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Classical Molecular Dynamics Simulation with the Velocity Verlet Algorithm at Strong External Magnetic Fields

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We present a new method for incorporating arbitrarily strong static homogeneous external magnetic fields into molecular dynamics computer simulations. Conventional techniques dealing with magnetic fields demand the simulation time step Δt to be small compared to the Larmor oscillation time $2\pi/\Omega$. In our method, in contrast, the magnetic field is built into the propagation equations in such a way as to make the choice of Δt entirely independent of $2\pi/\Omega$. Thus, the time step is determined only by the internal physical properties of the system under consideration. This property of our method is essential for simulating strongly magnetized systems of charged particles in an efficient way. The method is developed in the framework of the second-order Velocity Verlet propagation scheme. However, the underlying concept is independent of this choice, and a generalization to arbitrary order without any reference to a specific propagation scheme is also given.

1. INTRODUCTION

At its very heart, classical (i.e., non-quantum-mechanical and nonrelativistic) molecular dynamics (MD) is the problem of numerically solving Newton's equations of motion for a system of many particles interacting with each other, possibly under the influence of external fields.

Here we consider systems of charged particles exposed to a static (i.e., time-independent) homogeneous external magnetic field. Implementing an external magnetic field into a MD simulation is not difficult a priori, but since MD follows the trajectory of each individual simulation particle, the time step Δt of the simulation has to be chosen small enough to have a sufficient number of steps per Larmor oscillation in order to follow the spiralling motion of the particles correctly: A particle of specific charge q/m performs Larmor oscillations of

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frequency $\Omega = qB/m$ when influenced by a magnetic field B. The condition for the choice of Δt in a straightforward implementation is therefore

$$\Omega \Delta t \overset{!}{\ll} 2\pi. \tag{1}$$

When the magnetic field is weak, i.e., when the time scale τ_{int} defined by the interactions within the system itself is small compared to $2\pi/\Omega$, the choice of Δt is dominated by τ_{int}, and (1) is automatically fulfilled: $\Delta t \overset{!}{\ll} \tau_{\text{int}} \ll 2\pi/\Omega$. At strong magnetic field, however, where $2\pi/\Omega \ll \tau_{\text{int}}$, the MD simulation would have to perform a huge number of very small time steps to cover time intervals of the order of τ_{int} while obeying (1), and it would thus be numerically very expensive to simulate the internal evolution of the system under the influence of a strong magnetic field.

The aim of this paper is to present a numerical algorithm which allows one to simulate systems of charged particles under the influence of strong static external magnetic fields without having to fulfill condition (1); i.e., there may be an arbitrary number of Larmor oscillations per time step, yet still the particle trajectory is sampled correctly to within the order of the propagation scheme. Consequently, the time step is limited only by the bold internal physical restriction $\Delta t \overset{!}{\ll} \tau_{\text{int}}$, independently of the size of the external $2\pi/\Omega$ time scale.

Hence, in the context of this paper, a magnetic field shall be called "strong" if it is desirable for reasons of numerical efficiency to use an algorithm which is not restricted to condition (1).

Owing to the widespread use of the Velocity Verlet (VV) propagation scheme in MD codes, we will develop this algorithm within the VV framework, but the concept is more general and independent of the actual propagation scheme.

This paper is organized as follows:

- First, we briefly outline the basic concepts of the VV (Section 2).
- In Section 3 we show that the VV has to be modified to allow for magnetic fields, and we present three different ways of doing so.
- A numerical example (Section 4) serves to compare these modifications.
- We finally show (Section 5) how the algorithm presented here can be incorporated into propagation schemes of arbitrary order.

2. THE VELOCITY VERLET ALGORITHM

Let N be the number of particles in the system. The positions, velocities, and accelerations of the particles at time t are given by the three-dimensional vectors $\mathbf{r}_i(t)$, $\mathbf{v}_i(t)$, and $\mathbf{a}_i(t)$, respectively. The particle index i ($i = 1, 2, \ldots, N$) will be omitted in formulae which apply to all particles independently. The components of the vectors are referred to by subscripts x, y, and z.

Since $\mathbf{v} = d\mathbf{r}/dt$ and $\mathbf{a} = d\mathbf{v}/dt$, we can write Newton's equations as a system of $6N$ first-order ordinary differential equations,

$$\dot{\mathbf{r}}_i \equiv \frac{d}{dt}\mathbf{r}_i = \mathbf{v}_i \tag{2}$$

$$\dot{\mathbf{v}}_i \equiv \frac{d}{dt}\mathbf{v}_i = \mathbf{a}_i = \frac{\mathbf{F}_i}{m_i}, \tag{3}$$

where m_i is the mass of particle i, and $\mathbf{F}_i$ is the force acting on particle i. In the most general case, $\mathbf{a}_i$ can be a function of all particle positions and velocities, and it may be explicitly time-dependent.

Among the variety of numerical algorithms for solving systems of first-order ordinary differential equations [1–5], the VV scheme [5, p. 81] is one of the most popular for MD simulations. In the notation of this paper it can be written as

$$\mathbf{r}(t+\Delta t) = \mathbf{r}(t) + \Delta t\mathbf{v}(t) + \tfrac{1}{2}(\Delta t)^2\mathbf{a}(t) + O((\Delta t)^3) \tag{4}$$

$$\mathbf{a}(t+\Delta t) = \mathbf{a}(\mathbf{r}_1(t+\Delta t), \ldots, \mathbf{r}_N(t+\Delta t); \mathbf{v}_1(t+\Delta t), \ldots, \mathbf{v}_N(t+\Delta t); t+\Delta t) \tag{5}$$

$$\mathbf{v}(t+\Delta t) = \mathbf{v}(t) + \tfrac{1}{2}\Delta t[\mathbf{a}(t) + \mathbf{a}(t+\Delta t)] + O((\Delta t)^3). \tag{6}$$

At first glance, this seems to be an implicit scheme, as references to $t+\Delta t$ appear on both sides of Eq. (6). However, in many simple MD problems without external magnetic fields, the particle accelerations do not depend on the particle velocities, allowing (5) to be replaced by

$$\mathbf{a}(t+\Delta t) = \mathbf{a}(\mathbf{r}_1(t+\Delta t), \ldots, \mathbf{r}_N(t+\Delta t);\ t+\Delta t). \tag{7}$$

The order of evaluation of Eqs. (4), (6), and (7) is now crucial: At time t, we can calculate $\mathbf{r}(t+\Delta t)$ through Eq. (4), then $\mathbf{a}(t+\Delta t)$ using (7), and finally $\mathbf{v}(t+\Delta t)$ via (6). The implicit character of Eq. (6) thus disappears when the special structure (7) applies for the acceleration. In this case, the VV

- is explicit, i.e., without reference into the future: The system at time $t+\Delta t$ can be calculated directly from quantities known at time t.
- is self-starting, i.e., without reference into the far past: The system at time Δt can be calculated directly knowing only the system at time $t=0$.
- allows Δt to be chosen differently for each time step. This can be very useful when the accelerations vary strongly over time, as is often the case in the simulation of Coulomb systems. For details on how to choose Δt adaptively, cf. [2, p. 714].
- is a second-order integration scheme; i.e., the error term is $O((\Delta t)^3)$.
- is time reversal invariant and symplectic [6–8].
- requires only one evaluation of the accelerations per time step.

Since calculating the accelerations is usually the most time-consuming part of a MD simulation code, its combination of advantageous features makes the VV the algorithm of choice for a wide range of MD applications.

3. VELOCITY VERLET AND MAGNETIC FIELD

In the presence of a magnetic field acting on charged particles, the accelerations explicitly depend on the velocities. Consequently, (7) no longer holds, and the VV is reduced to the implicit scheme (4)–(6). However, in the case of a static homogeneous external magnetic field acting on a system which would fulfill (7) if the external field were absent, the VV can be modified to restore the explicit character.

