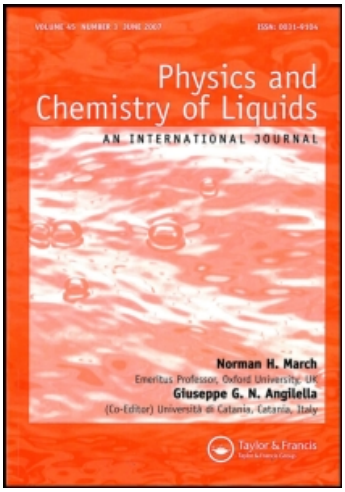

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DIFFUSION OF ONE-COMPONENT PLASMA IN A MAGNETIC FIELD – MOLECULAR DYNAMICS STUDY

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Molecular dynamics calculations have been performed on a classical, 3-dimensional one-component plasma, subjected to a magnetic field, which is uniform and constant in magnitude and direction; various values of the plasma parameter and magnetic field strength were considered. The Ewald sum technique was used to deal with the long-range Coulomb force, while the effects of the magnetic field were incorporated using a recently developed algorithm. This algorithm takes into account the effects of the magnetic field *exactly* and thus is more accurate than ones used previously. The two diffusion coefficients D_z and D_x, respectively parallel and perpendicular to the magnetic field have been calculated. Both coefficients decrease as a function of the magnetic field strength, but they differ considerably, with D_x always less than D_z. A noticeable plateau is observed in the plots of the diffusion coefficients, especially for intermediate values of the plasma parameter. A simple theoretical model based on the generalized Langevin equation is presented; its results are in reasonable qualitative agreement with the values obtained from molecular dynamics.

Keywords: One-component plasma; Molecular dynamics; Diffusion; Langevin equation

I. INTRODUCTION

The one-component plasma (OCP) is the simplest model of an ionic fluid in which classical, identical point ions move in a uniform and rigid neutralizing background of electrons. The static properties of the OCP depend on a single dimensionless plasma parameter $\Gamma = e^2/r_0 k_B T$, where $r_0 = (3/4\pi\rho)^{1/3}$ is the ion-sphere radius, e is the electronic charge, T is the temperature and ρ is the number density. Various static and dynamic properties of this system have been studied using Monte Carlo and Molecular Dynamics (MD) techniques. The reader is directed to an article by Baus and Hansen [1], for a comprehensive review and an extensive list of references.

However, the study of an OCP in a magnetic field has not received much attention. Such a system could serve as a prototype for some astrophysical and terrestrial plasmas. Bernu [2] performed rather limited MD simulations of the velocity correlation function

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and developed a primitive theoretical model. His simulation used an approximate algorithm to include the effects of a magnetic field and his model predicted that the diffusion parallel to the direction of the magnetic field is independent of the field strength; this is contrary to his own MD results.

Recently, we developed an exact algorithm [3] for the motion of a charged particle in a constant magnetic field and extended it to include position-dependent forces, of which the Coulomb force is an example. This algorithm was used in an MD calculation of the diffusion coefficient of a 2-dimensional electron fluid in the presence of a magnetic field [4]. The scarcity of data for a similar 3-dimensional system and our new algorithm provided an incentive for us to perform extensive MD calculations to study diffusion of a 3-dimensional OCP as a function of the plasma parameter and magnetic field. We have also developed a model for diffusion, based on the Langevin equation; it is a one-parameter model and produces a reasonable qualitative agreement for both diffusion coefficients, D_x (perpendicular to the field direction) and D_z (parallel).

II. SIMULATION DETAILS

The system is a classical 3-dimensional OCP with electrons of charge e and mass m embedded in a uniform neutralizing background of opposite charge. There is a uniform, constant magnetic field strength B in the z-direction. In our MD simulation there are N electrons in a cube of side length L, interacting through the Coulomb potential $\phi(r) = e^2/r$. The problem of the long-range nature of the potential in MD simulations is handled using the Ewald technique for effectively summing the interaction of an electron with all of its infinite periodic images [5]. It expresses the potential energy U in terms of two convergent summations, one in real space and one in reciprocal lattice space. The well-known result [6] is

