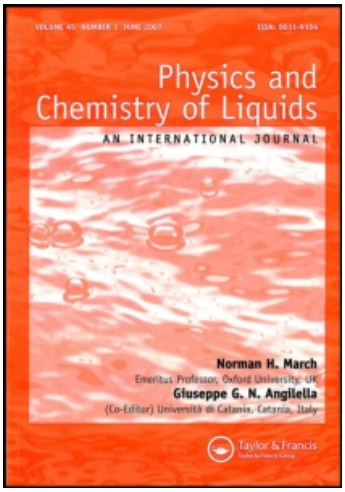

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EXACT ALGORITHM FOR DYNAMICS OF CHARGED PARTICLES IN A MAGNETIC FIELD

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A new and exact algorithm for the two-dimensional motion of an electron in a constant, perpendicular magnetic field has been derived. It is then extended to include a position-dependent force, of which the Coulomb force is an example. Such an algorithm can be readily used in any molecular dynamics simulation.

Keywords: One-component plasma; Algorithm; Magnetic field effects

I. INTRODUCTION

There has been considerable interest in studying the effect of a magnetic field on static, dynamic and transport properties of one-component plasmas [1–4]. The systems of interest include three-dimensional, two-dimensional and, more recently, bilayer and multilayer electron gas. Analysis of such systems using molecular dynamics computer simulation methods requires an algorithm for the motion of the particles which is efficient and as accurate as possible. The effect of the long-range ion–ion interaction potential may be modelled through the use of the Ewald sum [5]; this expresses the potential energy in terms of two convergent summations, one in real space and the other in reciprocal-lattice space. The force on each particle is then

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obtained from this expression and inserted in the dynamics algorithm. When a magnetic field is introduced, changes to the algorithm are required. The two known adjustments, a simple extension of the Verlet algorithm [6] and the one used by Bernu [1] have deficiencies.

In this paper, we derive an algorithm that can be used to determine the motion of a charged particle in both a constant external magnetic field and the electric field created by other particles in the system. The result is exact in the case of a magnetic field alone. It is presented here in the context of electrons in a plane, but can easily be extended to three-dimensional systems.

II. DERIVATION FOR MAGNETIC FORCE ONLY

Consider a constant, uniform transverse magnetic field of strength B which acts on electrons constrained to move in the xy-plane. The equations of motion are

$$\ddot{x}(t) = -B\dot{y}(t), \qquad \ddot{y}(t) = B\dot{x}(t). \tag{1}$$

It follows that the even time derivatives are given for $n \in \mathbb{N}$ by

$$x^{(2n)}(t) = (-1)^n B^{2n-1}\dot{y}(t), \qquad y^{(2n)}(t) = (-1)^{n+1} B^{2n-1}\dot{x}(t), \tag{2}$$

and the odd for $n = 0$ or $n \in \mathbb{N}$ by

$$x^{(2n+1)}(t) = (-1)^n B^{2n}\dot{x}(t), \qquad y^{(2n+1)}(t) = (-1)^n B^{2n}\dot{y}(t). \tag{3}$$

Using Taylor series about t in powers of h we obtain

$$\begin{aligned} x(t+h) + x(t-h) &= 2\sum_{n=0}^{\infty} \frac{h^{2n}}{(2n)!} x^{(2n)}(t) \\ &= 2x(t) + \frac{2}{B}\dot{y}(t) \sum_{n=1}^{\infty} \frac{(-1)^n (Bh)^{2n}}{(2n)!} \\ &= 2x(t) - 2B^{-1}(1 - \cos Bh)\dot{y}(t), \\ y(t+h) + y(t-h) &= 2y(t) + 2B^{-1}(1 - \cos Bh)\dot{x}(t). \end{aligned} \tag{4}$$

$$\begin{aligned} x(t+h) - x(t-h) &= 2\sum_{n=0}^{\infty} \frac{h^{2n+1}}{(2n+1)!} x^{(2n+1)}(t) \\ &= \frac{2}{B}\dot{x}(t) \sum_{n=0}^{\infty} \frac{(-1)^n (Bh)^{2n+1}}{(2n+1)!} \\ &= 2B^{-1} \sin Bh\, \dot{x}(t), \\ y(t+h) - y(t-h) &= 2B^{-1} \sin Bh\, \dot{y}(t). \end{aligned} \tag{5}$$

