Sustainable numerical scheme for molecular dynamics simulation of the dusty plasmas in an external magnetic field

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Abstract. The method, which allows one to carry out computer simulation of a system of charged particles in a strong external homogeneous magnetic field with a time step that is independent on the Larmor oscillation time, was generalized for the case of the presence of the surrounding background for the moving particles. Correctly taking into account a strong magnetic field and friction force, which both depend on the particles velocities, we obtained solution resistant to a change in the time step within the second-order Velocity Verlet propagation scheme.

1. Introduction

Classical molecular dynamics is a problem of numerical solving of the Newton equations of motion for the many particle systems. The particles interact with each other and often turn up under an influence of the external fields. Additionally, the particles can be immersed in any external stationary environment, for example, one may consider the suspended Brownian particles in a liquid or the charged particles in a neutral gas (weakly ionized plasma), and finally, the charged particles of the condensed material in the background plasma (dusty plasma) [1,2]. If the concentration of the particles of the background medium itself is much higher than the concentration of the immersed particles, the environment can be considered as a continuum which makes some averaged effect on the immersed particles. This effect on the particle dynamics can be described by the friction force:

$$F_{fr}(t) = -\nu\vartheta(t) \ , \tag{1}$$

where ν is the friction coefficient, and $\vartheta(t)$ is the particle velocity, which is relative to the stationary background.

In this work, we considered a system of the charged particles exposed in a static uniform external magnetic field. Also the effect of the friction force was taken into account. Implementation of the external magnetic field and the friction force in the MD simulation is not a very difficult task. In Refs.[3-6] the different properties of a system of charged particles in a magnetic field were investigated on the basis of the molecular dynamics. In Refs.[7-10] the simulations of the dusty plasmas with taking into account of the background plasma and random force were performed on the basis of the Langevin dynamics.

In Ref.[11] authors described the way for obtaining of the sustainable numerical scheme for simulation of the particle system in the presence of some forces, depending on the particle velocity. There also second-order Velocity Verlet scheme, taking into account the external uniform magnetic field, was presented. Since MD investigates the trajectory of each particle, time step Δt is chosen small enough to have the necessary number of steps in the period of the Larmor oscillation in order to properly monitor the movement of particles in a spiral. Under the influence of the magnetic field B particle with specific charge q/m performs the rotation with the Larmor frequency $\Omega = qB/m$. One of the conditions for selection of Δt is related to the magnetic field strength:

$$\Omega \Delta t < 2\pi \tag{2}$$

When the magnetic field is weak, the condition (2) is performed quite easily. In a strong magnetic field for the condition (2) one should select very small time steps, which leads to a sharp increase in the amount of calculations, sometimes critical. In work [11] the stable numerical scheme was obtained on the basis of the expansion of $\vec{r}(t+\Delta t)$ and $\vec{\vartheta}(t+\Delta t)$ in the Taylor series. This scheme as was shown is resistant to a change in the time step at large external magnetic fields. Time step in this scheme is independent of the Larmor period of oscillation. In this paper, we introduce the frictional force in the Velocity Verlet scheme, performing all steps described in [11] for obtaining of the stable scheme for the case with background.

2. The Velocity Verlet scheme for simulation of the charged particles in an external magnetic field and background medium

2.1 Explicit and implicit Velocity Verlet schemes

Lets consider the system of N charged particles. The position, velocity, and acceleration of the i - th particle at time t are given by the three-dimensional vectors $\vec{r}_i(t), \vec{\vartheta}_i(t), \vec{a}_i(t)$. The components of the vectors are *x*, *y*, and *z*, respectively. We can write Newton's equations of the all N particles as a system of 6N first-order differential equations:

$$\frac{d\vec{r}_i}{dt} = \vec{\vartheta}_i(t) \quad , \tag{3}$$

$$\frac{d\vec{\vartheta}_i}{dt} = \vec{a}_i(t) = \frac{\vec{F}_i}{m_i} \quad , \tag{4}$$

here m_i is the mass of the particle *i*, $\vec{F}_i$ is the force acting on the particle *i* and $i=1,2..N$. In general case, $\vec{a}_i$ can be a function of the coordinates and velocities of all particles. To solve first- order differential equations (3)-(4), there are many numerical algorithms, including the Velocity Verlet scheme (VV), which is one of the most popular for MD simulations.

