Covariant Hamiltonian approach for time-dependent potentials applied to a pill-box cavity

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The typical treatment of time-dependent potentials, such as those used for radio frequency cavities, is to average a potential's time component through the interval that a reference particle spends in the cavity. Such an approach, using the so-called transit-time factor, uses time as the independent variable in the Hamiltonian. In this paper, we instead propose a fully covariant Hamiltonian to treat a potential's time component like any other space component. We show how to calculate the dynamics of particles in a pill-box cavity using an explicit symplectic integrator. Finally, we compare the results with the simulator TraceWin.

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I. INTRODUCTION

When a charged particle passes through an accelerator element which generates a time-dependent field, the resulting Hamiltonian is no longer a constant of motion. This requires special techniques to handle the time component, such as the transit-time factor (TTF) for rf cavities, where the time component is averaged and removed from the Hamiltonian.

This time dependence can also be eliminated by using a covariant Hamiltonian. This implies tracking in eight-dimensional phase space, where together with the usual six-dimensions $(x, P_x; y, P_y; z, P_z)$ we include time and its canonical conjugate (t, P_t) . In this case, the Hamiltonian $H = H(x, y, z, t, P_x, P_y, P_z, P_t)$ is always a constant of motion and will satisfy four pairs of Hamilton's equations

$$\frac{dx^\mu}{d\tau} = \frac{\partial H}{\partial P^\mu} \quad (1)$$

$$\frac{dP^\mu}{d\tau} = -\frac{\partial H}{\partial x^\mu} \quad (2)$$

where τ is the “proper” time of the particle (time in a reference frame comoving with the particle); $x^\mu = ct, x, y, z$ where $\mu = 0, 1, 2, 3$; and P^μ , defined rigorously in the next section, are the corresponding momenta.

The solutions to these Hamilton's equations can be obtained in many ways, the technique used to solve them depends on the form of the potential. Expanding on

preliminary studies [1], the potential considered in the example of this paper is that of a simple pill-box cavity. Such a potential can be split as shown in [2]; we will adopt this technique to construct an explicit symplectic integrator.

The results obtained with this method will be compared with the standard simulator used at the European Spallation Source, TraceWin [3].

II. HAMILTONIAN

The Lorentz invariant

$$ds^2 = -c^2 dt^2 + dx^2 + dy^2 + dz^2 = -c^2 d\tau^2 \quad (3)$$

leads to the Lagrangian

$$L = \frac{m}{2} v_\mu v^\mu \quad (4)$$

where

$$v^\mu = \left(c \frac{dt}{d\tau}, \frac{dx}{d\tau}, \frac{dy}{d\tau}, \frac{dz}{d\tau} \right) \quad (5)$$

$$v_\mu = \left(-c \frac{dt}{d\tau}, \frac{dx}{d\tau}, \frac{dy}{d\tau}, \frac{dz}{d\tau} \right). \quad (6)$$

With an external electromagnetic four-potential $A^\mu = (\frac{\phi}{c}, A_x, A_y, A_z)$ the Lagrangian is [4]

$$L = \frac{m}{2} v_\mu v^\mu + e v^\mu A_\mu \quad (7)$$

where e is the particle's electric charge. The corresponding Hamiltonian is calculated with the Legendre transform as

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$$P_\mu = \frac{\partial L}{\partial v^\mu} \quad (8)$$

$$H = P_\mu v^\mu - L. \quad (9)$$

This Hamiltonian generates eight equations of motion with the constraint $v_\mu v^\mu = -c^2$ so not all the variables are independent.

III. THE PILL-BOX CAVITY

The case presented here is the rudimentary pill-box cavity with the simplest accelerating mode (TM₀₁). The electric and magnetic fields, expressed in cylindrical coordinates plus time (t, r, θ, z) are [5]

$$E_z = E_0 J_0 \left(\frac{b_{01}}{a} r \right) \sin(\omega t + \phi_0) \quad (10)$$

$$B_\theta = \frac{E_0}{c} J_1 \left(\frac{b_{01}}{a} r \right) \cos(\omega t + \phi_0) \quad (11)$$

$$E_r = E_\theta = B_r = B_z = 0. \quad (12)$$

J_0 and J_1 are the Bessel functions of kind 0 and 1; b_{01} is the first zero of J_0 , that is, $J_0(b_{01}) = 0$; a is the radius of the pill box cavity (this leaves the electric field as zero when $r = a$); $\omega/2\pi$ is the oscillation frequency of the field, which is fixed by the cavity aperture through the relationship $\omega = (cb_{01})/a$; and ϕ_0 is the phase that the particle encounters at the cavity entrance.