With a homogeneous magnetic field $\mathbf{B} = (0, 0, B)$ pointing in the z direction, the acceleration on each particle is

$$\mathbf{a}(t) = \mathbf{a}^{\mathrm{C}}(t) - \Omega\mathbf{e}_z \times \mathbf{v}(t), \tag{8}$$

where $\mathbf{a}^{\mathrm{C}}$ is the part of the acceleration which does not depend on the velocities,

$$\mathbf{a}^{\mathrm{C}}(t) = \mathbf{a}^{\mathrm{C}}(\mathbf{r}_1(t), \ldots, \mathbf{r}_N(t); t), \tag{9}$$

$\Omega = qB/m$ is the Larmor frequency, and $\mathbf{e}_z = (0, 0, 1)$ is the unit vector in the z direction. To simplify notation, we will assume a system where all the particles have the same charge-to-mass ratio q/m. The argumentation can easily be extended to individual values $\Omega_i = q_i B/m_i$ per particle.

An important example for $\mathbf{a}^{\mathrm{C}}$ is $\mathbf{a}^{\mathrm{C}} = q\mathbf{E}/m$, where $\mathbf{E}$ is the electric field acting on the particle due to the pairwise Coulomb interactions within the N-particle system.

In the following subsections of this section, we present three different approaches to putting a magnetic field into the VV, which we shall call "inversion of $\mathbf{e}_z \times \mathbf{v}$," "Taylor expansion," and "velocity transformation."

We will find that inversion is valid only for weak magnetic fields, whereas the other two, by their very construction, apply for arbitrary magnetic field strengths. Second, Taylor expansion is equivalent to velocity transformation to within terms of order $O((\Delta t)^3)$. Finally, we will show that in the weak field limit all three approaches are consistent with each other.

3.1. Inversion of $\mathbf{e}_z \times \mathbf{v}$

Using the structure (8) of the acceleration with magnetic field, we can write the VV system (4)–(6) in a different way:

$$\mathbf{r}(t + \Delta t) = \mathbf{r}(t) + \Delta t\, \mathbf{v}(t) + \tfrac{1}{2}(\Delta t)^2 \left[\mathbf{a}^{\mathrm{C}}(t) - \Omega \mathbf{e}_z \times \mathbf{v}(t)\right] + O((\Delta t)^3) \tag{10}$$

$$\mathbf{a}^{\mathrm{C}}(t + \Delta t) = \mathbf{a}^{\mathrm{C}}(\mathbf{r}_1(t + \Delta t), \ldots, \mathbf{r}_N(t + \Delta t); t + \Delta t) \tag{11}$$

$$\begin{aligned}\mathbf{v}(t + \Delta t) = \mathbf{v}(t) + \tfrac{1}{2}\Delta t \big[&\mathbf{a}^{\mathrm{C}}(t) - \Omega \mathbf{e}_z \times \mathbf{v}(t) + \mathbf{a}^{\mathrm{C}}(t + \Delta t) \\ &- \Omega \mathbf{e}_z \times \mathbf{v}(t + \Delta t)\big] + O((\Delta t)^3).\end{aligned} \tag{12}$$

Since the cross product $\mathbf{e}_z \times \mathbf{v}$ only mixes the v_x and v_y components within each of the individual particles in a linear way, (12) is a set of three linear equations per particle, which can easily be solved for $\mathbf{v}(t + \Delta t)$ explicitly:

$$\begin{aligned}v_x(t + \Delta t) = \frac{1}{1 + \frac{1}{4}(\Omega \Delta t)^2} \big\{ &v_x(t) + \tfrac{1}{2}\Delta t \left[a_x^{\mathrm{C}}(t) + a_x^{\mathrm{C}}(t + \Delta t) + 2\Omega v_y(t)\right] \\ &+ \tfrac{1}{4}(\Delta t)^2 \Omega \left[a_y^{\mathrm{C}}(t) + a_y^{\mathrm{C}}(t + \Delta t) - \Omega v_x(t)\right] \big\} + O((\Delta t)^3)\end{aligned} \tag{13}$$

$$v_y(t + \Delta t) = \text{(like (13), exchange } x \leftrightarrow y\text{, replace } \Omega \to -\Omega) \tag{14}$$

$$v_z(t + \Delta t) = v_z(t) + \tfrac{1}{2}\Delta t \left[a_z^{\mathrm{C}}(t) + a_z^{\mathrm{C}}(t + \Delta t)\right] + O((\Delta t)^3). \tag{15}$$

Equations (10), (11), and (13)–(15) are an explicit, symplectic, and time reversal invariant algorithm including the magnetic field.

However, it can be seen that this algorithm becomes inefficient for a strong magnetic field; i.e., it fails for time steps of the order of $2\pi/\Omega$. For example, the most simple case of closed circular motion when $\mathbf{a}^{\mathrm{C}} \equiv 0$ and $v_z(0) = 0$ is not reproduced using Eqs. (10), (11), and (13)–(15) with a time step $\Delta t = 2\pi/\Omega$.

A more geometric rather than our algebraic derivation of (13)–(15) is given in [3, p. 58 ff.; 4, p. 111 ff.]; however, they do not write down the actual result (13)–(15) explicitly.

Reference [3, p. 59] states that this algorithm has "less than one percent error for $\Omega\Delta t < 0.35$." This is consistent with our numerical results in Section 4.

For purposes of comparison in Section 3.2.2, we cast Eqs. (13)–(15) into an alternative form by expanding $[1 + \frac{1}{4}(\Omega\Delta t)^2]^{-1}$ with respect to Δt:

$$v_x(t+\Delta t) = v_x(t) + \tfrac{1}{2}\Delta t\left[a_x^{\mathrm{C}}(t) + a_x^{\mathrm{C}}(t+\Delta t) + 2\Omega v_y(t)\right] + \tfrac{1}{4}(\Delta t)^2\Omega\left[a_y^{\mathrm{C}}(t) + a_y^{\mathrm{C}}(t+\Delta t) - 2\Omega v_x(t)\right] + O((\Delta t)^3) \tag{16}$$

$$v_y(t+\Delta t) = (\text{like (16), exchange } x \leftrightarrow y, \text{ replace } \Omega \to -\Omega) \tag{17}$$

$$v_z(t+\Delta t) = v_z(t) + \tfrac{1}{2}\Delta t\left[a_z^{\mathrm{C}}(t) + a_z^{\mathrm{C}}(t+\Delta t)\right] + O((\Delta t)^3). \tag{18}$$

3.2. Taylor Expansion

3.2.1. *Taylor Expansion Algorithm*

Let us now explicitly assume that the magnetic field is arbitrarily strong; i.e., $\Omega\Delta t \ll 2\pi$ no longer holds, where the inversion algorithm was found to fail. Consider the Taylor series for $\mathbf{r}(t+\Delta t)$,

$$\mathbf{r}(t+\Delta t) = \mathbf{r}(t) + \Delta t\,\mathbf{v}(t) + \sum_{n=2}^{\infty} \frac{(\Delta t)^n}{n!}\frac{d^{n-2}}{dt^{n-2}}\mathbf{a}(t), \tag{19}$$

where $\mathbf{a}(t)$ is given in (8). Instead of $\Omega\Delta t \ll 2\pi$, we assume that $\Omega\Delta t = O((\Delta t)^0)$ or

$$\Omega = O((\Delta t)^{-1}) \Rightarrow \mathbf{a} = O((\Delta t)^{-1}), \tag{20}$$

while we still have

$$\mathbf{r},\ \mathbf{v},\ \mathbf{a}^{\mathrm{C}},\ \frac{d^n}{dt^n}\mathbf{a}^{\mathrm{C}} = O((\Delta t)^0). \tag{21}$$

Under these assumptions, we will

a. show that (19) is no longer properly sorted in ascending orders of Δt;
b. expand the general term of (19) in orders of Δt; and
c. perform the $\sum_{n=2}^{\infty}$ for the first and second order of Δt as obtained in step b.

This will result in a new arrangement of the summation terms in (19) which is properly sorted in orders of Δt with a remainder $O((\Delta t)^3)$, and which must therefore replace (4) in the VV.