$$\vec{r}(t+\Delta t) = \vec{r}(t) + \Delta t \vec{\vartheta}(t) + \frac{1}{2}(\Delta t)^2 \vec{a}(t) + O\left((\Delta t)^3\right), \tag{5}$$

$$\vec{a}(t+\Delta t) = \vec{a}(\vec{r}_1(t+\Delta t), \ldots, \vec{r}_N(t+\Delta t), \vec{\vartheta}_1(t+\Delta t), \ldots, \vec{\vartheta}_N(t+\Delta t), t+\Delta t) \ , \tag{6}$$

$$\vec{\vartheta}(t+\Delta t) = \vec{\vartheta}(t) + \frac{1}{2}\Delta t(\vec{a}(t) + \vec{a}(t+\Delta t)) + O\left((\Delta t)^3\right) . \tag{7}$$

In scheme (5) - (7) one can see $t+\Delta t$ on both sides of Eqs. (6) and (7), so it appears as implicit scheme. In many simple tasks when a magnetic field and friction are absent particle acceleration does not depend on the particle velocity and the equation (6) can be written as follows:

$$\vec{a}(t+\Delta t) = \vec{a}(\vec{r}_1(t+\Delta t), \ldots, \vec{r}_N(t+\Delta t), t+\Delta t) \tag{8}$$

From equation (5) one can calculate $\vec{r}(t+\Delta t)$ at time *t*. Using (8) $\vec{a}(t+\Delta t)$ can be found, and finally $\vec{\vartheta}(t+\Delta t)$ via (7). Thus, implicit form of equations (5) - (8) disappears. In this case, VV scheme is a second- order integration scheme, i.e., the error term is $O((\Delta t)^2)$.

Obviously, when the magnetic field affects on the charged particles, and (or) the particles undergo the friction force in the background medium, the acceleration depends on the velocity, and (8) is not correct, we have an implicit scheme (5) - (7). As was shown in Ref.[11], in the case of a static homogeneous external magnetic field acting on the system, VV can be modified in order to repair an explicit form. We performed this taking into account the friction force. In a homogeneous magnetic field $\vec{B}(0,0,B)$ directed along the axis *z*, the acceleration of each particle, also experiencing the friction in the background gas, can be written as follows:

$$\vec{a}(t)=\vec{a}^{C}(t)-\Omega\vec{e}_{z}\times\vec{\vartheta}(t)-\nu\vec{\vartheta}(t), \tag{9}$$

here $\vec{a}^{C}(t)$ is part of acceleration which does not depend on the velocity:

$$\vec{a}^{C}(t)=\vec{a}^{C}(\vec{r}_{1}(t),...,\vec{r}_{N}(t);t), \tag{10}$$

$\Omega=qB/m$ is the Larmor frequency, $\vec{e}_{z}=(0,0,1)$ is the unit vector directed along the *z* axis. To simplify the notation, we considered a system where all the particles have the same charge- to-mass ratio. In subsections 2.2 and 2.3, we described two different approaches, taking into account the magnetic field and the friction force in the VV scheme, which we in agreement with Ref.[11] called as "inversion $\vec{e}_{z}\times\vec{\vartheta}$" and "Taylor expansion".

2.2 Inversion $\vec{e}_{z}\times\vec{\vartheta}$

In expression (9), we have the cross product $\vec{e}_{z}\times\vec{\vartheta}$, which after substitution in Eqs. (5) - (7) mixes the ϑ_{x} and ϑ_{y} components of the each individual particle. Rewriting Eq.(7) in an explicit form for $\vec{\vartheta}(t+\Delta t)$, we have the following equations of the explicit VV scheme with the acceleration given by (9):

$$r_{x}(t+\Delta t)=r_{x}(t)+\Delta t\vartheta_{x}(t)+\frac{1}{2}(\Delta t)^{2}\left[a_{x}^{C}(t)-\nu\vartheta_{x}(t)+\Omega\vartheta_{y}(t)\right]+O((\Delta t)^{3}), \tag{11}$$