$$\begin{aligned} U &= \frac{1}{2}{\sum_{\boldsymbol{p}}}' \sum_{i=1}^{N} \sum_{j=1}^{N} \phi(|\boldsymbol{r}_i - \boldsymbol{r}_j + \boldsymbol{p}|) \\ &= \frac{e^2}{2}{\sum_{\boldsymbol{p}}}' \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{\operatorname{erfc}(\alpha|\boldsymbol{r}_i - \boldsymbol{r}_j + \boldsymbol{p}|)}{|\boldsymbol{r}_i - \boldsymbol{r}_j + \boldsymbol{p}|} - N\frac{e^2\alpha}{\sqrt{\pi}} \\ &\quad + \frac{e^2}{\pi L^3} \sum_{\boldsymbol{g}\neq\boldsymbol{0}} \frac{4\pi^2}{g^2} \exp\left(-\frac{g^2}{4\alpha^2}\right)\left(\sum_{i=1}^{N}\sum_{j=1}^{N} \cos[\boldsymbol{g}\circ(\boldsymbol{r}_i - \boldsymbol{r}_j)]\right). \end{aligned} \tag{1}$$

The sum over $\boldsymbol{p}$ is taken over all lattice points, $\boldsymbol{p} = L(\lambda_1, \lambda_2, \lambda_3)$ with $(\lambda_1, \lambda_2, \lambda_3)$ integers; the prime on this sum implies that if $i = j$, the $\boldsymbol{p} = 0$ term is to be omitted; $\boldsymbol{g}$ is the reciprocal lattice vector given by $\boldsymbol{g} = (2\pi/L)(\lambda_1, \lambda_2, \lambda_3)$. The parameter α is chosen so that both series in (1) converge rapidly. Including the effect of the magnetic field, the force on particle 1, say, is given by

$$\begin{aligned} \boldsymbol{F}(\boldsymbol{r}_1) = -\nabla_{r_1} U &= e^2 \frac{2\pi}{L^3} \sum_{\boldsymbol{g}\neq\boldsymbol{0}} \boldsymbol{g}\left\{\frac{1}{g^2}\exp(-g^2/4\alpha^2)\sum_{j=2}^{N}\sin[\boldsymbol{g}\circ(\boldsymbol{r}_1 - \boldsymbol{r}_j)]\right\} \\ &\quad + e^2 {\sum_{\boldsymbol{p}}}' \sum_{j=1}^{N} \frac{\boldsymbol{s}_{1j}}{|\boldsymbol{s}_{1j}|^3}\left\{\operatorname{erfc}(\alpha|\boldsymbol{s}_{1j}|) + \alpha|\boldsymbol{s}_{1j}|\frac{2}{\sqrt{\pi}}\exp(-\alpha^2|\boldsymbol{s}_{1j}|^2)\right\} \\ &\quad - \frac{eB}{c}\dot{\boldsymbol{r}}_1 \times \hat{z} \end{aligned} \tag{2}$$

where $\boldsymbol{s}_{1j} = \boldsymbol{r}_1 - \boldsymbol{r}_j + \boldsymbol{p}$ and c is the speed of light. If α is chosen large enough, the only term that contributes to the sum in real-space is that with $\boldsymbol{p} = 0$, and so the real-space sum reduces to the usual minimum image convention. We chose $\alpha = 5/L$ and truncated the real-space sum at $\boldsymbol{p} = 0$, as is normally done in such simulations. A large value of α would require a large number of terms in the reciprocal-space sum. As per previous simulations, we fixed the maximum value of the integer set $(\lambda_1,\lambda_2,\lambda_3)$ at 5, with the constraint that $\lambda_1^2 + \lambda_2^2 + \lambda_3^2 \leq 27$. In the simulation we use dimensionless parameters: distances in units of the ion-sphere radius r_0, energies in units of e^2/r_0, time in units of $\tau = \sqrt{mr_0^3/e^2}$ and magnetic field B in units of $mc/e\tau$. The following algorithm for the particle dynamics in dimensionless units includes the effects of the Coulomb force and the magnetic field [3].

$$
\begin{aligned}
x(t+h) &= \frac{1}{1+a^2}\{2x(t) - x(t-h) - 2a[y(t) - y(t-h)] + a^2 x(t-h) + Ah^2[f_x(t) - af_y(t)]\} \\
y(t+h) &= \frac{1}{1+a^2}\{2y(t) - y(t-h) + 2a[x(t) - x(t-h)] + a^2 y(t-h) + Ah^2[f_y(t) + af_x(t)]\} \\
z(t+h) &= \{2z(t) - z(t-h)\} + h^2 f_z(t).
\end{aligned} \tag{3}
$$