Using (5) to express $\dot{x}(t)$ and $\dot{y}(t)$ in terms of $[x(t+h) - x(t-h)]$ and $[y(t+h) - y(t-h)]$, substituting this into (4) and setting $a = (1 - \cos Bh)/\sin Bh$, we obtain

$$\begin{aligned} x(t+h) &= 2x(t) - x(t-h) - a[y(t+h) - y(t-h)], \\ y(t+h) &= 2y(t) - y(t-h) + a[x(t+h) - x(t-h)]. \end{aligned} \tag{6}$$

The solution of this linear system for $x(t+h)$ and $y(t+h)$ is

$$\begin{aligned} x(t+h) &= \{2x(t) - x(t-h) - 2a[y(t) - y(t-h)] + a^2 x(t-h)\}/(1+a^2) \\ &= x(t) + \cos Bh[x(t) - x(t-h)] - \sin Bh[y(t) - y(t-h)], \\ y(t+h) &= \{2y(t) - y(t-h) + 2a[x(t) - x(t-h)] + a^2 y(t-h)\}/(1+a^2) \\ &= y(t) + \cos Bh[y(t) - y(t-h)] + \sin Bh[x(t) - x(t-h)]. \end{aligned} \tag{7}$$

This is the algorithm which yields the exact motion of each electron due to the magnetic field only. The corresponding expressions for velocity components are

$$\dot{x}(t) = \frac{Bh}{\sin Bh} \frac{x(t+h) - x(t-h)}{2h}, \qquad \dot{y}(t) = \frac{Bh}{\sin Bh} \frac{y(t+h) - y(t-h)}{2h}. \tag{8}$$

Assume that the dynamics calculation is started by specifying the coordinates at times $-h$ and 0. The orbit of each electron will be the circle which passes through $(x(-h), y(-h))$, $(x(0), y(0))$ as prescribed and $(x(h), y(h))$ as obtained from (7); let d be the distance between the first two points. From (7) and (8) it can be shown that the radius

of the circle and the speed of the electron are, respectively,

$$r_1 = d/\sqrt{2(1-\cos Bh)} \quad \text{and} \quad s_1 = Br_1. \tag{9}$$

It can be shown that the position given by (7) for any multiple of h is the same as that given for the same instant by the known solution for continuous time variable.

III. COMBINATION OF MAGNETIC FORCE AND POSITION-DEPENDENT FORCE

Now consider the equations of motion

$$\ddot{x}(t) = f_x(t) - B\dot{y}(t), \qquad \ddot{y}(t) = f_y(t) + B\dot{x}(t), \tag{10}$$

where $f_x(t)$ and $f_y(t)$ are components of an interaction force depending on the position coordinates $(x(t), y(t))$. For example, this force could be the Ewald sum expression for the Coulomb interactions among the electrons.

Higher order time derivatives can be computed:

$$\begin{aligned} x^{(3)}(t) &= \dot{f}_x(t) - B\ddot{y}(t) \approx -B(f_y(t) + B\dot{x}(t)) \\ y^{(3)}(t) &= \dot{f}_y(t) + B\ddot{x}(t) \approx B(f_x(t) - B\dot{y}(t)), \end{aligned}$$

in which time derivatives of f are neglected; this is consistent with standard dynamics algorithms. Now, of course, h must be sufficiently small to yield accurate results.