An analogous procedure will then have to be carried out with the series

$$\mathbf{v}(t+\Delta t) = \mathbf{v}(t) + \Delta t\mathbf{a}(t) + \sum_{n=2}^{\infty} \frac{(\Delta t)^n}{n!}\frac{d^{n-1}}{dt^{n-1}}\mathbf{a}(t), \tag{22}$$

replacing (6).

a. The general term of the infinite sum in (19) is

$$\frac{(\Delta t)^n}{n!}\frac{d^{n-2}}{dt^{n-2}}\mathbf{a}(t). \tag{23}$$

Since $\mathbf{a} = \mathbf{a}^{\mathrm{C}} - \Omega \mathbf{e}_z \times \mathbf{v}$ and $\mathbf{a} = d\mathbf{v}/dt$, we have

$$\begin{aligned} \frac{d^{n-2}}{dt^{n-2}}\mathbf{a} &= \frac{d^{n-2}}{dt^{n-2}}\mathbf{a}^{\mathrm{C}} - \Omega \mathbf{e}_z \times \frac{d^{n-2}}{dt^{n-2}}\mathbf{v} \\ &= \frac{d^{n-2}}{dt^{n-2}}\mathbf{a}^{\mathrm{C}} - \Omega \mathbf{e}_z \times \frac{d^{n-3}}{dt^{n-3}}\mathbf{a}. \end{aligned} \tag{24}$$

By induction, we can derive

$$\frac{d^{n-2}}{dt^{n-2}}\mathbf{a} = O((\Delta t)^{-n+1})$$

from (20), (21), and (24), and therefore the order of the general term (23) is

$$\frac{(\Delta t)^n}{n!}\frac{d^{n-2}}{dt^{n-2}}\mathbf{a}(t) = O((\Delta t)^n)\, O((\Delta t)^{-n+1}) = O((\Delta t)^1),$$

so clearly the Taylor series (19) is no longer sorted in ascending orders of Δt, as every single term is $O((\Delta t)^1)$.

b. Having found that (23) is of the order $O((\Delta t)^1)$, we now proceed to explicitly calculate its Δt and $(\Delta t)^2$ components. The z component of Eq. (19) is unaffected by the magnetic field. To deal with the action of the cross product on the x and y components in a convenient way, we introduce a complex notation by the mapping

$$\mathcal{M}\colon \mathbb{R}^3 \to \mathbb{C}; \qquad \mathbf{b} \mapsto b = b_x + i b_y, \tag{25}$$

where $\mathbf{b} \in \mathbb{R}^3$ is an arbitrary three-dimensional vector. $\mathcal{M}$ maps the cross product $\mathbf{e}_z \times \mathbf{b}$ into a simple multiplication: $\mathbf{e}_z \times \mathbf{b} \mapsto -b_y + i b_x = ib$. $\mathcal{M}$ is not bijective, but as long as we only consider cross products with $\mathbf{e}_z$, we know that the z component of the result is zero, and we can define an inverse mapping by

$$\mathcal{M}^{-1}\colon \mathbb{C} \to \mathbb{R}^3; \qquad b = \Re b + i \Im b \mapsto \mathbf{b} = (\Re b, \Im b, 0). \tag{26}$$

Equation (24) is thus mapped into

$$\frac{d^{n-2}}{dt^{n-2}}a = \frac{d^{n-2}}{dt^{n-2}}a^{\mathrm{C}} - i\Omega \frac{d^{n-3}}{dt^{n-3}}a. \tag{27}$$

Recursively putting (27) into itself $(n-3)$ times and finally applying (8), we obtain

$$\frac{d^{n-2}}{dt^{n-2}}a = \frac{d^{n-2}}{dt^{n-2}}a^{\mathrm{C}} - i\Omega\left\{\frac{d^{n-3}}{dt^{n-3}}a^{\mathrm{C}} - i\Omega\left[\frac{d^{n-4}}{dt^{n-4}}a^{\mathrm{C}} \cdots - i\Omega(a^{\mathrm{C}} - i\Omega v)\right]\right\}.$$

As a^{C}, $v = O((\Delta t)^0)$ and $\Omega = O((\Delta t)^{-1})$, we can find the lowest orders of Δt by collecting the highest orders of Ω:

$$\begin{aligned} \frac{d^{n-2}}{dt^{n-2}}a &= (-i\Omega)^{n-1} v + (-i\Omega)^{n-2} a^{\mathrm{C}} + \sum_{k=1}^{n-2} (-i\Omega)^{n-2-k} \frac{d^k}{dt^k} a^{\mathrm{C}} \\ &= (-i\Omega)^{n-1} v + (-i\Omega)^{n-2} a^{\mathrm{C}} + O((\Delta t)^{3-n}). \end{aligned}$$

The general term (23) is now

$$\frac{(\Delta t)^n}{n!}\frac{d^{n-2}}{dt^{n-2}}a = \frac{(-i\Omega\Delta t)^n}{n!}\left(\frac{v}{-i\Omega}+\frac{a^{\mathrm{C}}}{(-i\Omega)^2}\right)+O((\Delta t)^3).$$

c. This result can finally be put into the original Taylor expansion (19), yielding, in complex notation,

$$\begin{aligned} r(t+\Delta t) &= r(t)+\Delta t v(t)+\sum_{n=2}^{\infty}\left[\frac{(-i\Omega\Delta t)^n}{n!}\left(\frac{v(t)}{-i\Omega}+\frac{a^{\mathrm{C}}(t)}{(-i\Omega)^2}\right)+O((\Delta t)^3)\right] \\ &= r(t)+\Delta t v(t)+[\exp(-i\Omega\Delta t)-1+i\Omega\Delta t]\left(\frac{v(t)}{-i\Omega}+\frac{a^{\mathrm{C}}(t)}{(-i\Omega)^2}\right) \\ &\quad +O((\Delta t)^3). \end{aligned}$$

We now apply $\mathcal{M}^{-1}$ to retrieve the x and y components, while the propagation formula for the z component remains unchanged,

$$\begin{aligned} r_x(t+\Delta t) &= r_x(t)+\frac{1}{\Omega}[v_x(t)\sin(\Omega\Delta t)-v_y(t)C(\Omega\Delta t)] \\ &\quad +\frac{1}{\Omega^2}\left[-a_x^{\mathrm{C}}(t)C(\Omega\Delta t)-a_y^{\mathrm{C}}(t)S(\Omega\Delta t)\right]+O((\Delta t)^3) \qquad (28) \\ r_y(t+\Delta t) &= (\text{like (28), exchange } x\leftrightarrow y, \text{ replace } \Omega\rightarrow-\Omega) \qquad (29) \\ r_z(t+\Delta t) &= r_z(t)+\Delta t v_z(t)+\tfrac{1}{2}(\Delta t)^2 a_z^{\mathrm{C}}(t)+O((\Delta t)^3), \qquad (30) \end{aligned}$$

where we have defined

$$S(\Omega\Delta t) \equiv \sin(\Omega\Delta t)-\Omega\Delta t \qquad (31)$$

$$C(\Omega\Delta t) \equiv \cos(\Omega\Delta t)-1. \qquad (32)$$

The analogous expansion of (22) is done in Appendix A. The result is

$$\begin{aligned} v_x(t+\Delta t) &= v_x(t)\cos(\Omega\Delta t)+v_y(t)\sin(\Omega\Delta t)+\frac{1}{\Omega}\left[-a_y^{\mathrm{C}}(t)C(\Omega\Delta t)\right. \\ &\quad \left.+a_x^{\mathrm{C}}(t)\sin(\Omega\Delta t)\right]+\frac{1}{\Omega^2}\left[-\frac{a_x^{\mathrm{C}}(t+\Delta t)-a_x^{\mathrm{C}}(t)}{\Delta t}C(\Omega\Delta t)\right. \\ &\quad \left.-\frac{a_y^{\mathrm{C}}(t+\Delta t)-a_y^{\mathrm{C}}(t)}{\Delta t}S(\Omega\Delta t)\right]+O((\Delta t)^3) \qquad (33) \\ v_y(t+\Delta t) &= (\text{like (33), exchange } x\leftrightarrow y, \text{ replace } \Omega\rightarrow-\Omega) \qquad (34) \\ v_z(t+\Delta t) &= v_z(t)+\tfrac{1}{2}\Delta t\left[a_z^{\mathrm{C}}(t)+a_z^{\mathrm{C}}(t+\Delta t)\right]+O((\Delta t)^3). \qquad (35) \end{aligned}$$

The set (28)–(30), (11), and (33)–(35) of propagation equations is now a proper second-order integration algorithm at arbitrary $\Omega\Delta t$ which is *not* restricted to $\Omega\Delta t \ll 2\pi$. Note that these propagation equations do not refer to $\mathbf{a}$, but only to $\mathbf{a}^{\mathrm{C}}$; i.e., the magnetic field is entirely incorporated into the propagation equations. Irrespective of the strength of the magnetic field, the choice of the time step Δt is now determined only by the time scale imposed by $\mathbf{a}^{\mathrm{C}}$, i.e., by the internal physical properties of the system under consideration.