The velocity components are

$$
\begin{aligned}
v_x(t) &= c_1 \frac{1}{2h}\{x(t+h) - x(t-h)\} - c_2 h f_y(t) \\
v_y(t) &= c_1 \frac{1}{2h}\{y(t+h) - y(t-h)\} + c_2 h f_x(t) \\
v_z(t) &= \frac{1}{2h}\{z(t+h) - z(t-h)\}.
\end{aligned} \tag{4}
$$

Here $a = (1 - \cos(Bh))/\sin(Bh)$, $A = 2a/Bh$, $c_1 = Bh/\sin(Bh)$ and $c_2 = (\sin(Bh) - Bh)/Bh\sin(Bh)$ where h is the time step; $f_x(t)$, $f_y(t)$ and $f_z(t)$ are the components of the Ewald sum expression for the Coulomb force. The z-component is not affected by the magnetic field and hence is given by the usual Verlet algorithm. The velocity results are used to control the temperature and confirm total energy conservation of the system during the calculation.

We use the algorithm given by Eqs. (3) and (4) in our MD simulation. The basic cell is a cube with side $L = (N/\rho r_0^3)^{1/3}$ and containing 108 electrons; this translates to $L = 7.68$ in dimensionless units. The starting configuration for the electrons was a face-centered cubic structure, with velocities given by the Maxwellian distribution determined by the given plasma parameter Γ (i.e. inverse temperature). The time step h was chosen to be 0.04 in dimensionless units. Temperature scaling was done every 50-time steps. The equilibrium configuration was reached after running the MD simulation typically for 15 000 time steps (in 5 cycles of 2000 time steps with scaling and 1000 without). Then, with the temperature scaling off, the position co-ordinates of the 108 electrons for 20 000 time steps were stored. We were able to maintain the temperature to within 2% of the desired temperature. These co-ordinates were later used to obtain the mean-square displacement from which the diffusion coefficients were obtained. Simulations were performed for various values of Γ from 10 to 110; for each Γ several

values of B between 0 and 4 were considered. For some typical numbers, one can refer to the phase diagram of the OCP [7]. From the diagram, one can deduce, for example, that an electron density of $\rho = 10^{16}\,\mathrm{cm}^{-3}$ and a temperature of 10 K falls in the domain of classical plasma; this corresponds to $\Gamma \sim 60$. B in Tesla then is approximately 20 times the B in dimensionless units, and $h = 0.04$ corresponds to about 0.01 ps.

III. DIFFUSION MODEL

Bernu [2] developed a model for the diffusion coefficients D_x and D_z by taking for the memory function of the velocity correlation function (VCF), a Gaussian form determined by the exact short-time behaviour of the appropriate VCF. This model is not satisfactory, as it predicts D_z to be independent of the magnetic field, contrary to the results of our MD simulation. In a recent paper [4], we developed a model based on the Langevin equation for diffusion of a 2-dimensional electron gas subjected to a magnetic field. Here we present an extension of this model for the system under consideration. The Langevin equation with a magnetic field can be written as

$$\frac{d\boldsymbol{v}}{dt} = -\int_0^t \gamma_B(t-s)\boldsymbol{v}(s)ds - \frac{e}{mc}\boldsymbol{v}\times\boldsymbol{B} + \boldsymbol{R}(t) \tag{5}$$

where $\boldsymbol{v}(t)$ is the velocity of the tagged particle, $\gamma_B(t)$ is a time-dependent friction coefficient which depends on the magnetic field $\boldsymbol{B}$, and $\boldsymbol{R}(t)$ is a random force (per unit mass) which averages to zero and is not correlated with the velocity of the particle. Since $\boldsymbol{B}$ is in the z-direction we have

$$\boldsymbol{v}\times\boldsymbol{B} = B\underline{\underline{\sigma}}\boldsymbol{v}, \quad \text{where} \quad \underline{\underline{\sigma}} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Taking the Laplace transform of (5), noting that the contribution from the random force to each diffusion coefficient is zero and simplifying, we obtain

$$\hat{\boldsymbol{v}}(\omega) = (\underline{\underline{I}} - b(\omega)\underline{\underline{\sigma}})^{-1}\frac{\boldsymbol{v}(0)}{i\omega + \hat{\gamma}_B(\omega)}, \tag{6}$$

where $\underline{\underline{I}}$ is the unit matrix and $b(\omega) = (e/mc)(B/(i\omega + \hat{\gamma}_B(\omega)))$. It can be easily shown that

