RK4 is also shown for a reference. The time step was $\Delta t/(2\pi/\omega_c) = 8 \times 10^{-3}$ except for S_2. We observe that S_4 gives almost same result with S_8 for this calculation. We also observe the deviation of S_2 and RK4 results from S_4 and S_8 results.

extend the formulation to a time-dependent field's case by using an extended phase space [6]. In this case, we adopt $\bar{z}' := (x, y, z, t, v_x, v_y, v_z, -\mathcal{E})^{\mathrm{T}}$ as the non-canonical variables where $\mathcal{E}$ is the energy. The Hamiltonian is $\bar{H}'[\bar{z}'] = \frac{m}{2}\boldsymbol{v}^2 + e\phi(\boldsymbol{x}, t) - \mathcal{E}$. Noting that the time-like variable as τ, we obtain the time evolution equation as $\dot{\bar{z}}' = \bar{\mathcal{J}}'\partial_{\bar{z}'}\bar{H}'[\bar{z}']$. The dot $\dot{}$ denotes τ derivative here. By decomposing the Poisson tensor by each row, we can obtain easy and exact integration algorithm as same as above. Of course, the recurrence formula is applicable to obtain an arbitrary high order algorithm.

Below we will show numerical results. In this paragraph, we present a numerical test for demonstrating the accuracy of the algorithm; A charged particle orbit in a uniform magnetic field was calculated during 10^4 times the cyclotron period. We adopted $r = 5$ for the recurrence formula. The relative change of energy was measured by

$$\frac{\langle \Delta E \rangle}{E_0} := \frac{1}{(t_1 - t_0)E_0} \int_{t_0}^{t_1} |E(t) - E_0| \mathrm{d}t,$$

where t_0 and t_1 are the start and the end of time, E_0 is the initial value of the energy. Figure 1 plots $\langle \Delta E \rangle / E_0$ by changing Δt. G_1 is first-order and is not time-reversal symmetric. S_{2m} is $2m$th-order and is time-reversal symmetric. RK4 denotes 4th-order Runge-Kutta method shown for a reference. The cyclotron frequency is denoted by $\omega_c := |e|B_0/m$, where B_0 is a typical value of the magnetic field. We confirmed that the algorithm developed here showed good scaling property. Note that the relative energy change of S_4 scales as Δt^4 as the theory predicts. The relative energy change scales as Δt^5 for RK4, however, its magnitude is much larger than S_4. An important thing is that the developed algorithm does not accumulate the energy change; it just oscillates in time. On the contrary, RK4 accumulated the energy change. It is not surprising that a good numerical accuracy is obtained even for $\Delta t/(2\pi/\omega_c) > 1$, because S_{2m} is composed of r steps of S_{2m-2} and so on; actual one step is smaller than the cyclotron period. Some spiky behavior is observed especially for higher order algorithms. It seems to happen when Δt is an integer times the cyclotron period. In [4], we examined a trade-off between the accuracy and the computational cost. If we adopt higher-order algorithm, we may need more computational time for one step, although we can take a larger Δt. Thus there should be an optimum order of accuracy for obtaining a result for a given error tolerance. For the same test calculation as Fig. 1, we found S_4 was optimum. S_6 was even better than RK4.

We also examined basic drift motions such as $E \times B$, ∇B and curvature drifts. The drift motion was successfully calculated [7]. The velocities agreed with the theoretical values. This will be reported elsewhere.

In this paragraph, another numerical test is presented. A charged particle motion in a rapidly oscillating electromagnetic field is calculated, by using the formulation in the extended phase space. By averaging the equation of motion in time, we obtain an equation showing that the ponderomotive force acts on the oscillation center of the charged particle. If we write the oscillation center velocity as $\boldsymbol{U}$, the averaged equation of motion is $m\frac{\mathrm{d}\boldsymbol{U}}{\mathrm{d}t} = -e\nabla\Phi_{\mathrm{pond}}$, with $\Phi_{\mathrm{pond}} := \frac{1}{4}\frac{e}{m\omega^2}|\boldsymbol{E}_0|^2$, where ω and $\boldsymbol{E}_0(\boldsymbol{x})$ are the angular frequency and the amplitude of the oscillating electric field, respectively [8]. In our test calculation, we apply an external field with $\boldsymbol{E}(\boldsymbol{x}, t) = \bar{E}\sin kx \cos\omega t\, \hat{\boldsymbol{y}}$ and $\boldsymbol{B}(\boldsymbol{x}, t) = -\frac{k}{\omega}\bar{E}\cos kx \sin\omega t\, \hat{\boldsymbol{z}}$, where $\bar{E}$ is an amplitude of the electric field, k is the wave number, $\hat{\boldsymbol{y}}$ and $\hat{\boldsymbol{z}}$ are the unit vectors in y and z directions, respectively. This is a standing wave, and Φ_{pond} is zero at $kx = n\pi$ with n being an integer and is maximum at $kx = (n + \frac{1}{2})\pi$. Therefore, we expect that a charged particle is confined in the well of Φ_{pond} for an appropriate initial condition.

