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

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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

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Suppose we try to advance time by small $\Delta t$. Since the operator $V_{li}$ and $V_{ji}$ do not commute, we recognize that
\[ e^{\Delta V_{li}} e^{\Delta V_{ji}} = e^{\Delta V_{li}} e^{\Delta V_{ji}} + O(\Delta t^2). \] (1)

The right-hand side, except for the $O(\Delta t^2)$ term, expresses a sequential operation of $e^{\Delta V_{li}}$ followed by $e^{\Delta V_{ji}}$. The exponential operator $e^{\Delta V_{li}}$ gives us time evolution only by $H_2$, which can be easily and exactly integrated as we observed. Similarly, $e^{\Delta V_{ji}}$ 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
\[ e^{\Delta V_{li}} = e^{\Delta V_{li}} e^{\Delta V_{i}} e^{\Delta V_{i}} + O(\Delta t^3). \] (2)

Since the error term scales as $O(\Delta t^3)$, this gives us the second-order algorithm $S_2(\Delta t) := e^{\Delta V_{li}} e^{\Delta V_{i}} e^{\Delta V_{i}}$. We easily verify that $S_2(\Delta t) S_2(\Delta t) S_2(-\Delta t) = 1$; 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
\[ S_{2m}(\Delta t) = S_{2m-2}(p_{m1}\Delta t) \cdots S_{2m-2}(p_{m3}\Delta t), \] (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 $k_m := \frac{1}{4+4\pi}$.

The order of accuracy is not affected by the choice of $r$, however, the numerical factor of the error term may be different on $r$. 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 $H[z] = (p - eA(q))^2/2m + e\phi(q)$, where $q = (q^1, q^2, q^3)^T$ and $p = (p_1, p_2, p_3)^T$ are canonical coordinates and momenta, respectively, and $z = (q^1, q^2, q^3, p_1, p_2, p_3)^T$. The mass and the charge are denoted by $m$ and $e$, respectively, $A$ and $\phi$ are vector and scalar potentials, respectively. Note that a static electromagnetic field is assumed. This Hamiltonian includes $p \cdot A(q)$. 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 $x$ and $u$, where $x$ is the same as $q$ and $v$ is the velocity. Then the Hamiltonian can be written in a summation of two terms, where one depends only on $v$ and the other only on $x$. 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 $x$ to a set of new variables $\tilde{x}' = \tilde{x}'(x)$, and we obtain a resultant evolution equation as $\dot{\tilde{x}}' = J' \partial_\tilde{x}' H'[\tilde{x}']$. The Poisson tensor $J' = (J'_{\tilde{a} \tilde{b}})$ with $\alpha, \beta = 1, \cdots, 6$ is a $6 \times 6$, anti-symmetric tensor. For $\alpha$th component of this evolution equation, the right-hand side is $\sum_{\beta=1}^6 J'_{\alpha \beta} \partial_{\tilde{x}}' H'[\tilde{x}']$. If this is a constant, the evolution equation can be integrated easily and exactly. In order to realize it, we firstly decompose $J'$, not the Hamiltonian as in the previous studies, as $J' = \sum_{a=1}^6 J_a$, where the $a$th row of $J_a$ is the same as $J'$ and the other rows are set to be zero. Then the formal solution of the evolution equation becomes $\dot{\tilde{x}}' = \sum_{a=1}^6 J_a \partial_{\tilde{x}}' H'[\tilde{x}'](0)$. Considering a small time step $\Delta t$, the first-order approximation to the exponential operator is $e^{\Delta t \sum_{a=1}^6 J_a \partial_{\tilde{x}}' H'[\tilde{x}'](0)} = \sum_{a=1}^6 \prod_{\beta=1}^6 e^{\Delta t J_{\alpha \beta} \partial_{\tilde{x}}' H'[\tilde{x}'](0)} + O(\Delta t^2)$. For the decomposed $J_a$ described above, the time evolution by an exponential operator $e^{\Delta t J_a \partial_{\tilde{x}}' H'[\tilde{x}'](0)}$ does not change variables $\tilde{x}'_a$ with $\beta \neq \alpha$. Therefore, if $\sum_{\beta=1}^6 J_{\alpha \beta} \partial_{\tilde{x}}' H'[\tilde{x}'](0)$ does not depend on $\tilde{x}'_a$, $\tilde{x}'_a$ can be easily and exactly time advanced by the operator $e^{\Delta t J_a \partial_{\tilde{x}}' H'[\tilde{x}'](0)}$. The sequential operations of $e^{\Delta t J_a \partial_{\tilde{x}}' H'[\tilde{x}'](0)}$ with $\alpha = 1, \cdots, 6$ enables us the easy and exact time integration of $\tilde{x}'_a$ 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 $x = (x^1, y, z)^T$ and $v = (v_x, v_y, v_z)^T$. Then the Hamiltonian is rewritten as $H'[\tilde{x}'] = -\frac{m}{2} \dot{v}^2 + e\phi(x)$, and the Poisson tensor $J'$ transforms to
\[ J' := \frac{1}{m} \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & mB_z \\ 1 & mB_z & 0 \end{pmatrix}. \]