$$(\underline{\underline{I}} - b(\omega)\underline{\underline{\sigma}})^{-1} = \frac{1}{1+b^2}\underline{\underline{P}} \quad \text{where} \quad \underline{\underline{P}} = \begin{pmatrix} 1 & b & 0 \\ -b & 1 & 0 \\ 0 & 0 & 1+b^2 \end{pmatrix};$$

we have dropped the dependence of b on ω for clarity. The self-diffusion coefficient, defined as

$$D = \int_0^\infty \langle \boldsymbol{v}(t)\circ\boldsymbol{v}(0)\rangle dt = \langle \hat{\boldsymbol{v}}(0)\circ\boldsymbol{v}(0)\rangle, \tag{7}$$

can now be written as

$$D = \frac{1}{1+b^2}\frac{1}{\hat{\gamma}_B(0)}\Big[\langle v_x^2(0)\rangle + \langle v_y^2(0)\rangle + (1+b^2)\langle v_z^2(0)\rangle\Big]. \tag{8}$$

This expression can naturally be broken into x, y and z-components of diffusion. For the system being considered all results are symmetric in x and y; we label the diffusion coefficient perpendicular to the magnetic field by x. Since $\langle v_x^2(0)\rangle = (k_B T/m)$, the diffusion coefficients can be written as

$$\begin{aligned} D_z(B) &= \frac{1}{\Gamma}\frac{1}{\hat{\gamma}_B(0)} = \frac{1}{\Gamma}\frac{1}{\hat{\gamma}_0(0)}\frac{\hat{\gamma}_0(0)}{\hat{\gamma}_B(0)} = \frac{D_z(0)}{f_B} \quad \text{where} \quad f_B = \frac{\hat{\gamma}_B(0)}{\hat{\gamma}_0(0)} \\ D_x(B) &= \frac{1}{\Gamma}\frac{\hat{\gamma}_B(0)}{\hat{\gamma}_B^2(0)+B^2} = \frac{D_z(0) f_B}{f_B^2 + [B\Gamma D_z(0)]^2}. \end{aligned} \tag{9}$$

These equations are in dimensionless units and their results are to be compared with the corresponding MD values.

Equation (9) indicate that *both* diffusion coefficients depend on the magnetic field strength B; the only unknown parameter is f_B, which also depends on Γ. Note that f_B denotes the functional dependence of the friction coefficient γ(at $\omega = 0$) on B. The value of $D_z(0)$ was taken from the MD result for each value of Γ. Based on our analysis of a similar 2-dimensional system [4], we chose a quadratic dependence for f_B on magnetic field, viz. $f_B = 1 + \delta^2 B^2$, and determined δ from a best fit of the MD values of $D_z(B)$. Having done this, the expression for $D_x(B)$ is free of any parameters and is specified completely.

IV. RESULTS AND DISCUSSION

The stored (x, y, z) position co-ordinates of the 108 electrons for 20 000 time steps are utilized to calculate quantities of interest. The mean-square displacement (MSD) has x-component $\langle \Delta x^2(t)\rangle = (1/N)\langle \sum_{j=1}^{N} [x_j(t) - x_j(0)]^2\rangle$ and so on. The diffusion coefficients D_x and D_z can be calculated using the corresponding MSD component at large times, either by computing its slope or by dividing it by time.

$$D_x = \lim_{t\to\infty} \frac{\langle \Delta x^2(t)\rangle}{2t} = \lim_{t\to\infty} \frac{1}{2}\frac{d}{dt}\langle \Delta x^2(t)\rangle, \tag{10}$$

and similar expressions can be written for D_y and D_z; symmetry requires that $D_y = D_x$.

We have performed extensive simulations and obtained diffusion coefficients for several values of Γ ranging from 10 to 110, and for magnetic field strengths B ranging from 0 to 4. Results are presented here for three representative values from hotter to cooler: $\Gamma = 20$, 50 and 80. Figure 1 shows a plot of the two diffusion coefficients as a function of B for $\Gamma = 20$; MD values for D_z and D_x are displayed by triangles and diamonds, respectively. The predictions of our theoretical diffusion model as given by Eqs. (9), are indicated by a solid curve of D_z and a dashed curve of D_x. As stated earlier, our model depends on one parameter δ; we chose this parameter so

