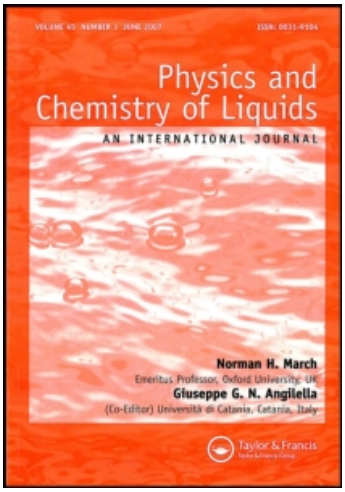

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MAGNETIC FIELD EFFECTS ON DIFFUSION IN 2-DIMENSIONAL ELECTRON FLUID

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Molecular Dynamics calculations have been performed on a 2-dimensional (2D) electron fluid interacting with a $1/r$ potential, and subjected to a perpendicular, uniform and constant magnetic field, for various values of the plasma parameter Γ. A new and more accurate algorithm, that takes into account the effects of the magnetic field exactly, has been used in the simulation. The diffusion coefficient has been calculated and the results show a monotonic decrease as a function of the magnetic field strength. A simple theoretical model based on a generalized Langevin equation predicts a Lorentzian dependence. The model results are in reasonable agreement with the Molecular Dynamics results, especially for higher values of Γ.

Keywords: Electron fluid; Molecular dynamics; Diffusion; Langevin equation

INTRODUCTION

Static, dynamic and transport properties of classical 2-dimensional (2D), one-component plasma (OCP) have been studied using Monte Carlo and Molecular Dynamics (MD) techniques for a number of

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years [1–3]. The electrons interact through the Coulomb potential and, to ensure charge neutrality, the particles are immersed in a uniform background of positive charge. The thermodynamic state of the OCP is completely determined by the dimensionless plasma parameter $\Gamma = e^2/r_0 k_B T$, where r_0 is Wigner–Seitz disk radius, related to the number density n through $nr_0^2 = 1/\pi$, e is the charge of the electron, T is the temperature and k_B is the Boltzmann constant. Studies have shown that the system exhibits fluid–solid transition around $\Gamma = 130$.

When it comes to transport coefficients, some fundamental difficulties remain. Theory predicts that time-correlation functions (TCF) in 2D should decay as $1/t$ for large times, so that transport coefficients, which are the time-integrals of TCF, would then diverge. However, one can estimate a value for the diffusion coefficient, for example, from the long-time slope of the mean-square displacement (msd) of a particle. MD simulations on 2D, classical electron fluid, indicate that the msd is linear at long times and hence support the existence of a diffusion constant. Using such an approach, diffusion coefficients for a 2D OCP, for a range of values of Γ, have been obtained [4,5].

In this paper, we investigate the effect of a magnetic field on diffusion of a 2D OCP. Hansen *et al.* [4] claimed that the diffusion in such a system obtained through MD methods is *not* affected by magnetic fields. The standard treatment of such MD simulations is to use periodic boundary conditions in conjunction with Ewald summations of the Coulomb interaction with the infinite array of periodic images of the other particles and the background. However, they chose to place the electrons on the surface of a three-dimensional sphere and thus avoid boundary conditions from the start. They have verified their methodology, but their conclusion on the independence of diffusion on magnetic field is in variance with expected behaviour. Since the effect of a magnetic field is to make the electrons go in a circular path, it is to be anticipated that the diffusion coefficient should decrease as the magnetic field strength is increased. Bernu [6] studied a three-dimensional OCP in a magnetic field and concluded that the magnetic field effect is to decrease the diffusion coefficient. But in this case, there are two diffusion coefficients to consider, one parallel and the other perpendicular to the magnetic field.

In addition, there are different algorithms to take into account the effect of a magnetic field on the motion of the electron. It seems that Bernu [6] has used one that does yield a circular path (in 2 dimensions) for a pure magnetic field motion, but the circle is not the one that is obtained based on exact dynamics. Hansen *et al.* [4] do not indicate the algorithm they used in their simulation. We have developed an algorithm [7] that takes into account the effects of a magnetic field *exactly*. Based on these developments, we felt it would be constructive to investigate again, through MD simulation methods, magnetic field effects on diffusion in a 2D OCP.