However, this Taylor expansion algorithm is not invariant under time reversal, and the determinant of the Jacobian is $1+O((\Delta t)^4)$ in cases where $\mathbf{a}^{\mathrm{C}}$ is generated by a conservative force (i.e., $\nabla \times \mathbf{a}^{\mathrm{C}} = 0$), and $1 + O((\Delta t)^2)$ otherwise.

3.2.2. *Weak Field Limit*

In the limit $\Omega \Delta t \ll 1$, the trigonometric functions in Eqs. (28)–(29) and (33)–(34) can be expanded into their power series up to and including terms of the order $O((\Omega \Delta t)^2)$, yielding

$$r_x(t+\Delta t) = r_x(t) + \Delta t v_x(t) + \tfrac{1}{2}(\Delta t)^2\left[a_x^{\mathrm{C}}(t) + \Omega v_y(t)\right] + O((\Delta t)^3) \tag{36}$$

$$r_y(t+\Delta t) = (\text{like (36), exchange } x \leftrightarrow y, \text{ replace } \Omega \to -\Omega) \tag{37}$$

$$r_z(t+\Delta t) = r_z(t) + \Delta t v_z(t) + \tfrac{1}{2}(\Delta t)^2 a_z^{\mathrm{C}}(t) + O((\Delta t)^3), \tag{38}$$

which is precisely the $\mathbf{r}$ propagation equation (10), and

$$\begin{aligned} v_x(t+\Delta t) = {} & v_x(t) + \tfrac{1}{2}\Delta t\left[a_x^{\mathrm{C}}(t) + a_x^{\mathrm{C}}(t+\Delta t) + 2\Omega v_y(t)\right] \\ & + \tfrac{1}{4}(\Delta t)^2\Omega\left[\tfrac{4}{3}a_y^{\mathrm{C}}(t) + \tfrac{2}{3}a_y^{\mathrm{C}}(t+\Delta t) - 2\Omega v_x(t)\right] + O((\Delta t)^3) \end{aligned} \tag{39}$$

$$v_y(t+\Delta t) = (\text{like (39), exchange } x \leftrightarrow y, \text{ replace } \Omega \to -\Omega) \tag{40}$$

$$v_z(t+\Delta t) = v_z(t) + \tfrac{1}{2}\Delta t\left[a_z^{\mathrm{C}}(t) + a_z^{\mathrm{C}}(t+\Delta t)\right] + O((\Delta t)^3), \tag{41}$$

which looks subtly different from (16)–(17) due to the $\frac{4}{3}$ and $\frac{2}{3}$ weights in the $(\Delta t)^2$ terms of (39)–(40). However, this is not a true difference to within order $O((\Delta t)^3)$: Substituting $a_y^{\mathrm{C}}(t+\Delta t) = a_y^{\mathrm{C}}(t) + \Delta t\, da_y^{\mathrm{C}}(t)/dt + O((\Delta t)^2)$ into either (39) or (16) yields in both cases

$$\begin{aligned} v_x(t+\Delta t) = {} & v_x(t) + \tfrac{1}{2}\Delta t\left[a_x^{\mathrm{C}}(t) + a_x^{\mathrm{C}}(t+\Delta t) + 2\Omega v_y(t)\right] \\ & + \tfrac{1}{4}(\Delta t)^2\Omega\left[2a_y^{\mathrm{C}}(t) - 2\Omega v_x(t)\right] + O((\Delta t)^3). \end{aligned}$$

Furthermore, at $\Omega = 0$, the Taylor expansion algorithm simplifies into the field-free VV (4), (9), and (6).

This clearly shows that the Taylor expansion algorithm (and, equivalently, the velocity transformation algorithm to be presented in the following section) is the most general implementation of a static homogeneous external magnetic field in the VV algorithm.

3.3. Velocity Transformation

In this section we introduce a slightly more physical approach inspired by classical electrodynamics which reproduces the propagation equations (28)–(30) and (33)–(35) from a different point of view, and which also yields an elegant generalization to arbitrary order.

Again, we consider an N-particle system under the influence of a static homogeneous external magnetic field, with the acceleration on the particles given by Eq. (8). Here, however, we first solve the velocity propagation equations to desired accuracy, and then we obtain the corresponding equations for the particle position by integration:

$$\mathbf{r}(t+\Delta t) = \mathbf{r}(t) + \int_t^{t+\Delta t} \mathbf{v}(t')\, dt'. \tag{42}$$

In the following, we first review the harmonic oscillator solution obtained for non-interacting particles affected only by a magnetic field. As a next step, a time-independent acceleration $\mathbf{a}^{\mathrm{C}} = \text{const.}$ is incorporated by means of a transformation in velocity space. Finally, we present a generalization of this transformation suitable for time-dependent accelerations $\mathbf{a}^{\mathrm{C}}(t)$ and derive propagation equations from this transformation.

3.3.1. *Simple Harmonic Oscillator Motion*

A multiparticle system of N particles without interaction between the particles (i.e., $\mathbf{a}^{\mathrm{C}} = 0$) can be described by N independent equations of motion. Therefore it suffices to solve the equation of motion of one single particle. In this case, Eq. (8) simplifies to $\mathbf{a}(t) = \dot{\mathbf{v}}(t) = -\Omega \mathbf{e}_z \times \mathbf{v}(t)$. The v_z equation is $\dot{v}_z(t) = 0$, yielding $v_z(t) = v_z(0) = \text{const.}$ The v_x and v_y equations can be combined using the complex mapping (25),

$$\dot{v}(t) = -i\Omega v(t), \tag{43}$$

which is the differential equation of the simple harmonic oscillator. Given $v(t)$ and $r(t)$ at some time t, we thus know $v(t + \Delta t)$ analytically:

$$v(t + \Delta t) = v(t) \exp(-i\Omega \Delta t). \tag{44}$$

Rewriting this equation as $v(t') = v(t) \exp[-i\Omega(t' - t)]$ and integrating it according to (42) leads to

$$r(t + \Delta t) = r(t) + \frac{i}{\Omega} v(t)[\exp(-i\Omega \Delta t) - 1].$$

The particles move with constant velocity v_z along the direction of the magnetic field (the z direction) and gyrate around $\mathbf{B}$ with the Larmor radius $r_{\mathrm{L}} = v_\perp / \Omega$ (where $v_\perp = \sqrt{v_x^2 + v_y^2} = \text{const.}$) and the Larmor frequency Ω. If desired, the inverse mapping (26) provides propagation equations.