$r_{y}(t+\Delta t)$ can be obtained from (11) by replacing $x\rightarrow y$ and $\Omega\rightarrow-\Omega$

$$r_{z}(t+\Delta t)=r_{z}(t)+\Delta t\vartheta_{z}(t)+\frac{1}{2}(\Delta t)^{2}\left[a_{z}^{C}(t)-\nu\vartheta_{z}(t)\right]+O((\Delta t)^{3}), \tag{12}$$

$$\vartheta_{x}(t+\Delta t)=\frac{1}{K}\left[\vartheta_{x}(t)+\frac{1}{2}\Delta t\left(\begin{array}{l}a_{x}^{C}(t)+a_{x}^{C}(t+\Delta t)+\Omega\vartheta_{y}(t)-\nu\vartheta_{x}(t)+\\ \dfrac{\Omega}{1+\nu\Delta t/2}\left(\begin{array}{l}\vartheta_{y}(t)+\dfrac{\Delta t}{2}a_{y}(t)+\dfrac{\Delta t}{2}a_{y}(t+\Delta t)-\\ \dfrac{\Delta t}{2}\Omega\vartheta_{x}(t)-\dfrac{\Delta t}{2}\nu\vartheta_{y}(t)\end{array}\right)\end{array}\right)\right]+O((\Delta t)^{3}), \tag{13}$$

where $K=1+\frac{\Omega^{2}(\Delta t)^{2}}{4+2\nu\Delta t}+\frac{\nu\Delta t}{2}$, $\vartheta_{y}(t+\Delta t)$ can be obtained from (13) by replacing $x\rightarrow y$ and $\Omega\rightarrow-\Omega$

$$\vartheta_{z}(t+\Delta t)=\frac{1}{1+\nu\Delta t/2}\left[\vartheta_{z}(t)+\frac{1}{2}\Delta t\left(a_{z}^{C}(t)+a_{z}^{C}(t+\Delta t)\right)\right]+O((\Delta t)^{3}) \tag{14}$$

It is shown below the scheme (11) - (14) is stable only in the case of weak magnetic fields. When a strong magnetic field is applied, it becomes unstable with respect to the time step and requires a large amount of calculations with a small time step.

2.3 The Taylor expansion

In work [11] for an arbitrary value of magnetic field the authors developed the robust numerical scheme based on the Taylor expansion of the particle acceleration and velocity, followed by the correct choice of all the terms that are not higher than $O((\Delta t)^2)$. This scheme has been successfully used in many studies, for example in Ref.[12]. Applying the same technique for the case when the particles are immersed in a homogeneous stationary environment we obtained the following equations for the positions and velocities of the particles:

$$\begin{aligned} r_x(t+\Delta t) = r_x(t) - \frac{1}{(\Omega^2+\nu^2)} \begin{bmatrix} \left(\nu\vartheta_x(t)+\Omega\vartheta_y(t)\right)\cdot\left(\exp(-\nu\Delta t)\cos(\Omega\Delta t)-1\right)+ \\ \left(\nu\vartheta_y(t)-\Omega\vartheta_x(t)\right)\exp(-\nu\Delta t)\sin(\Omega\Delta t) \end{bmatrix} \\ + \frac{1}{(\Omega^2+\nu^2)^2} \begin{bmatrix} C(\Omega\Delta t)\left((\nu^2-\Omega^2)a_x^C(t)+2\nu\Omega a_y^C(t)\right)+ \\ S(\Omega\Delta t)\left((\nu^2-\Omega^2)a_y^C(t)-2\nu\Omega a_x^C(t)\right) \end{bmatrix} + O((\Delta t)^3) \end{aligned} \tag{15}$$

$r_y(t+\Delta t)$ can be obtained from (15) by replacing $x \to y$ and $\Omega \to -\Omega$)

$$r_z(t+\Delta t) = r_z(t) + \Delta t\vartheta_z(t) + \frac{1}{2}(\Delta t)^2\left[a_z^C(t) - \nu\vartheta_z(t)\right] + O((\Delta t)^3), \tag{16}$$

where we have defined:

$$S(\Omega\Delta t) \equiv \exp(-\nu\Delta t)\sin(\Omega\Delta t) - \Omega\Delta t \tag{17}$$

$$C(\Omega\Delta t) \equiv \exp(-\nu\Delta t)\cos(\Omega\Delta t) - 1 + \nu\Delta t \tag{18}$$