SIMULATION DETAILS

The system is a classical 2D OCP with N electrons of charge e and mass m embedded in a uniform neutralizing background. The electrons are in a square box of side length L and interact 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 [8] sum, a technique for effectively summing the interaction of an electron with all of its infinite periodic images. 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 [1] is

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

The sum over $\bar{p}$ is a sum over integers λ_1, λ_2 with $\bar{p} = L(\lambda_1, \lambda_2)$; the prime on this sum implies that if $i=j$, the $\bar{p} = 0$ term is to be omitted. The parameter α is to be chosen that both series in (1) converge

rapidly. The force on particle 1, say, is then given by [9]

$$\bar{F}(\bar{r}_1) = -\nabla_{\bar{r}_1} U = \frac{2\pi}{L^2} \sum_{\bar{g}\neq\bar{0}} \bar{g} \left\{ \frac{1}{g} \operatorname{erfc}\left(\frac{g}{2\alpha}\right) \sum_{j=2}^{N} \sin[\bar{g} \circ (\bar{r}_1 - \bar{r}_j)] \right\}$$

$$+ \sum_{\bar{p}}{}' \sum_{j=1}^{N} \frac{\bar{s}_{1j}}{|\bar{s}_{1j}|^3} \left\{ \operatorname{erfc}(\alpha|\bar{s}_{1j}|) + \alpha|\bar{s}_{1j}| \frac{2}{\sqrt{\pi}} \exp(-\alpha^2|\bar{s}_{1j}|^2) \right\} \qquad (2)$$

where $\bar{s}_{1j} = \bar{r}_1 - \bar{r}_j + \bar{p}$.

In addition, the electrons in our system are subjected to uniform and constant magnetic field acting perpendicular to the 2D plane. The force is given by the Lorentz term. We have developed a new algorithm that takes into account the effects of the magnetic field exactly. This result, which includes the effects of the Coulomb force and the magnetic field, is [7]

$$\begin{aligned} x(t+h) &= \{2x(t) - x(t-h) - 2a[y(t) - y(t-h)] + a^2 x(t-h) \\ &\quad + Ah^2[f_x(t) - a f_y(t)]\}/(1+a^2) \\ y(t+h) &= \{2y(t) - y(t-h) + 2a[x(t) - x(t-h)] + a^2 y(t-h) \\ &\quad + Ah^2[f_y(t) + a f_x(t)]\}/(1+a^2) \end{aligned} \qquad (3)$$

Here $a = 1 - \cos(Bh)/\sin(Bh)$ and $A = 2a/Bh$ where B is the magnetic field strength and h is the time step; $f_x(t)$ and $f_y(t)$ are the components of the Ewald sum expression for the Coulomb force. In the simulation, we use dimensionless parameters: distances in units of the Wigner-Seitz radius r_0, energies in units of e^2/r_0, time in units of $\tau = (mr_0^3/e^2)^{1/2}$ and magnetic field B in units of $mc/e\tau$, with c being the velocity of light. We use the above algorithm (3) in our MD simulation.

The basic cell is a square with side $L = (N/nr_0^2)^{1/2}$ and containing 128 electrons. The starting configuration for the electrons was a face-centered 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 for

30,000 time steps (in five cycles of 6000 time steps). We were able to maintain the temperature to within about 2% of the desired temperature. The magnetic field was now turned on and the temperature scaling removed. The position co-ordinates of the 128 electrons for 60,000 time steps were stored. These co-ordinates were later used to obtain the pair distribution function and mean square displacement. Simulations were performed for $\Gamma = 10$, 50 and 90, and for each value of Γ, we considered $B = 0$, 1, 2, 3 and 4. For a typical areal electron density of 8×10^{12} per square meter, B in dimensionless units is approximately the same as B in Teslas, and $h = 0.04$ corresponds to about 0.22 ps.

DIFFUSION MODEL

We have developed a simple model, based on the generalized Langevin equation, to describe diffusion in presence of a magnetic field. The equation can be written as

$$\frac{d\bar{v}}{dt} = -\int_0^t \gamma(t-s)\bar{v}(s)\,ds - \frac{e}{mc}\bar{v} \times \bar{B} + \bar{R}(t), \tag{4}$$

where $\bar{v}(t)$ is the velocity of the tagged particle, $\gamma(t)$ is the time-dependent friction coefficient, $\bar{B}$ is the magnetic field, and $\bar{R}(t)$ is a random force (per unit mass) which averages to zero and is not correlated with the velocity of the particle. Since $\bar{B}$ is along the z-axis and the motion of the electron is along the x–y plane, we have

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

Taking Laplace transform of (4), we get

$$\bar{\hat{v}}(\omega) = (\underline{\underline{I}} - b(\omega)\underline{\underline{\sigma}})^{-1}\frac{\bar{\hat{R}}(\omega) + \bar{v}(0)}{i\omega + \hat{\gamma}(\omega)}, \tag{5}$$

where $\underline{\underline{I}}$ is the unit matrix and $b(\omega) = (e/mc)(B/(i\omega + \hat{\gamma}(\omega)))$.