3.3.2. *Static Acceleration*

In a second step we will assume that the interaction between the N particles can be approximated by a time-independent, homogeneous acceleration $\mathbf{a}^{\mathrm{C}}(t) = \mathbf{a}^{\mathrm{C}} = \text{const.}$ per particle during one time step. Now we have to take into account all terms of (8) and the equations of motion become, in complex notation for v_x and v_y,

$$\dot{v}(t) = -i\Omega v(t) + a^{\mathrm{C}} \tag{45}$$

$$\dot{v}_z(t) = a_z^{\mathrm{C}}. \tag{46}$$

Equations (45) looks quite similar to (43), except for the additional term caused by the static acceleration. However, by means of a suitable velocity transformation, the equation of motion (45)–(46) can be cast into the simple harmonic oscillator form. This is accomplished by

$$\tilde{v}(t) = v(t) + \frac{i}{\Omega} a^{\mathrm{C}} \tag{47}$$

$$\tilde{v}_z(t) = v_z(t). \tag{48}$$

For a physical interpretation of this transformation, see Appendix C. Note that v_z is not influenced and Eq. (46) is solved by $v_z(t+\Delta t) = v_z(t) + \Delta t a_z^{\mathrm{C}}$. The transformation (47) yields $\dot{\tilde{v}}(t) = -i\Omega\,\tilde{v}(t)$, as desired. This can immediately be solved and backtransformed, resulting in

$$v(t+\Delta t) = \left(v(t) + \frac{i}{\Omega}a^{\mathrm{C}}\right)\exp(-i\Omega\Delta t) - \frac{i}{\Omega}a^{\mathrm{C}},$$

and integration (42) leads to

$$r(t+\Delta t) = r(t) + \frac{i}{\Omega}\left(v(t) + \frac{i}{\Omega}a^{\mathrm{C}}\right)[\exp(-i\Omega\Delta t) - 1] - \frac{i}{\Omega}a^{\mathrm{C}}\Delta t.$$

Again, propagation equations can be derived from these results with the inverse mapping (26). These propagation equations are the same as (28)–(30) and (33)–(35) except for the finite differences $a^{\mathrm{C}}(t+\Delta t) - a^{\mathrm{C}}(t)$ in the second-order terms of (33)–(34): The finite differences vanish here since a^{C} is assumed to be constant. Thus we find that under this assumption we arrive at a propagation scheme which is second order in **r**, but only first order in **v**, which would not be efficient for MD simulation purposes in the VV framework. In order to obtain propagation algorithms of arbitrary order k, the time evolution of the acceleration has to be taken into account.

3.3.3. *Generalized Velocity Transformation*

Let us first focus on the x and y directions. We start from

$$\dot{v}(t+\Delta t) = -i\Omega v(t+\Delta t) + a^{\mathrm{C}}(t+\Delta t)$$

(cf. Eq. (45), with a^{C} time-dependent), and put in the Taylor series for $a^{\mathrm{C}}(t+\Delta t)$,

$$a^{\mathrm{C}}(t+\Delta t) = \sum_{n=0}^{k}\frac{(\Delta t)^n}{n!}\frac{d^n}{dt^n}a^{\mathrm{C}}(t) + O((\Delta t)^{k+1}),$$

to arrive at

$$\dot{v}(t+\Delta t) = -i\Omega v(t+\Delta t) + \sum_{n=0}^{k}\frac{(\Delta t)^n}{n!}\frac{d^n}{dt^n}a^{\mathrm{C}}(t) + O((\Delta t)^{k+1}). \tag{49}$$

The aim is now once more to find a transformation of the velocity $v \to \tilde{v}$ which simplifies (49) to a harmonic oscillator equation $\dot{\tilde{v}}(t+\Delta t) = -i\Omega\,\tilde{v}(t+\Delta t) + O((\Delta t)^{k+1})$ within the order $O((\Delta t)^{k+1})$. This is provided by

$$\tilde{v}(t+\Delta t) = v(t+\Delta t) + \sum_{n=0}^{k}\left[\left(\frac{i}{\Omega}\right)^{n+1}\left(\frac{d^n}{dt^n}a^{\mathrm{C}}(t)\right)\sum_{m=0}^{n}\frac{(-i\Omega\Delta t)^m}{m!}\right]. \tag{50}$$

An analytic proof of this property is given in Appendix B. The solution is $\tilde{v}(t+\Delta t) = \tilde{v}(t)\exp(-i\Omega\Delta t)$ as in (44); after backtransformation with respect to (50) and integration

according to (42) we get

$$v(t+\Delta t) = v(t)\exp(-i\Omega\Delta t) + \sum_{n=0}^{k-1}\left[\left(\frac{i}{\Omega}\right)^{n+1}\left(\frac{d^n}{dt^n}a^{\mathrm{C}}(t)\right)\exp_n(-i\Omega\Delta t)\right] + O((\Delta t)^{k+1}) \tag{51}$$

$$r(t+\Delta t) = r(t) + \sum_{n=0}^{k-1}\left[\left(\frac{i}{\Omega}\right)^{n+1}\left(\frac{d^n}{dt^n}v(t)\right)\exp_n(-i\Omega\Delta t)\right] + O((\Delta t)^{k+1}), \tag{52}$$

with the definition $\exp_n(x) \equiv \exp(x) - \sum_{m=0}^{n}\frac{x^m}{m!}$. As usual, the inverse mapping (26) provides the x and y propagation equations. The appropriate propagation equations for r_z and v_z to the same order are

$$v_z(t+\Delta t) = v_z(t) + \sum_{n=0}^{k-1}\left(\frac{d^n}{dt^n}a_z^{\mathrm{C}}(t)\right)\frac{(\Delta t)^{n+1}}{(n+1)!} + O((\Delta t)^{k+1}) \tag{53}$$

$$r_z(t+\Delta t) = r_z(t) + \Delta t\, v_z(t) + \sum_{n=0}^{k-2}\left(\frac{d^n}{dt^n}a_z^{\mathrm{C}}(t)\right)\frac{(\Delta t)^{n+2}}{(n+2)!} + O((\Delta t)^{k+1}). \tag{54}$$

The derivatives $d^n\mathbf{a}^{\mathrm{C}}(t)/dt^n$ must be provided by the actual propagation scheme; they have to be known at least up to and including order $O((\Delta t)^{k-n-2})$ and $O((\Delta t)^{k-n-1})$ for the **r** and **v** propagation equations, respectively.

For example, if we choose $k = 2$ and

$$\frac{d}{dt}\mathbf{a}^{\mathrm{C}}(t) = \frac{\mathbf{a}^{\mathrm{C}}(t+\Delta t) - \mathbf{a}^{\mathrm{C}}(t)}{\Delta t} + O((\Delta t)^1),$$

Eqs. (51)–(52) and (53)–(54) are exactly the same as (28)–(30) and (33)–(35) in Section 3.2; i.e., the Taylor expansion and velocity transformation approaches arrive at the same results for the VV algorithm including a static homogeneous external magnetic field; both are valid for arbitrarily strong magnetic fields.

4. NUMERICAL EXAMPLE

To give an illustration of the performance of the algorithms presented in Section 3, we calculate the trajectory of one single particle in an attractive Coulomb-like central potential $-|\mathbf{r}|^{-1}$ under the influence of a static homogeneous external magnetic field.

At $t = 0$, the dimensionless particle position and velocity vectors are arbitrarily chosen to be $\mathbf{r}(0) = (-1, 0, -1)$ and $\mathbf{v}(0) = (0, 1, 0.1)$, respectively. The acceleration of the particle is given by

$$\mathbf{a} = -\Omega\mathbf{e}_z \times \mathbf{v} - \frac{\mathbf{r}}{|\mathbf{r}|^3}.$$

We integrate the equations of motion (2)–(3) numerically from $t = 0$ to $t = 20$ for different combinations of the parameters Ω and Δt as listed in Table I, exploring a range of $\Omega\Delta t = 10^{-3}\cdots 10^{+3}$. For each pair of parameters, we use both the inversion algorithm [propagation equations (10), (11), and (13)–(15)] and the Taylor expansion algorithm

TABLE I
Choice of Parameters Ω and Δt for the Numerical Example

	$\Omega = 1$	$\Omega = 100$	$\Omega = 10{,}000$
$\Delta t = 0.001$	0.001	0.1	10
$\Delta t = 0.003$	0.003	0.3	30
$\Delta t = 0.01$	0.01	1	100
$\Delta t = 0.03$	0.03	3	300
$\Delta t = 0.1$	0.1	10	1000

Note. Column and row headings are Ω and Δt, respectively; table entries are $\Omega \Delta t$.