This procedure gives the following approximate formulas for even and odd time derivatives for $n \in \mathbb{N}$

$$\begin{aligned} x^{(2n)}(t) &= (-1)^n(-B^{2n-2}f_x(t) + B^{2n-1}\dot{y}(t)) \\ y^{(2n)}(t) &= (-1)^{n+1}(B^{2n-2}f_y(t) + B^{2n-1}\dot{x}(t)) \\ x^{(2n+1)}(t) &= (-1)^n(B^{2n-1}f_y(t) + B^{2n}\dot{x}(t)) \\ y^{(2n+1)}(t) &= (-1)^n(-B^{2n-1}f_x(t) + B^{2n}\dot{y}(t)). \end{aligned} \tag{11}$$

The Taylor series now give

$$\begin{aligned} x(t+h)+x(t-h) &= 2x(t)-2\frac{1-\cos Bh}{Bh}h\dot{y}(t) \\ &\quad +2\frac{1-\cos Bh}{(Bh)^2}h^2 f_x(t), \\ y(t+h)+y(t-h) &= 2y(t)+2\frac{1-\cos Bh}{Bh}h\dot{x}(t) \\ &\quad +2\frac{1-\cos Bh}{(Bh)^2}h^2 f_y(t), \end{aligned} \tag{12}$$

$$\begin{aligned} x(t+h)-x(t-h) &= 2\frac{\sin Bh}{Bh}h\,\dot{x}\,(t)+2\frac{\sin Bh-Bh}{(Bh)^2}h^2 f_y(t), \\ y(t+h)-y(t-h) &= 2\frac{\sin Bh}{Bh}h\,\dot{y}\,(t)-2\frac{\sin Bh-Bh}{(Bh)^2}h^2 f_x(t). \end{aligned} \tag{13}$$

Using (13) to express $\dot{x}(t)$ in terms of $[x(t+h)-x(t-h)]$ and $f_y(t)$ and $\dot{y}(t)$ in terms of $[y(t+h)-y(t-h)]$ and $f_x(t)$, then substituting into (12) and letting $A=2a/Bh$, we obtain

$$\begin{aligned} x(t+h) &= 2x(t)-x(t-h)-a[y(t+h)-y(t-h)] \\ &\quad +Ah^2 f_x(t), \\ y(t+h) &= 2y(t)-y(t-h)+a[x(t+h)-x(t-h) \\ &\quad +Ah^2 f_y(t). \end{aligned} \tag{14}$$

The solution of the linear system (14) yields the desired algorithm: it is

$$\begin{aligned} x(t+h) &= \{2x(t)-x(t-h)-2a[y(t)-y(t-h)]+a^2x(t-h) \\ &\quad +Ah^2[f_x(t)-af_y(t)]\}/(1+a^2), \\ y(t+h) &= \{2y(t)-y(t-h)+2a[x(t)-x(t-h)]+a^2y(t-h) \\ &\quad +Ah^2[f_y(t)+af_x(t)]\}/(1+a^2). \end{aligned} \tag{15}$$

This agrees with the standard Verlet algorithm in the limit $B \to 0$ since $a \to 0$ and $A \to 1$, and can also be expressed as

$$\begin{aligned} x(t+h) &= x(t) + \cos Bh\,[x(t) - x(t-h)] - \sin Bh\,[y(t) - y(t-h)] \\ &\quad + h^2\left[\frac{\sin Bh}{Bh} f_x(t) - \frac{1-\cos Bh}{Bh} f_y(t)\right], \\ y(t+h) &= y(t) + \cos Bh\,[y(t) - y(t-h)] + \sin Bh\,[x(t) - x(t-h)] \\ &\quad + h^2\left[\frac{\sin Bh}{Bh} f_y(t) + \frac{1-\cos Bh}{Bh} f_x(t)\right]. \end{aligned} \tag{16}$$

The corresponding expressions for velocity components are

$$\begin{aligned} \dot{x}(t) &= \frac{Bh}{\sin Bh}\frac{x(t+h) - x(t-h)}{2h} - \frac{\sin Bh - Bh}{Bh \sin Bh} h f_y(t), \\ \dot{y}(t) &= \frac{Bh}{\sin Bh}\frac{y(t+h) - y(t-h)}{2h} + \frac{\sin Bh - Bh}{Bh \sin Bh} h f_x(t). \end{aligned} \tag{17}$$

In a recent study of the effects of a magnetic field on diffusion in a two-dimensional one-component plasma [7], we have used Eq. (16) in the molecular dynamics calculation.