where 0 and 1 denote $3 \times 3$ zero and unit matrices, respectively. We can confirm that $\partial_{\tilde{x}}' \sum_{\beta=1}^6 J'_{a \beta} \partial_{\tilde{x}}' H'[\tilde{x}'] = 0$. 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
extend the formulation to a time-dependent field's case by using an extended phase space [6]. In this case, we adopt \( \mathbf{r}' := (x, y, z, t, v_x, v_y, v_z, -E) \) as the non-canonical variables where \( E \) is the energy. The Hamiltonian is 
\[
\mathcal{H}^r[\mathbf{r}'] = \frac{1}{2} \mathbf{p}^2 + \mathcal{V}(\mathbf{r}, t) - E.
\]
Noting that the time-like variable as \( \tau \), we obtain the time evolution equation as \( \mathbf{r}' = \frac{\partial}{\partial \tau} \mathcal{H}^r[\mathbf{r}'] \). The dot \( ' \) denotes \( \tau \) 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
\[
\frac{\langle \Delta E \rangle}{E_0} := \frac{1}{(t_1 - t_0)E_0} \int_{t_0}^{t_1} |E(t) - E_0| dt,
\]
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 \( \Delta t \). \( S_{2m} \) is first-order and is not time-reversal symmetric. \( S_{2m} \) is 2nth-order and is time-reversal symmetric. RK4 denotes 4th-order Runge-Kutta method shown for a reference. The cyclotron frequency is denoted by \( \omega_c \). RK4 denotes 4th-order Runge-Kutta method.

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 \( \Delta t \) 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 \( \Delta t \). 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 \( E \times B \), \( \nabla B \) 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 \( U \), the averaged equation of motion is
\[
\frac{dU}{dt} = -e \nabla \Phi_{\text{pond}}, \quad \Phi_{\text{pond}} := \frac{1}{2} \frac{m}{r_{\text{mag}}^2} |E|^2,
\]
where \( \omega \) and \( r_{\text{mag}}(x) \) are the angular frequency and the amplitude of the oscillating electric field, respectively [8]. In our test calculation, we apply an external field with \( E(x, t) = \hat{E} \sin k x \cos \omega t \hat{y} \) and \( B(x, t) = -\frac{1}{c} \hat{E} \cos k x \sin \omega t \hat{z} \), where \( \hat{E} \) is an amplitude of the electric field, \( k \) is the wave number, \( \hat{y} \) and \( \hat{z} \) are the unit vectors in \( y \) and \( z \) directions, respectively. This is a standing wave, and \( \Phi_{\text{pond}} \) is zero at \( k x = n \pi \) with \( n \) being an integer and is maximum at \( k x = (n + \frac{1}{2})\pi \). Therefore, we expect that a charged particle is confined in the well of \( \Phi_{\text{pond}} \) for an appropriate initial condition.

Figure 2 shows the oscillation.
period of the electromagnetic field, starting with \( x(0)/L_0 = \pi/4 \), \( y(0) = z(0) = 0 \), \( u(0) = 0 \). 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 \( \Delta t/(2\pi/\omega_c) = 8 \times 10^3 \). 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 \( \Phi_{\text{pond}} \). As we observe, \( S_4 \) almost overlaps \( S_8 \). Note that the result of \( S_8 \) did not change by choosing smaller \( \Delta t \). 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 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.

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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.