[propagation equations (28)–(30), (11), and (33)–(35)] and compare their performance by evaluating the following two observables:

A. Maximum relative deviation of the modulus of the radius vector $\mathbf{r}_{\Omega,\,\Delta t}(t)$ from the "exact" trajectory $\mathbf{r}_{\Omega,\,\mathrm{ex}}(t)$, i.e., from the trajectory calculated with the Taylor expansion algorithm at the smallest step size $\Delta t = 0.001$:

$$\Delta r \equiv \max_{0 \le t \le 20} \left| \frac{|\mathbf{r}_{\Omega,\,\Delta t}(t)| - |\mathbf{r}_{\Omega,\,\mathrm{ex}}(t)|}{|\mathbf{r}_{\Omega,\,\mathrm{ex}}(t)|} \right|. \tag{55}$$

B. Maximum deviation of total energy,

$$\Delta E \equiv \max_{0 \le t \le 20} \left| \frac{E(t) - E(t=0)}{E(t=0)} \right|, \tag{56}$$

where $E(t)$ is the sum of kinetic and potential energy, $E(t) = \frac{1}{2}|\mathbf{v}(t)|^2 - |\mathbf{r}(t)|^{-1}$.

4.1. Position Deviation Δr

Figure 1 shows the behaviour of the position deviation (55) as a function of Δt and Ω for both integration algorithms. In both algorithms the deviation scales like $(\Delta t)^2$, as is to be expected for second-order methods. Except for the smallest magnetic field $\Omega = 1$, the Taylor expansion algorithm performs better than the inversion algorithm by several orders of magnitude, regardless of the size of the time step Δt. This difference in quality grows with increasing magnetic field: Inversion performs the better, the *weaker* the magnetic field, whereas Taylor expansion performs the better, the *stronger* the magnetic field. At weak magnetic field ($\Omega = 1$), the position deviations of both algorithms are practically the same. This could have been expected, as we showed in Section 3.2.2 that both algorithms are equal in the weak field limit.

A closer look at an actual particle trajectory is given in Fig. 2, which shows the time evolution of $|\mathbf{r}(t)|$ at $\Omega = 1000$, calculated with the inversion algorithm at three different step sizes. The results of the Taylor expansion algorithm for any of these step sizes are indistinguishable from the $\Delta t = 0.001$ curve. The inversion algorithm is drastically wrong at large time steps.

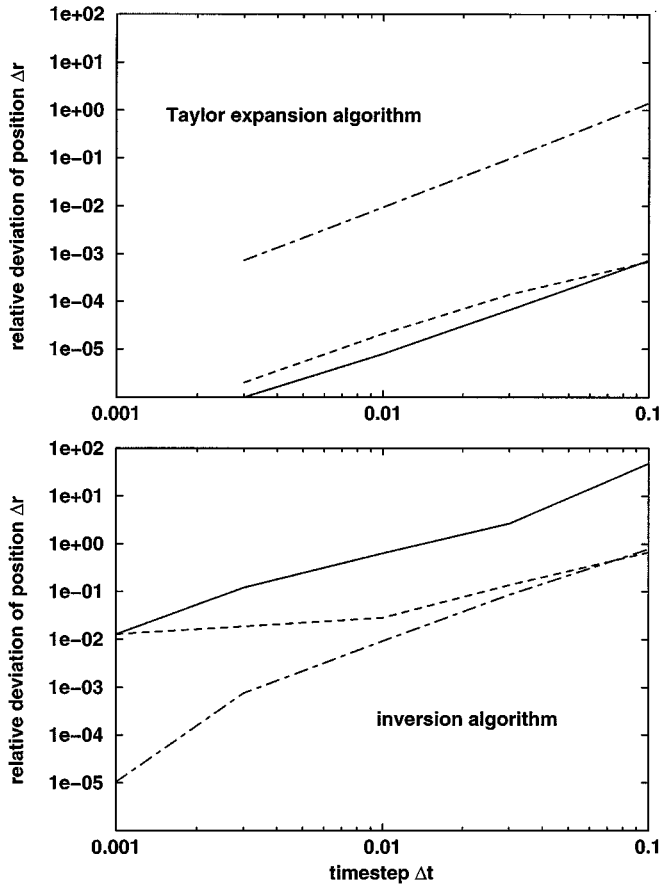

FIG. 1. Relative deviation of position as defined in (55) as a function of step size Δt. Lower panel: inversion algorithm; upper panel: Taylor expansion algorithm. Lines indicate the magnetic field strength: $\Omega = 1$ (dot dashed), $\Omega = 100$ (dashed), and $\Omega = 10{,}000$ (solid).

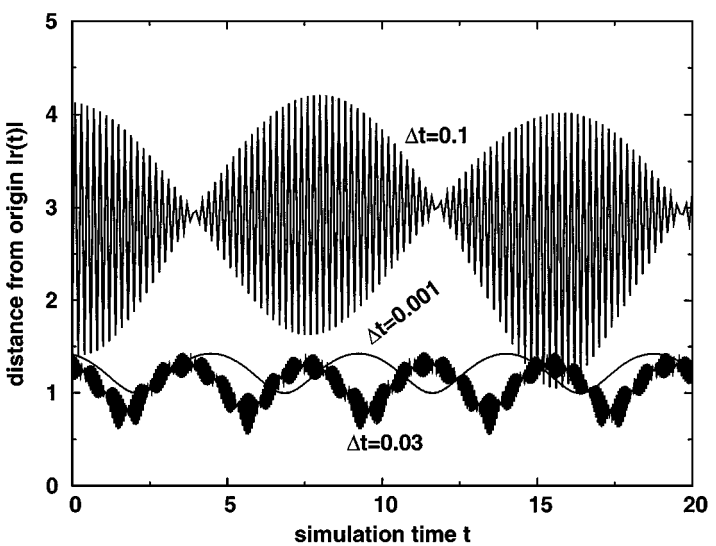

FIG. 2. Time evolution of the distance from the origin $|\mathbf{r}(t)|$ at $\Omega = 1000$. Solid line: Taylor expansion algorithm with any step size and inversion algorithm at $\Delta t = 0.001$; wriggly line close to the solid line: inversion algorithm at $\Delta t = 0.03$; fringes far from the solid line: inversion algorithm at $\Delta t = 0.1$.

4.2. Energy Deviation ΔE

For most many-particle MD simulations, the position deviation is not a sensible measure of integrator accuracy, since the individual particle trajectories behave (deterministically) chaotically; i.e., small changes in Δt can create entirely different particle trajectories when the simulation time is large compared to the time scale of collisions in the system.

In conservative systems, the relative deviation of the total energy from its initial value (56) is a useful tool for monitoring the accuracy of the integration algorithm. Figure 3 shows this energy deviation in our example as a function of Δt and Ω for both integration algorithms.

The results are qualitatively the same as for the position deviation:

- The error scaling is proportional to $(\Delta t)^2$ in both cases.
- Taylor expansion improves with growing magnetic field.
- Inversion gets worse with growing magnetic field.
- There is no combination of parameters where inversion outperforms Taylor expansion.

At strong fields Taylor expansion performs better by several orders of magnitude.