IV. COMPARISON WITH OTHER ALGORITHMS

We have studied two ways of comparing this algorithm with others. One uses each algorithm to compute the orbit of a particle subject to a magnetic force only: the exact result is well known. The second considers a two-dimensional system of electrons interacting through Coulomb forces and subject to a constant magnetic field normal to the plane. Results using our algorithm were compared to those obtained from a simple Verlet algorithm and from an improvement reported by Hansen [8] to have been used in the work of Bernu [1].

The simplest Verlet algorithm [6] for this problem is

$$\begin{aligned} x(t+h) &= 2x(t) - x(t-h) - Bh^2 \dot{y}(t) + h^2 f_x(t), \\ y(t+h) &= 2y(t) - y(t-h) + Bh^2 \dot{x}(t) + h^2 f_y(t), \\ \dot{x}(t) &= (x(t+h) - x(t-h))/2h, \\ \dot{y}(t) &= (y(t+h) - y(t-h))/2h. \end{aligned} \tag{18}$$

It is easy to show that this is unsatisfactory because it does not yield circular orbits for the magnetic force only.

The Bernu algorithm is obtained by solving the system (18) for $x(t+h)$ and $y(t+h)$; the result, with $\alpha = Bh/2$, is

$$\begin{aligned} x(t+h) &= x(t) + \frac{1-\alpha^2}{1+\alpha^2}[x(t) - x(t-h)] - \frac{2\alpha}{1+\alpha^2}[y(t) - y(t-h)] \\ &\quad + \frac{h^2}{1+\alpha^2}[f_x(t) - \alpha f_y(t)], \\ y(t+h) &= y(t) + \frac{1-\alpha^2}{1+\alpha^2}[y(t) - y(t-h)] + \frac{2\alpha}{1+\alpha^2}[x(t) - x(t-h)] \\ &\quad + \frac{h^2}{1+\alpha^2}[f_y(t) + \alpha f_x(t)]. \end{aligned} \tag{19}$$

If the magnetic force only is considered, the electron orbit produced by this algorithm will, in fact, be a circle passing through the two given initial points; however, with $(x(h), y(h))$ determined by (19) the radius and electron speed are

$$r_2 = d\sqrt{(1 + (Bh/2)^2)/(Bh)^2} \quad \text{and} \quad s_2 = dh^{-1}/\sqrt{1 + (Bh/2)^2}. \tag{20}$$

These results are not exact. Figure 1 shows the ratio of these radii and speeds to those obtained by our exact algorithm for $Bh \in (0, \pi)$.

The differences are small for values of $Bh < 1$ which are likely to be used in molecular dynamics calculations; however, the effect of different speeds causes the positions obtained from (19) to lag behind those obtained from (16). Thus, when particle interactions are included, the slight differences in coordinates for small time can eventually yield very different trajectories.

The second comparison involved calculations for a two-dimensional system of electrons with a standard molecular dynamics configuration: an infinite lattice of square boxes each containing 128 particles. The interelectronic Coulomb forces were treated using the Ewald sum method with minimum imaging convention [9]; a magnetic field of constant strength B perpendicular to the plane was included. Let n be the areal density, m the mass and e the charge of an electron and c the speed