$$\begin{aligned} &\vartheta_x(t+\Delta t) = \exp(-\nu\Delta t)\left(\vartheta_x(t)\cos(\Omega\Delta t)+\vartheta_y(t)\sin(\Omega\Delta t)\right)+ \\ &\frac{1}{\Omega^2+\nu^2}\begin{bmatrix} \exp(-\nu\Delta t)\left(\Omega\sin(\Omega\Delta t)-\nu\cos(\Omega\Delta t)\right)a_x^C(t)+\nu a_x^C(t)- \\ \exp(-\nu\Delta t)\left(\Omega\cos(\Omega\Delta t)+\nu\sin(\Omega\Delta t)\right)a_y^C(t)+\Omega a_y^C(t) \end{bmatrix}+ \\ &\frac{1}{\left(\Omega^2+\nu^2\right)^2}\begin{bmatrix} \left\{\exp(-\nu\Delta t)\left((\nu^2-\Omega^2)\cos(\Omega\Delta t)-2\nu\Omega\sin(\Omega\Delta t)\right)+(\Omega^2-\nu^2)+(\Omega^2+\nu^2)\nu\Delta t\right\}\frac{d}{dt}a_x^C(t)+ \\ \left\{\exp(-\nu\Delta t)\left((\nu^2-\Omega^2)\sin(\Omega\Delta t)+2\nu\Omega\cos(\Omega\Delta t)\right)-2\nu\Omega+(\Omega^2+\nu^2)\nu\Delta t\right\}\frac{d}{dt}a_y^C(t) \end{bmatrix}+ \\ &O((\Delta t)^3) \end{aligned} \tag{19}$$

$\vartheta_y(t+\Delta t)$ can be obtained from (19) by replacing $x \to y$ и $\Omega \to -\Omega$

$$\vartheta_z(t+\Delta t) = \frac{1}{1+\nu\Delta t/2}\left[\vartheta_z(t)+\frac{1}{2}\Delta t\left(a_z^C(t)+a_z^C(t+\Delta t)\right)\right]+O((\Delta t)^3) \tag{20}$$

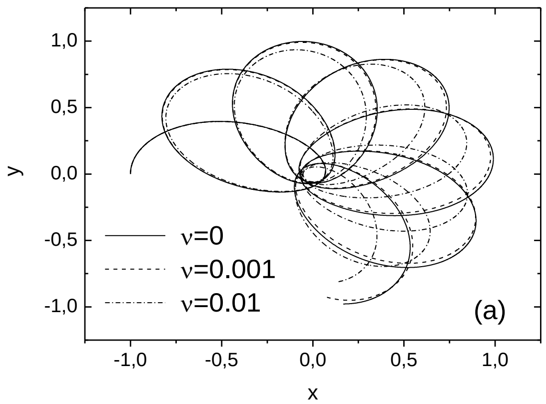
The system of Eqs. (15) - (20) is a sustainable second-order numerical scheme for simulation of the charged particles in an external homogeneous stationary magnetic field and background environment. The choice of the integration step for it is not limited to a condition $\Omega\Delta t << 2\pi$. In these equations, there are not references to the acceleration caused by the Lorentz force and by frictional force, they are fully integrated into these equations. There are references only on $\vec{a}^C$ caused by the interaction of the particles, as well as by the external forces beyond the control of the particles velocities. The choice of the time step is now depends only on the time scale conditioned by $\vec{a}^C$. At $\nu = 0$ Eqs.(15) - (20) transform to the corresponding equations presented in [11] for the case without the background.

3. Numerical example

Lets consider the following example. We calculated the trajectory of the first charged particle (charge and mass are $q_1 = -1, m_1 = 1$), moving in a gaseous environment with a friction coefficient ν in the Coulomb field of the second stationary charged particle ($q_2 = 1$), and in a static homogeneous external magnetic field. At the initial time $t = 0$ position and velocity of the first particle are determined by the vectors $\vec{r}(0) = (-1,0,0)$ and $\vec{\vartheta}(0) = (0,1,0)$, respectively. The second particle is at the origin (0,0,0). Then, the acceleration of the first particle is given by:

$$\vec{a}(t) = -\frac{\vec{r}}{|\vec{r}|^3} - \Omega\vec{e}_z \times \vec{\vartheta}(t) - \nu\vec{\vartheta}(t) \tag{21}$$

We numerically calculated the equations of motion from $t = 0$ to $t = 20$ in a wide range of variation of the parameters $\Omega, \Delta t$ and ν on the basis of both methods, by an algorithm (11) - (14) and the algorithm of the Taylor expansion (15) - (20). Fig. 1 shows the trajectories calculated for different values Ω and ν on the basis of the equations (15) - (20), the trajectories calculated by the scheme of the Taylor series expansion [11], which does not take into account the friction force ($\nu = 0$), are also given. As can be seen from these graphs at $\nu = 0.001$ the trajectories, calculated by (15) - (20) and [11], are almost the same. With an increase in ν noticeable differences occur. It is also shown that with an increase in the magnetic field the Larmor rotations occur in addition to the rotation around of the force center of the electric field.