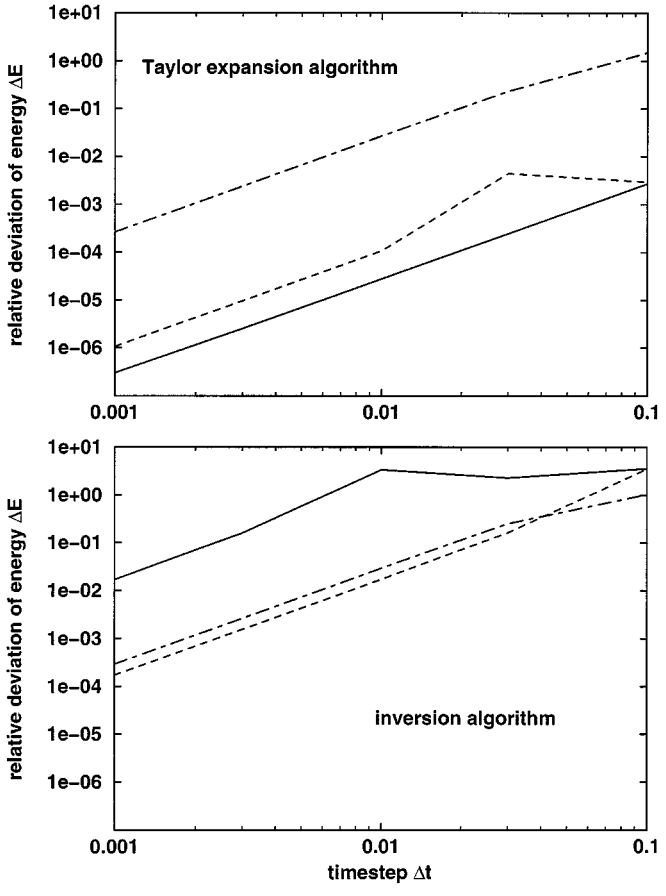

FIG. 3. Relative deviation of total energy as defined in (56) as a function of step size Δt. Lower panel: inversion algorithm; upper panel: Taylor expansion algorithm. Lines indicate the magnetic field strength: $\Omega = 1$ (dot dashed), $\Omega = 100$ (dashed), and $\Omega = 10{,}000$ (solid).

5. BEYOND VELOCITY VERLET: EXPANSION TO ARBITRARY ORDER

In some MD applications it may be desirable to use higher order propagation schemes, such as Runge–Kutta or predictor–corrector methods, instead of the second-order VV. Care must then be taken to incorporate the magnetic field to at least the same order into the propagation equations.

It is straightforward to push both the Taylor expansion and the velocity transformation to an arbitrary order k, and one finds that the resulting propagation equations obtained from the two methods are identical at any k.

For the velocity transformation algorithm, the general result has already been presented in Eqs. (51)–(52) and (53)–(54). The generalization of the Taylor expansion is conceptually simple, but rather clumsy to write down; therefore it will be omitted here.

6. CONCLUSION

We have presented a method for incorporating arbitrarily strong static homogeneous external magnetic fields into the second-order Velocity Verlet propagation algorithm. Our method can be derived either from a suitable Taylor expansion or from a generalized velocity transformation. It results in a scheme where the choice of the time step is entirely independent of the strength of the magnetic field. If desired, the method also allows the development of analogous schemes for higher order propagation algorithms.

The second-order scheme has been incorporated successfully into various MD simulation codes, investigating both stopping power [9–11] and radiative recombination [12] of highly charged ions in magnetized electron plasmas, and electron beam dynamics in electron coolers [13].

Currently, we are trying to improve the Taylor expansion algorithm by additionally including time reversibility and symplecticity conditions into the construction a priori.

APPENDIX A: DERIVATION OF EQUATIONS (33) AND (34)

Equations (33) and (34) can be derived from (22) as follows:

Replacing n by $n+1$ in (27), we get

$$\frac{d^{n-1}}{dt^{n-1}}a = \frac{d^{n-1}}{dt^{n-1}}a^{\mathrm{C}} - i\Omega\frac{d^{n-2}}{dt^{n-2}}a,$$

which we recursively put into itself $(n-2)$ times to arrive at

$$\frac{d^{n-1}}{dt^{n-1}}a = \frac{d^{n-1}}{dt^{n-1}}a^{\mathrm{C}} - i\Omega\left\{\frac{d^{n-2}}{dt^{n-2}}a^{\mathrm{C}} - i\Omega\left[\frac{d^{n-3}}{dt^{n-3}}a^{\mathrm{C}} \cdots - i\Omega(a^{\mathrm{C}} - i\Omega v)\right]\right\}.$$

We obtain the lowest orders of Δt by collecting the highest orders of Ω:

$$\begin{aligned}\frac{d^{n-1}}{dt^{n-1}}a &= (-i\Omega)^n v + (-i\Omega)^{n-1}a^{\mathrm{C}} + (-i\Omega)^{n-2}\frac{d}{dt}a^{\mathrm{C}} + \sum_{k=2}^{n-1}(-i\Omega)^{n-1-k}\frac{d^k}{dt^k}a^{\mathrm{C}} \\ &= (-i\Omega)^n v + (-i\Omega)^{n-1}a^{\mathrm{C}} + (-i\Omega)^{n-2}\frac{d}{dt}a^{\mathrm{C}} + O((\Delta t)^{3-n}).\end{aligned}$$

Thus we have

$$\frac{(\Delta t)^n}{n!}\frac{d^{n-1}}{dt^{n-1}}a = \frac{(-i\Omega\Delta t)^n}{n!}\left(v + \frac{a^{\mathrm{C}}}{-i\Omega} + \frac{da^{\mathrm{C}}/dt}{(-i\Omega)^2}\right) + O((\Delta t)^3),$$

which we put into (22) to get

$$\begin{aligned} v(t+\Delta t) &= v(t) + \Delta t[a^{\mathrm{C}}(t) - i\Omega v(t)] \\ &\quad + \sum_{n=2}^{\infty}\left[\frac{(-i\Omega\Delta t)^n}{n!}\left(v(t) + \frac{a^{\mathrm{C}}(t)}{-i\Omega} + \frac{da^{\mathrm{C}}(t)/dt}{(-i\Omega)^2}\right) + O((\Delta t)^3)\right] \\ &= v(t) + \Delta t a^{\mathrm{C}}(t) - i\Omega\Delta t v(t) + [\exp(-i\Omega\Delta t) - 1 + i\Omega\Delta t] \\ &\quad \times\left(v(t) + \frac{a^{\mathrm{C}}(t)}{-i\Omega} + \frac{da^{\mathrm{C}}(t)/dt}{(-i\Omega)^2}\right) + O((\Delta t)^3). \end{aligned}$$

Application of $\mathcal{M}^{-1}$ results in

$$\begin{aligned} v_x(t+\Delta t) &= v_x(t)\cos(\Omega\Delta t) + v_y(t)\sin(\Omega\Delta t) + \frac{1}{\Omega}\left[-a_y^{\mathrm{C}}(t)C(\Omega\Delta t) + a_x^{\mathrm{C}}(t)\sin(\Omega\Delta t)\right] \\ &\quad + \frac{1}{\Omega^2}\left[-\frac{d}{dt}a_x^{\mathrm{C}}(t)C(\Omega\Delta t) - \frac{d}{dt}a_y^{\mathrm{C}}(t)S(\Omega\Delta t)\right] + O((\Delta t)^3) \\ v_y(t+\Delta t) &= (\text{like } v_x(t+\Delta t), \text{ exchange } x \leftrightarrow y \text{ and replace } \Omega \to -\Omega) \end{aligned}$$

with S and C as defined in Eqs. (31) and (32). The derivative da^{C}/dt appears only in the term $1/\Omega^2[\cdots]$, which is of the order $O((\Delta t)^2)$. It is therefore sufficient to replace da^{C}/dt by the approximation $da^{\mathrm{C}}(t)/dt = [a^{\mathrm{C}}(t+\Delta t) - a^{\mathrm{C}}(t)]/\Delta t + O((\Delta t)^1)$, which leads to Eqs. (33) and (34).