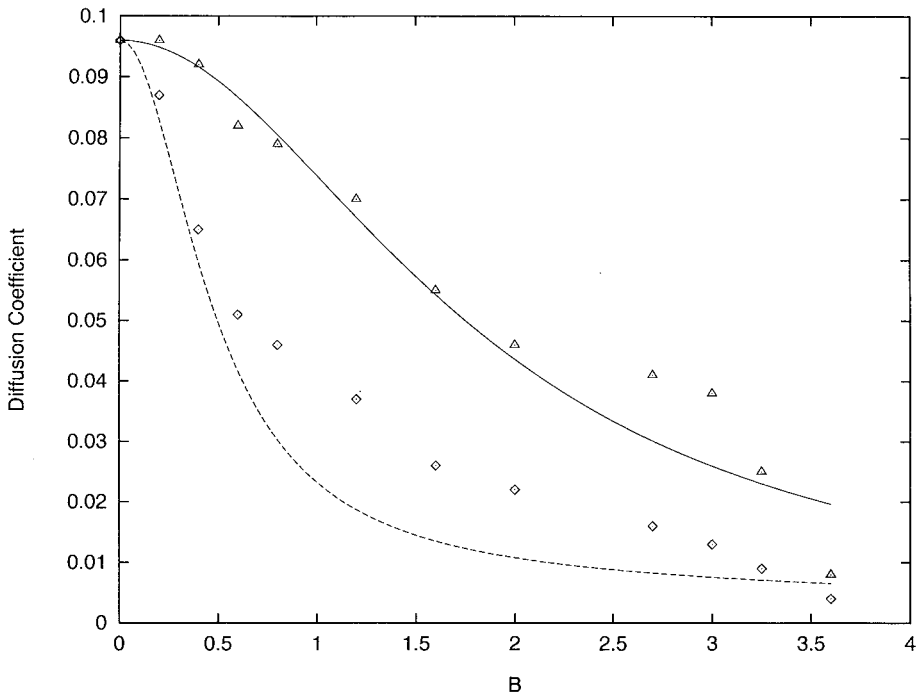

FIGURE 1 Plot of the two diffusion coefficients as a function of the magnetic field strength B for $\Gamma = 20$. MD results are denoted by triangles for D_z and by diamonds for D_x. The model results are denoted by the solid curve for D_z and by the dashed curve for D_x.

as to get the best fit to the MD results for D_z. The MD results indicate that. D_x is always less than D_z, and both coefficients show a monotonic decrease as B is increased. The effect of the magnetic field is to constrain the translational motion of the electron, and thus the behaviour of D_x is roughly as expected since the x and y components are directly affected by the magnetic field. Although the z-component of the equation of motion does not contain B explicitly, the time-dependence of each z-coordinate is, nevertheless, coupled to the variations of the x and y coordinates since the force in the z-direction depends on all three components of the position. Thus D_z is expected to decrease with B, albeit at a slower rate than D_x.

A careful look at Fig. 1 reveals an interesting feature, in that the decrease in the diffusion coefficients is not uniform. For small B the decrease is uniform and monotonic, then there is a region of B in which the diffusion coefficient decreases much more slowly; this is followed by a rather steep decrease leading to almost zero diffusion for large B. This plateau feature is more pronounced for D_z than D_x. We have observed this behaviour for all values of Γ, not just those presented here, and feel that this feature is real and not an artefact of our MD programme. It is more prominent at intermediate values of Γ. For large values of Γ, the diffusion coefficient is small to start with, and hence the plateau is not so obvious. For small values of Γ, the decrease in the diffusion coefficient is very gradual which masks the plateau effect.

Our simple theoretical model predicts that D_x is always less than D_z, and its results agree qualitatively with the MD values for both diffusion coefficients. The MD results, which show a plateau followed by a rather sharp decrease of the diffusion coefficient,

especially for D_z, suggest that more complex physical processes are involved. Therefore, a simple Langevin model is not sufficient to describe the process of diffusion in a 3-dimensional OCP in the presence of a magnetic field.

Figures 2 and 3 show similar plots of the two diffusion coefficients for $\Gamma = 50$ and 80, respectively; the symbols are the same as in Fig. 1. The behaviour is similar to what was seen for $\Gamma = 20$. However, the values of B where the plateau starts and where the diffusion falls off sharply are smaller than in Fig. 1.