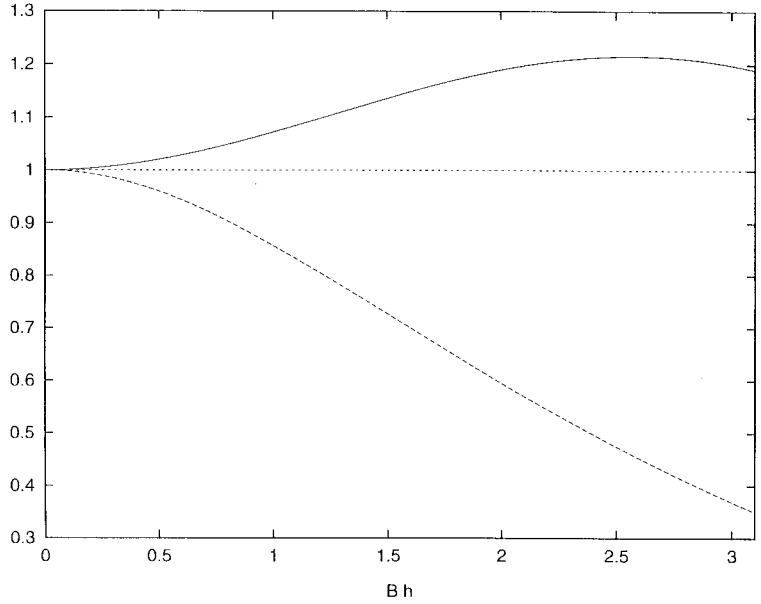


FIGURE 1 Comparison of results using algorithms (16) and (19) for magnetic force only. Both give circular orbits; the ratios of the radii and speeds are the same for any particle. As defined by Eqs. (9) and (20) the solid curve shows r_2/r_1 and the dashed curve shows s_2/s_1 for $Bh \in (0, \pi)$.

of light. Our dimensionless units correspond to lengths in units of $r_0 = (\pi n)^{-1/2}$ and times in units of $(mr_0^3/e^2)^{1/2}$; B is in units of $(mc^2/r_0^3)^{1/2}$. We chose the time increment $h = 0.03$ and box side length 20.2. For a typical areal density of $8 \times 10^{12}\,\mathrm{m}^{-2}$, $h = 0.03$ corresponds to 0.15 ps, and B in dimensionless units is almost equal to B in Teslas. Electron trajectories for our algorithm (16) and for algorithm (19) were obtained for various values of B.

The corresponding trajectories of a typical electron using (16) and (19) are shown in Fig. 2 for $B = 1$ and Fig. 3 for $B = 4$. For small B the trajectories are nearly identical for a certain initial time interval, but they eventually diverge because slightly different positions produce different interactions with the other electrons. The effect of a larger magnetic force is to reduce the diffusion of the electrons; this causes the trajectories produced by the different algorithms to stay together longer.