These fields can be expressed as a potential:

$$A_r = A_\theta = 0 \quad (13)$$

$$A_z = \frac{E_0}{\omega} J_0 \left(\frac{b_{01}}{a} r \right) \cos(\omega t + \phi_0). \quad (14)$$

Since the potential is only in the z direction, we do not need to transform the Lagrangian in cylindrical coordinates. We can instead continue in Cartesian coordinates, recalling that $r = \sqrt{x^2 + y^2}$. The Lagrangian is

$$L = \frac{m}{2} (v_0 v^0 + v_1 v^1 + v_2 v^2 + v_3 v^3) + e v^3 A_3. \quad (15)$$

The conjugate momenta are then

$$\begin{aligned} P_0 &= \frac{\partial L}{\partial v^0} = m v_0 \\ P_1 &= \frac{\partial L}{\partial v^1} = m v_1 \\ P_2 &= \frac{\partial L}{\partial v^2} = m v_2 \\ P_3 &= \frac{\partial L}{\partial v^3} = m v_3 + e A_3 \end{aligned} \quad (16)$$

so we can rewrite the 4-velocity as

$$v^\mu = \left(\frac{P^0}{m}, \frac{P^1}{m}, \frac{P^2}{m}, \frac{P^3 - e A^3}{m} \right). \quad (17)$$

The Hamiltonian is

$$\begin{aligned} H &= \frac{P_0 P^0}{m} + \frac{P_1 P^1}{m} + \frac{P_2 P^2}{m} + \frac{P_3 (P^3 - e A^3)}{m} - L \\ &= \frac{P_0 P^0}{2m} + \frac{P_1 P^1}{2m} + \frac{P_2 P^2}{2m} + \frac{(P_3 - e A_3)(P^3 - e A^3)}{2m} \end{aligned} \quad (18)$$

or explicitly

$$H = -\frac{P_t^2}{2m} + \frac{P_x^2}{2m} + \frac{P_y^2}{2m} + \frac{(P_z - e A_z)^2}{2m}. \quad (19)$$

The Hamiltonian (19) can be treated with the explicit symplectic integrator first developed in [2] and discussed in [6] Chap. 12 Sec. 9.

IV. THE ALGORITHM

The only problematic term in the Hamiltonian (19) is the one dependent on z because it mixes the momentum P_z with the position contained in A_z . The idea of our integrator is to create a new function $U_z(t, x, y, z)$ such that $A_z = \frac{\partial U_z}{\partial z}$. In our case

$$U_z = \frac{E_0}{\omega} J_0 \left(\frac{b_{01}}{a} r \right) \cos(\omega t + \phi_0) z. \quad (20)$$

The Lie transform of U_z has the property:

$$e^{-\epsilon: U_z}: z = z \quad (21)$$

$$e^{-\epsilon: U_z}: P_z = P_z - e \frac{\partial U_z}{\partial z} \quad (22)$$

and as a consequence, we have

$$e^{-\epsilon: U_z}: e^{-\frac{\hbar}{2} \frac{P_z^2}{2m}}: e^{\epsilon: U_z}: = e^{-\frac{\hbar}{2} \frac{(P_z - e A_z)^2}{2m}}: \quad (23)$$

This splitting technique is similar to the usual drift-kick-drift, but here the term U_z can be seen as a gauge transformation instead of a kick. Calling $K_t = \frac{P_t^2}{2m}$ and $K_i = \frac{P_i^2}{2m}$ with $i = x, y, z$ we define the second order explicit symplectic integrator as

$$\begin{aligned}
S_2 = & e^{-\frac{h}{2}K_x} e^{-\frac{h}{2}K_y} e^{-\epsilon U_z} e^{-\frac{h}{2}K_z} e^{\epsilon U_z} \\
& \times e^{-hK_t} \\
& \times e^{-\epsilon U_z} e^{-\frac{h}{2}K_z} e^{\epsilon U_z} e^{-\frac{h}{2}K_y} e^{-\frac{h}{2}K_x}, \quad (24)
\end{aligned}$$

This integrator can be extended to higher order integrators applying the techniques of Yoshida [7] or Suzuki [8]. Both approaches are explored in detail in [9].