The presence of the magnetic field shows itself in the plots of the MSD in an interesting fashion. In a central force field, MSD involves only translational motion and hence starts off in a quadratic fashion for small times and becomes linear at long times. The effect of the magnetic field alone is to make the charged particle go in circles, and the MSD of our system reflects both contributions. In Fig. 4 we show the MSD in the $x-y$ plane for very small times t in [0, 10] for $\Gamma = 20$ and $B = 3.0$, 3.6 and 4.4. One clearly sees sinusoidal oscillations, due to the magnetic field. The frequency of the oscillation is the cyclotron frequency, $\omega = eB/mc$, which in dimensionless units becomes simply $\omega = B$. The time period is thus given by $\tau_B = 2\pi/B$. The graph shows precisely this time period for the various values of B. It is also seen that the overall behaviour of the MSD is quadratic, as it should be. For longer times, this behaviour should go over to linear, and the effect of the magnetic field should be smeared out. This is exactly what is seen in Fig. 5, where the same MSD of Fig. 4 is extended to t in [0, 40]. The amplitude of oscillation decreases at longer times, though the time period of course stays the same.

It is realized that although the equation of motion for the z-component of the position does not involve magnetic field directly, it does depend on B. Figure 6 is intended

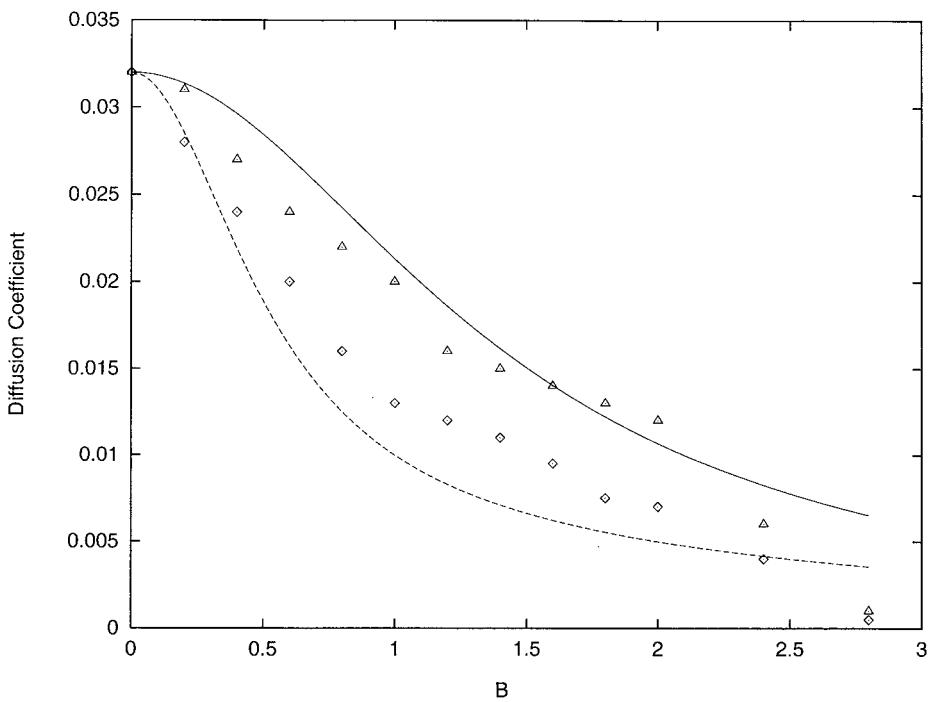

FIGURE 2 Same as Figure 1, except for $\Gamma = 50$.