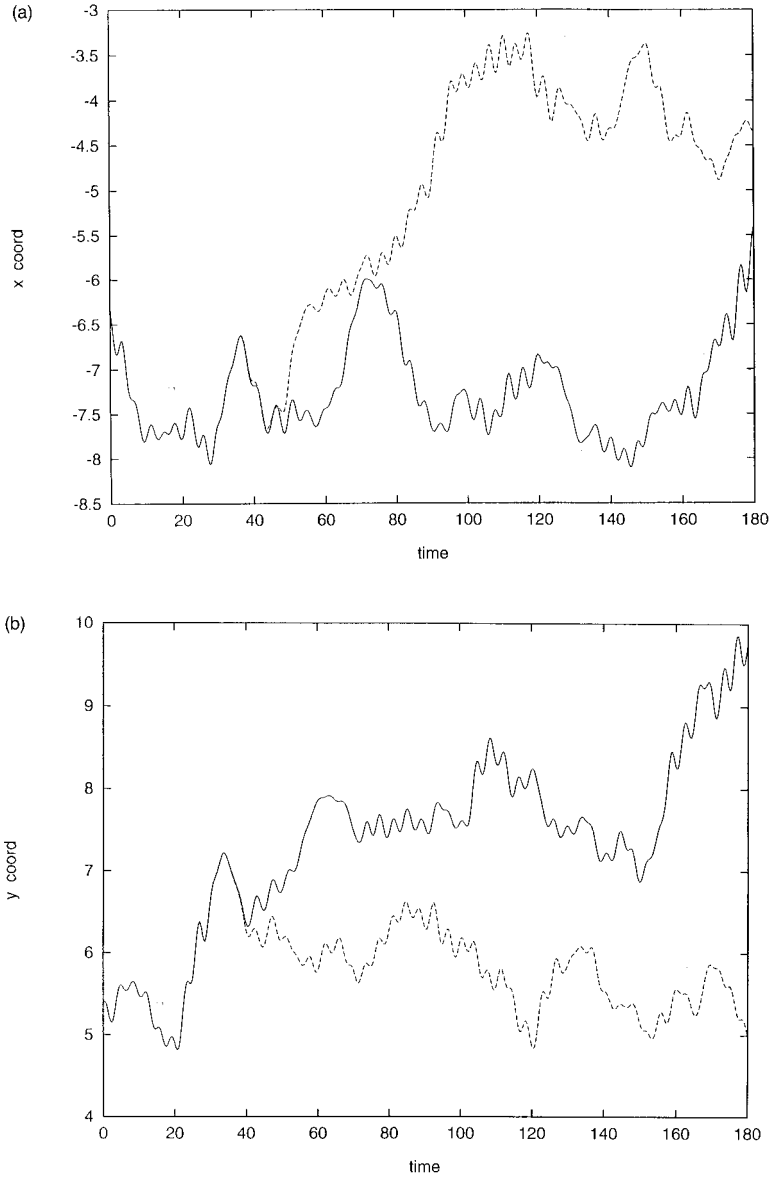


FIGURE 2 Comparison of results of (16) (solid) and (19) (dashed) for trajectory of a typical particle subject to both magnetic and Coulomb forces: (a) and (b) show x and y coordinates as functions of time and (c) shows the orbit starting at the point marked •. Magnetic field strength is $B = 1$.

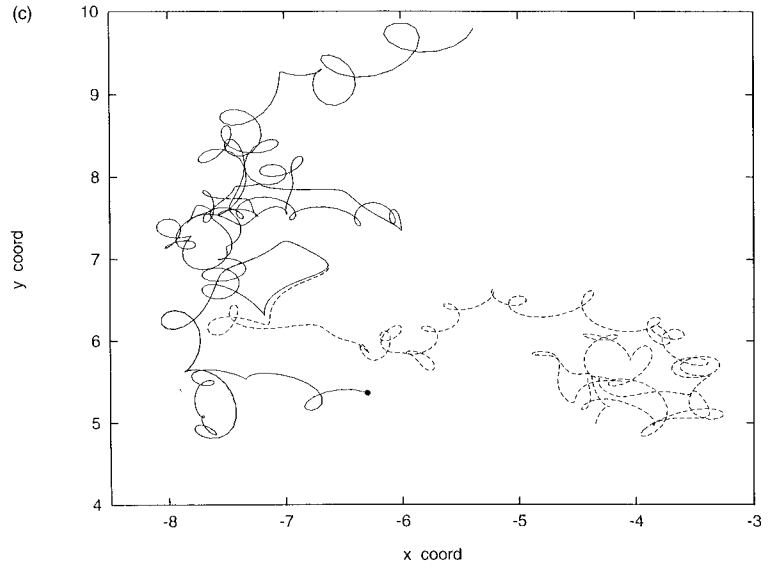


FIGURE 2 (Continued).