APPENDIX B: ANALYTIC PROOF OF TRANSFORMATION (50)

First we reorganize Eq. (50) and derive it with respect to t:

$$\begin{aligned} v(t+\Delta t) &= \tilde{v}(t+\Delta t) - \sum_{n=0}^{k}\left[\left(\frac{i}{\Omega}\right)^{n+1}\left(\frac{d^n}{dt^n}a^{\mathrm{C}}(t)\right)\sum_{m=0}^{n}\frac{(-i\Omega\Delta t)^m}{m!}\right] \\ \dot{v}(t+\Delta t) &= \dot{\tilde{v}}(t+\Delta t) - \sum_{n=0}^{k}\left[\left(\frac{i}{\Omega}\right)^{n+1}\left(\frac{d^{n+1}}{dt^{n+1}}a^{\mathrm{C}}(t)\right)\sum_{m=0}^{n}\frac{(-i\Omega\Delta t)^m}{m!}\right]. \end{aligned}$$

After putting both equations into Eq. (49), we get

$$\begin{aligned} \dot{\tilde{v}}(t+\Delta t) &= -i\Omega\tilde{v}(t+\Delta t) + \sum_{n=0}^{k}\frac{(\Delta t)^n}{n!}\frac{d^n}{dt^n}a^{\mathrm{C}}(t) \\ &\quad + \sum_{n=0}^{k-1}\left[\left(\frac{i}{\Omega}\right)^{n+1}\left(\frac{d^{n+1}}{dt^{n+1}}a^{\mathrm{C}}(t)\right)\sum_{m=0}^{n}\frac{(-i\Omega\Delta t)^m}{m!}\right] \\ &\quad + i\Omega\sum_{n=0}^{k}\left[\left(\frac{i}{\Omega}\right)^{n+1}\left(\frac{d^n}{dt^n}a^{\mathrm{C}}(t)\right)\sum_{m=0}^{n}\frac{(-i\Omega\Delta t)^m}{m!}\right] + O((\Delta t)^{k+1}). \quad (57) \end{aligned}$$

Note that, to within $O((\Delta t)^{k+1})$, it suffices to extend the second sum over $\sum_{n=0}^{k-1}$ instead of $\sum_{n=0}^{k}$, since the $(n=k)$ term is of the order $O(\Omega^{-k-1}) = O((\Delta t)^{k+1})$. Equation (57) is

the equation of the harmonic oscillator, if the three $\sum_n$ terms cancel to within $O((\Delta t)^{k+1})$. Indeed, rewriting $\sum_{n=0}^{k-1}$ into $\sum_{n=1}^{k}$, we find

$$\begin{aligned}
&\sum_{n=0}^{k} \frac{(\Delta t)^n}{n!} \frac{d^n}{dt^n} a^{\mathrm{C}}(t) + \sum_{n=1}^{k} \left[\left(\frac{i}{\Omega} \right)^n \left(\frac{d^n}{dt^n} a^{\mathrm{C}}(t) \right) \sum_{m=0}^{n-1} \frac{(-i\Omega\Delta t)^m}{m!} \right] \\
&\quad - \sum_{n=0}^{k} \left[\left(\frac{i}{\Omega} \right)^n \left(\frac{d^n}{dt^n} a^{\mathrm{C}}(t) \right) \sum_{m=0}^{n} \frac{(-i\Omega\Delta t)^m}{m!} \right] \\
&= \sum_{n=0}^{k} \frac{(\Delta t)^n}{n!} \frac{d^n}{dt^n} a^{\mathrm{C}}(t) + \sum_{n=1}^{k} \left(\frac{i}{\Omega} \right)^n \left(\frac{d^n}{dt^n} a^{\mathrm{C}}(t) \right) \\
&\quad \times \left[\sum_{m=0}^{n-1} \frac{(-i\Omega\Delta t)^m}{m!} - \sum_{m=0}^{n} \frac{(-i\Omega\Delta t)^m}{m!} \right] - a^{\mathrm{C}}(t) \\
&= \sum_{n=0}^{k} \frac{(\Delta t)^n}{n!} \frac{d^n}{dt^n} a^{\mathrm{C}}(t) + \sum_{n=1}^{k} \left(\frac{i}{\Omega} \right)^n \left(\frac{d^n}{dt^n} a^{\mathrm{C}}(t) \right) \left[- \frac{(-i\Omega\Delta t)^n}{n!} \right] - a^{\mathrm{C}}(t) = 0.
\end{aligned}$$

APPENDIX C: PHYSICAL INTERPRETATION

In this part we want to illuminate what has been done in Section 3.3.2 from a physical point of view. Assigning an equivalent electric field $\mathbf{E} = m\mathbf{a}^{\mathrm{C}}/q$ to the acceleration $\mathbf{a}^{\mathrm{C}}$, the transformation of the velocities in (47) can be interpreted as a special Lorentz transformation in the non-relativistic limit:

A Lorentz transformation to a coordinate frame K' moving with a velocity $\mathbf{u}$ with respect to the original frame K will transform the electric and magnetic fields according to [14, p. 552, here in SI units]:

$$\mathbf{E}' = \gamma(\mathbf{E} + \mathbf{u} \times \mathbf{B}) - \frac{\gamma^2}{\gamma + 1} \frac{\mathbf{u}}{c^2} (\mathbf{u} \cdot \mathbf{E}) \tag{58}$$

$$\mathbf{B}' = \gamma \left(\mathbf{B} - \frac{1}{c^2} (\mathbf{u} \times \mathbf{E}) \right) - \frac{\gamma^2}{\gamma + 1} \frac{\mathbf{u}}{c^2} (\mathbf{u} \cdot \mathbf{B}), \tag{59}$$

where $\gamma = 1/\sqrt{1 - (u/c)^2}$, and c is the velocity of light in vacuum. In the non-relativistic limit $c \to \infty$, Eqs. (58) and (59) simplify into

$$\mathbf{E}' = \mathbf{E} + \mathbf{u} \times \mathbf{B} \tag{60}$$

$$\mathbf{B}' = \mathbf{B}. \tag{61}$$

The aim is to obtain harmonic oscillator equations of motion in K'. To achieve this, the electric field components perpendicular to $\mathbf{B}$ must vanish in K'. With $\mathbf{B} = B\mathbf{e}_z$, we thus choose the relative velocity $\mathbf{u}$ to be

$$\mathbf{u} = \frac{\mathbf{E} \times \mathbf{B}}{B^2} = \frac{\mathbf{E} \times \mathbf{e}_z}{B}.$$

$\mathbf{u}$ is also called "drift velocity." Equations (60) and (61) now become

$$\mathbf{E}' = (\mathbf{E} \cdot \mathbf{e}_z)\mathbf{e}_z = (0, 0, E_z)$$

$$\mathbf{B}' = \mathbf{B} = (0, 0, B).$$

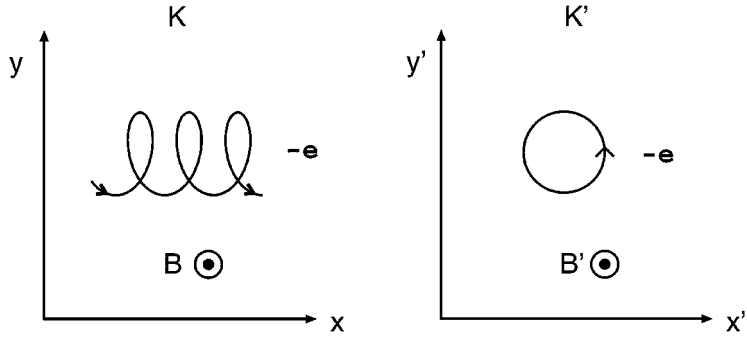

FIG. 4. $\mathbf{E} \times \mathbf{B}$ drift of a negatively charged particle projected onto the plane perpendicular to **B** in the frames of reference K and K'. The orientation of the plane is chosen to have $\mathbf{e}_x$ as the drift direction. The motion along **B** is not visible in this projection. Positive charges would rotate clockwise, but their drift direction in K is the same.

The motion in K' is made up of a gyration around **B** and an acceleration along **B** due to E_z. Additionally, in the original frame K, a uniform drift along $\mathbf{E} \times \mathbf{B}$ with velocity **u** is superimposed. Figure 4 gives a graphic representation of the particle orbit projected onto the plane perpendicular to **B**.

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