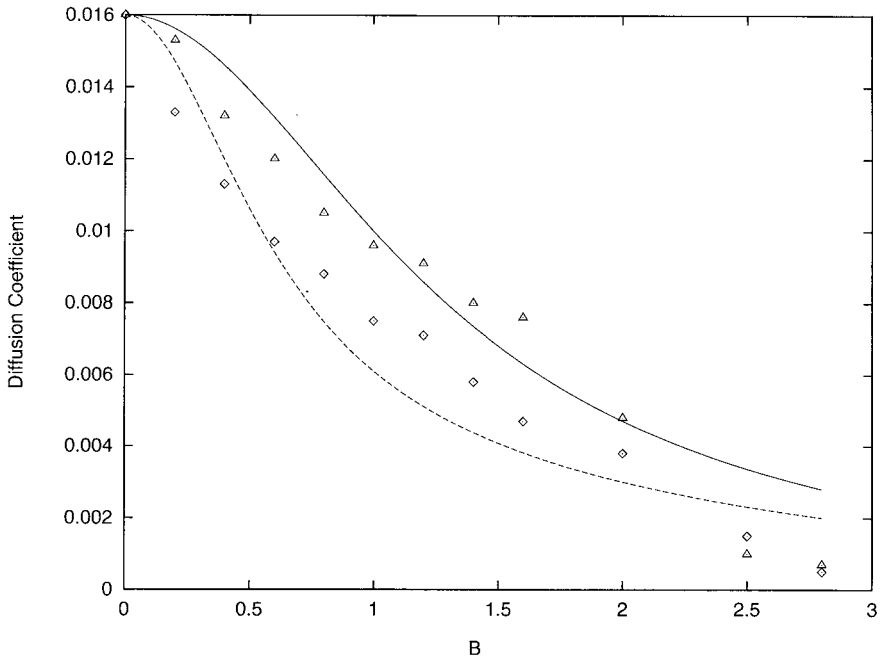

FIGURE 3 Same as Figure 1, except for $\Gamma = 80$.

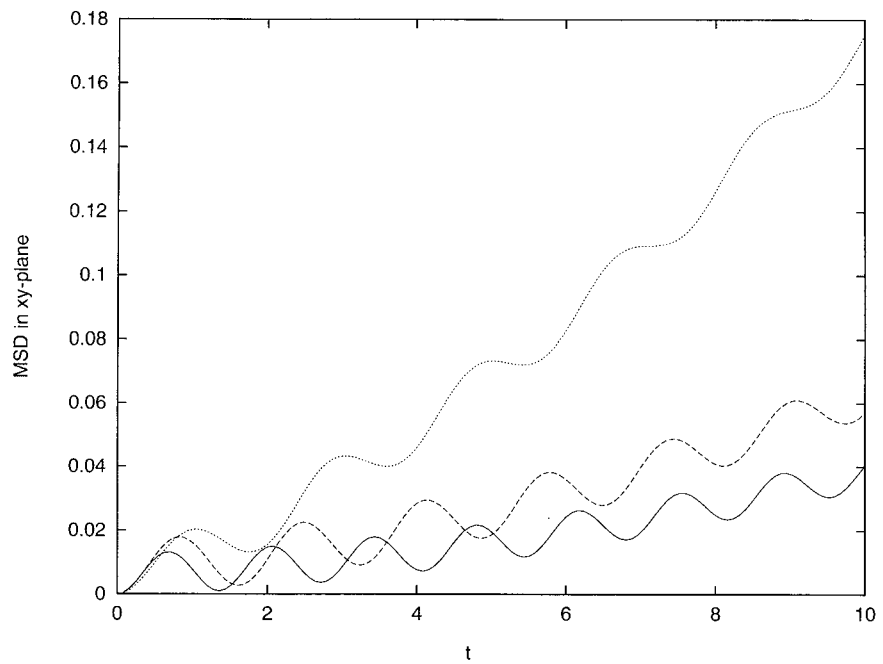

FIGURE 4 Plot of the mean-square displacement $< \Delta x^2 >$ as function of time t in $[0, 10]$, for $\Gamma = 20$. Solid curve represents $B = 4.4$, dashed curve represents $B = 3.6$ and dotted curve represents $B = 3.0$.