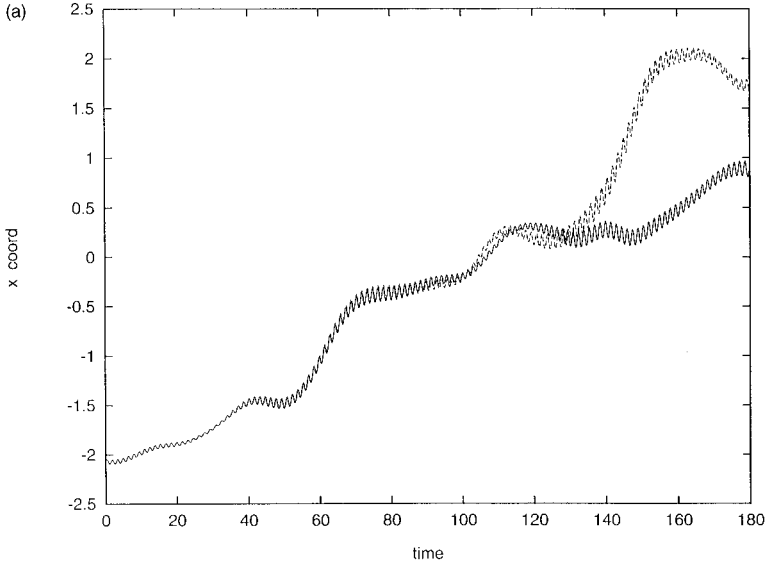
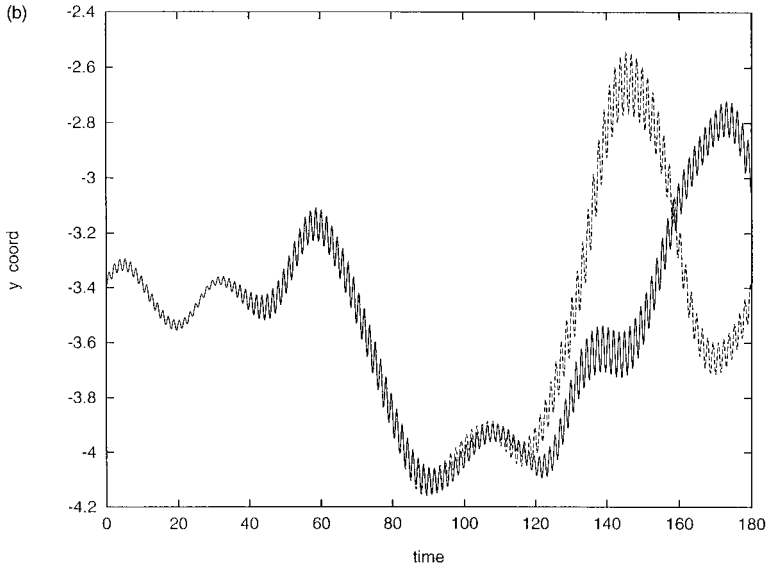


FIGURE 3 Same as Fig. 2 except $B = 4$.



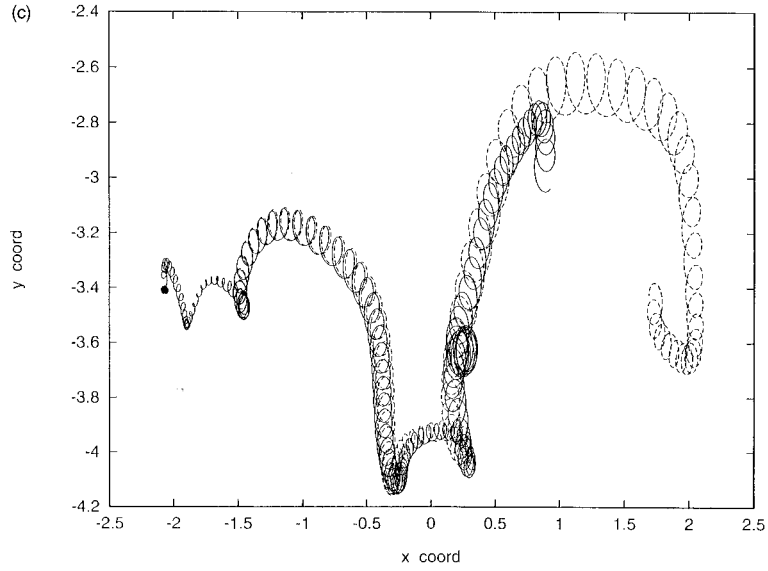


FIGURE 3 (Continued).

V. CONCLUSION

We assert that (16) provides the best algorithm for dynamics calculations for a system of charged particles in a constant external magnetic field. It is as simple to use as any of the alternatives, and it alone agrees with the exact solution for magnetic force only.

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