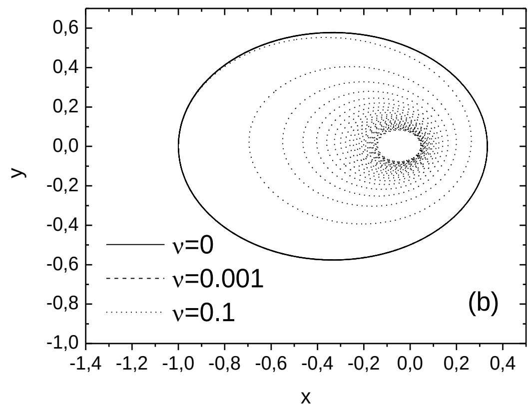


Figure 1. Trajectories of charged particle with acceleration (21). (a) - $\Omega = 1$ (b) - $\Omega = 0.001$

Fig. 2a shows the trajectories calculated for different values of the time step Δt on the basis of Eqs. (11) - (14), as well as Fig. 2b displays these calculated by a scheme of the Taylor expansion (15) - (20). In the first case on Fig. 2a it is visible that an increase in the time step results in the instability of the solution of the particle motion equations. Conversely, Fig. 2b shows that an algorithm of the Taylor series expansion (15) - (20) is resistant to a change in the time step. At $\Delta t = 0.1$ the trajectory becomes more polygonal in connection with a decrease in the number of the calculation points on the Larmor spiral, but the deviation of the solutions from the trajectory calculated at $\Delta t = 0.001$ remains within the margin of error. Thus solutions on the basis of the algorithm (11) - (14) depend strongly on Δt, while an algorithm of the Taylor expansion (15) - (20) is more stable relatively to a change in the time step, including range when $\Delta t > 0.1$. Recommended step is $\Delta t = 0.1$, since at its bigger values points of position still lie on the "exact" trajectory, but their number, attributable to a single coil, decreases.

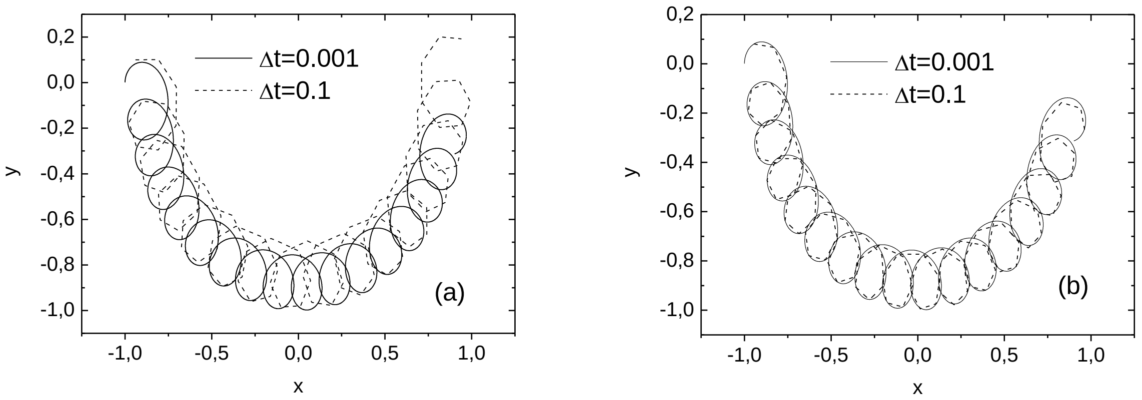


Figure 2. Trajectories of charged particle with acceleration (21). $\Omega = 10, \nu = 0.001$ (a) – algorithm (11)-(14), (b) - algorithm (15)-(20)

4. Conclusion

We presented a stable numerical scheme for solving of the equations of motion of charged particles in a background medium, as well as in a strong external static homogeneous magnetic field. To obtain it the method of the expansion in the Taylor series has been used. The Lorentz force and friction force depending on the particle velocity have been taken into account. In the resulting scheme the choice of the time step does not depend on the magnetic field.

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