Figure 2 shows $x(t)$ during 10^5 times the oscillation

period of the electromagnetic field, starting with $x(0)/L_0 = \pi/4$, $y(0) = z(0) = 0$, $\boldsymbol{v}(0) = 0$. Here, L_0 denotes a typical value of length, which coincides with the Larmor radius of a charged particle of its speed being a typical value V_0 in a constant magnetic field with typical value of magnitude. The angular frequency, the wave number and the amplitude of the oscillating field is $\omega/\omega_c = 10^2$, $kL_0 = 1$ and $\bar{E} = 1$, respectively. The time step was chosen as $\Delta t/(2\pi/\omega_c) = 8 \times 10^3$ for S_8, S_4 and RK4. For S_2, $\Delta t/(2\pi/\omega_c) = 4 \times 10^3$ was used because the calculation diverged for $\Delta t/(2\pi/\omega_c) = 8\times10^3$. Here, RK4 means that the evolution equation for $\bar{z}'$ is solved by the 4th-order Runge-Kutta method in this numerical test. As we expected, we observe that the particle oscillates in the potential well of $\Phi_{\rm pond}$. As we observe, S_4 almost overlaps S_8. Note that the result of S_8 did not change by choosing smaller Δt. We also observe that S_2 gives a longer oscillation period in the x direction. The RK4 result is closer to S_2 than S_4. Note that the RK4 result with $\Delta t/(2\pi/\omega_c) = 4 \times 10^3$ almost overlaps with the S_8 and S_4 results. In y direction, the particle oscillates rapidly due to the acceleration by the electric field itself.

Figure 3 shows the phase-space plots for the same data as Fig. 2. Used colors are also the same as Fig. 2. We observe that the amplitudes of v_x for S_2 and RK4 are much smaller than those of S_8 and S_4. The smaller v_x makes the motion in the x direction slower, giving the longer oscillation periods for those algorithms in Fig. 2.

In summary, we have extended the operator decomposition method for a charged particle motion. We have shown that the operator decomposition based on the Poisson tensor is effective, together with the appropriate choice of the variables. Here the non-canonical variables are adopted. The time-reversal symmetry leads to the second-order algorithm, and the recurrence formula leads to the arbitrary high-order algorithm. Note that one of the advantage of this algorithm is that it is explicit. Another advantage is that the algorithm does not accumulate error; the Hamiltonian just oscillates. We also extended the algorithm to the time-dependent field's case by introducing the extended phase space. We have examined the accuracy and effectiveness of the algorithm via two numerical tests. One was to follow pure cyclotron motion for a long time period. We observed the good scaling property of the developed algorithm. The other was to examine ponderomotive

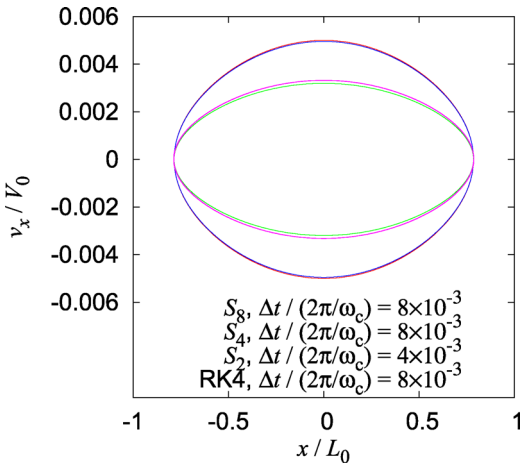

Fig. 3 Phase-space plots are shown for the same data as Fig. 2. Used colors are also the same as Fig. 2. Substantial difference in v_x is observed, that leads to the different oscillation periods in Fig. 2.

force on a charged particle in a rapidly oscillating electromagnetic field. We observed that the particle is trapped in the potential well of the field energy density as the theory predicts. The algorithm presented here can be extended even for a relativistic case. One of the important application may be runaway electrons in tokamaks. This will be reported in near future.

This work was supported by KAKENHI Grant No. 23760805 and No. 15K06647.

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