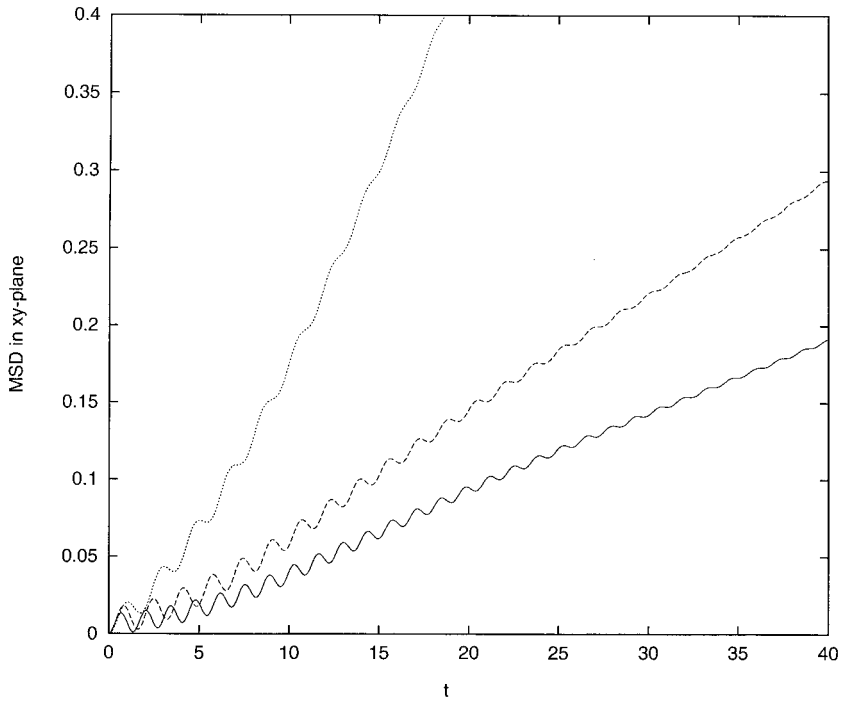

FIGURE 5 Same as Figure 4, except for t in [0, 40].

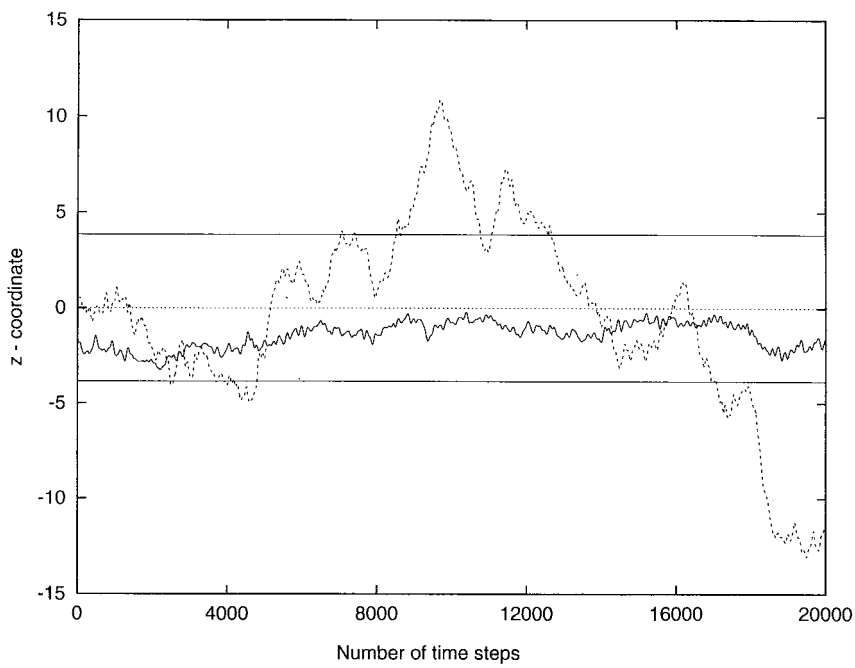

FIGURE 6 Plot of z-coordinate of a typical particle as a function of time. The solid curve is for $B=4.4$ and the dotted for $B=0$; both for $\Gamma=20$. The horizontal lines indicate the bounds of the basic simulation cell.

to display clearly the fact that diffusion parallel to the magnetic field is affected by the field. The z-coordinate of a typical particle is shown for the time interval used for diffusion calculations. The plots are for $B=0$ and 4.4, for $\Gamma=20$. The horizontal lines at ± 3.84 indicate the bounds of the basic cell. It is clear from the figure that for $B=4.4$, the z-coordinate is much constrained and this is reflected in the very small diffusion coefficient D_z.

V. CONCLUSION

We have performed extensive molecular dynamics simulation of a 3-dimensional, classical one-component plasma in the presence of a uniform, constant magnetic field. A recently developed algorithm that treats the effects of a magnetic field *exactly* has been used in the simulation. The diffusion coefficients, one parallel to and the other perpendicular to the magnetic field, have been computed for a number of values of the plasma parameter and the magnetic field strength. The diffusion coefficients fall off with magnetic field strength, but the decrease is not uniform. After an initial steady decrease, there seems to be a plateau followed by a steeper decrease, as the magnetic field strength is increased. This phenomenon occurs for all values for the plasma parameter, but is more pronounced at intermediate values, and for the diffusion coefficient parallel to the magnetic field. A simple theoretical model, based on the Langevin equation produced results that are in qualitative agreement with MD values. Further development of a model to explain all of the observed features would be valuable.

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