Every step of the integrator has to be evaluated for each coordinate and momentum component. The only terms differing from the identity map are:

$$\begin{aligned}
e^{-\frac{h}{2}K_x} i &= i + \frac{h}{2m} P_i \quad \text{for } i = x, y, z \\
e^{-hK_t} ct &= ct - \frac{h}{m} P_t \\
e^{\epsilon U_z} P_x &= P_x - \frac{\epsilon x z E_0 b_{01}}{a \omega} J_1\left(\frac{b_{01}}{a} r\right) \cos(\omega t + \phi_0) \\
e^{\epsilon U_z} P_y &= P_y - \frac{\epsilon y z E_0 b_{01}}{a \omega} J_1\left(\frac{b_{01}}{a} r\right) \cos(\omega t + \phi_0) \\
e^{\epsilon U_z} P_z &= P_z + \frac{\epsilon E_0}{\omega} J_0\left(\frac{b_{01}}{a} r\right) \cos(\omega t + \phi_0) \\
e^{\epsilon U_z} P_t &= P_t - \epsilon z E_0 J_0\left(\frac{b_{01}}{a} r\right) \sin(\omega t + \phi_0). \quad (25)
\end{aligned}$$

V. NUMERICAL RESULTS

We compared the results of this symplectic integrator with the well-established code TraceWin [3]. In particular, we benchmarked against a drift-gap-drift model, where we used TraceWin's "bunched cavity or thin gap" element for the gap. We also compared with a fieldmap model, but its divergence from the thin gap was negligible.

In order to compare the results of this symplectic integrator with TraceWin, we need results in the same reference frame. The first step is thus to find the transformation from the covariant Hamiltonian to a Hamiltonian in the laboratory frame which uses t as the independent variable. This can be done using Eq. (3) noting that $\frac{dt}{d\tau} = \gamma$. From the definition of the momenta Eq. (8) we have for the general Hamiltonian

$$P^0 = mv^0 + \epsilon A^0 = mc \frac{dt}{d\tau} + \epsilon \frac{\phi}{c} \quad (26)$$

$$P^i = mv^i + \epsilon A^i = m \frac{dx^i}{d\tau} + \epsilon A^i; \quad (i = 1, 2, 3) \quad (27)$$

and this is

$$cP^0 = \gamma mc^2 + \epsilon \phi \quad (28)$$

$$c^2(\vec{P} - \epsilon \vec{A})^2 = \gamma^2 m^2 c^2 v^2 \quad (29)$$

where the vector notation refers to the three spatial coordinates. Using the identity $v^2 = (1 - \frac{1}{\gamma^2})$, we can connect the spatial component with the time component

$$cP^0 = c\sqrt{(\vec{P} - \epsilon \vec{A})^2 + m^2 c^2} + \epsilon \phi \quad (30)$$

which is the desired time-independent Hamiltonian [4] if we identify cP^0 as the Hamiltonian.

From this Hamiltonian we can apply the transformations used in [5]. The first transformation normalizes the left and right sides of Eq. (30) by the reference momentum $P_r = \beta \gamma mc$. This momentum is well established for a time-independent Hamiltonian, but it is not uniquely defined throughout the motion of a time-dependent Hamiltonian because β and γ do not remain constant. Thus, for every instance in which we compare a step of the covariant Hamiltonian algorithm with TraceWin, we need to normalize the result to the reference momentum (of that step) calculated from the total energy cP^0 .

It is worth stressing here that the algorithm used for the integration of the covariant Hamiltonian is the one in Eqs. (24) and (25) where no normalization is applied, and only the final result (or an intermediate result as with energy plot in Fig. 1) is normalized for comparison with TraceWin. To introduce a normalization on each step may be useful for keeping the numerical quantities small in the execution of the algorithm, but it introduces an additional dependence of each step on energy, which does not come from the Hamiltonian itself and violates the symplectic nature of the Lie transform. This is why we use the normalization only on the final result for comparison purposes.

The last input we need for our simulator is the step size h . At the entrance of the cavity we have γ_i which can be calculated from the initial kinetic energy as $\gamma_i = \frac{E_{ki}}{mc^2} + 1$ while the speed in the laboratory frame is $\sqrt{1 - \frac{1}{\gamma_i^2}} c = \beta_i c$.

FIG. 1. Energy of a particle on the z-axis with an initial kinetic energy of 100 MeV. Comparison between the covariant Hamiltonian algorithm and the step function in a typical TTF algorithm (such as the one used in Tracewin).

FIG. 2. Comparison of phase space on three axes starting from the same initial distribution for Tracewin and our covariant Hamiltonian algorithm.

Without acceleration, the time to traverse the first length step dL of the pill-box cavity having a total length L is $dL = \beta_i c dt$ and we can again use the transformation $\frac{dt}{d\tau} = \gamma$ leaving

$$dL = \beta_i \gamma_i c d\tau. \quad (31)$$

We can thus divide the length L into segments and calculate the proper h in Eqs. (25) to evaluate the integrator. The β_i and γ_i must be recalculated at each step.

This manner of selecting h may seem to introduce a dependence on the energy that can break the symplectic nature of the algorithm because it does originate from the Hamiltonian. This is not true for the integrator used here because the step length is precalculated and used as a constant for each step of pure drifts (the only part of Eqs. (25) where h appears) and we know that the Lie transform always generates a canonical (and so symplectic) map, regardless the size of the integration step.

The symplecticity is preserved by this procedure, which keeps the momentum fixed along the drift sections,

but another issue is more subtle. The separation methods for symplectic integration, including the one used in this paper, minimize the error compared to the full Hamiltonian when the choice of the coefficients cancels the high-order terms of the Zassenhaus formula (which provides the expansion of the exponential of the Lie operator, see [5] p. 314). For our algorithm, this cancellation occurs when h is unchanged from the first to the last drift of the S_2 integrator.

However, in our case we want to change the value of h every time we pass through a kick given by the U_z potential. This procedure may break the symmetry of the S_2 integrator, which is no longer of second order, and introduces some error. To avoid this problem, one can use the same value for h along one full step of integrating S_2 , and then only recalculate h between integration steps.

The test case we use for comparison with `TraceWin` is a bunch consisting of 10^5 protons uniformly distributed around a kinetic energy of 100 MeV and passing through a pill-box cavity with a frequency of 200 MHz and a length of 1 m. The phase space for the three spatial dimensions x , y , z at the entrance and at the exit of the cavity is shown in Fig. 2, where z is colinear with the beamline. The comparison shows a strong matching, but this is not a surprise because such a cavity is primarily a drift space for our beam.

The interesting part here is in the behavior of the energy. The parameters selected for this numerical test are such that the cavity is working quite far from any ideal acceleration conditions. In fact, a proton of 100 MeV has a relativistic $\beta = 0.428$ and will take 7.79 ns to pass through the 1 m of length of the cavity. A cavity oscillating at 200 MHz will do 1.5 full oscillations in 7.79 ns. This oscillation becomes traceable (Fig. 1) in the energy gain of the covariant Hamiltonian algorithm if we track a reference particle with initial conditions set to zero for each coordinate and momenta component and with a kinetic energy of 100 MeV.

The TTF of such a field is 0.197, that is, the acceleration is only 20% of the peak field. In `TraceWin`, the incurs a total energy increase of 0.2 MeV, because its GAP element uses the TTF to calculate energy gain. In the simulator constructed

with the covariant Hamiltonian, we will have the same increase in energy at the end, but we can track the energy along the length of the cavity for each integration step.

VI. CONCLUSIONS

We presented an algorithm for performing symplectic integration of a Hamiltonian with a time-dependent external potential. The main concept is to use the full covariant Hamiltonian and to integrate the field in eight-dimensional phase space, applying a Lie-operator method to the field component as was done for s-dependent fields in [2]. A comparison with `TraceWin`, a well-established particle simulator, shows that the method reproduces the correct dynamics for the simple case of a pill-box cavity. More complicated potentials are feasible if they respect the separability of Eq. (23).

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