The inverse of the matrix can be easily evaluated to yield

$$\bar{\tilde{\boldsymbol{v}}}(\omega) = \frac{\underline{\underline{I}} - b(\omega)\underline{\underline{\sigma}}^{-1}}{1 + b^2(\omega)} \frac{\bar{\tilde{\boldsymbol{R}}}(\omega) + \bar{v}(0)}{i\omega + \hat{\gamma}(\omega)}. \tag{6}$$

The self-diffusion coefficient is defined as

$$D = \int_0^\infty \left\langle \bar{v}(t) \circ \bar{v}(0) \right\rangle dt = \left\langle \bar{\tilde{v}}(0) \circ \bar{v}(0) \right\rangle. \tag{7}$$

Since the random force satisfies the property $\langle \bar{\boldsymbol{R}}(t) \circ \bar{v}(0) \rangle = 0$, and since $\langle \underline{\underline{\sigma}}^{-1}\, \bar{v}(0) \circ \bar{v}(0) \rangle = 0$, we obtain

$$D = \frac{D_0}{(1 + (b(0)/\hat{\gamma}(0))^2)}, \tag{8}$$

where $D_0 = (\langle \bar{v}(0) \circ \bar{v}(0) \rangle)/\hat{\gamma}(0)$ is the diffusion coefficient in the absence of a magnetic field. For a 2D system, $\langle \bar{v}(0) \circ \bar{v}(0) \rangle = 2k_B T/m$ and thus the diffusion coefficient, in units of r_0^2/τ, can be written as

$$D(B) = \frac{D_0}{1 + (B\Gamma D_0/2)^2} \tag{9}$$

with all quantities in dimensionless units.

Thus this simple model depends on the plasma parameter Γ, and predicts a monotonic Lorentzian decrease in diffusion as a function of the magnetic field strength. Since the model does not predict the value of D_0, we match it to its MD value in order to compare with the rest of our MD results.

RESULTS AND DISCUSSION

The stored (x, y) position co-ordinates of the 128 electrons for 60,000 time steps are utilized to calculate quantities of interest. We calculated the pair distribution function $g(r)$, not only to check the accuracy of our algorithm and the quality of our data, but also to see if it depends

on the magnetic field strength. For a classical system, the partition function would be independent of the magnetic field. Since any equilibrium quantity can be obtained from the partition function, it should not be affected by magnetic field. The pair distribution function $g(r)$, is one such example and is calculated using the formula

$$\langle n(r)\rangle = 2\pi r \Delta r n g(r), \tag{10}$$

where $\langle n(r)\rangle$ is the average number of particles in an annulus of radius r and thickness Δr, centered at a given particle. Δr was taken to be 0.02, and averages were carried out over 20,000 time steps, with every fifth time step as a new origin.

In Fig. 1, we have plotted $g(r)$ for $\Gamma = 90$ and for $B = 0$ (solid line) and $B = 4$ (dashed line). The Monte Carlo results of Gann *et al.* [2] are indicated by diamonds. We notice that our results are in complete agree-

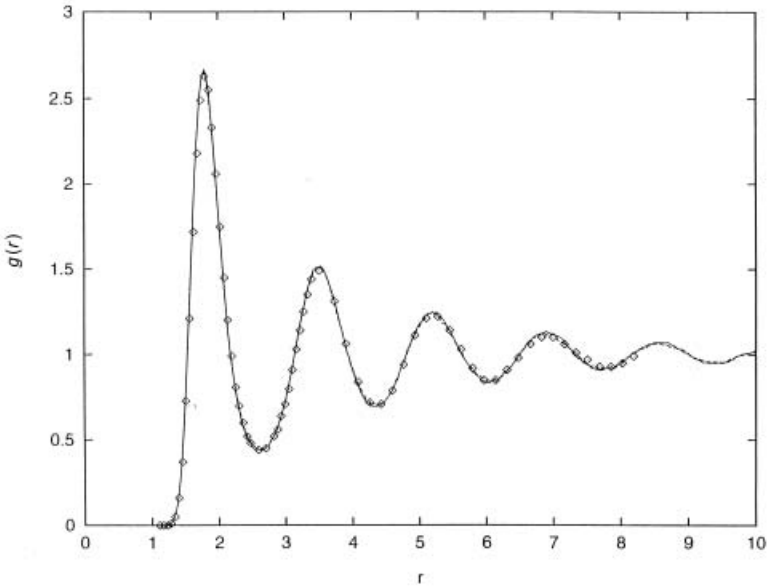


FIGURE 1 Plot, for $\Gamma = 90$, of the pair distribution function $g(r)$ as a function r in units of r_0. The solid line is for $B = 0$ and the dashed line for $B = 4$; note that these are nearly indistinguishable. The Monte Carlo results [2] are indicated by diamonds.

ment with those of Gann *et al.* and that, as expected, the pair distribution function is not affected by magnetic field.

The diffusion coefficient D can be calculated through the slope of the msd at large times, or equivalently from

$$D = \lim_{t\to\infty} \frac{\langle \Delta r^2(t)\rangle}{4t}$$

where

$$\langle \Delta r^2(t)\rangle = \frac{1}{N}\left\langle \sum_{j=1}^{N} \left|\bar{r}_j(t) - \bar{r}_j(0)\right|^2 \right\rangle \tag{11}$$

is the mean-square displacement.

The msd became linear and stayed linear, at times well before the 60,000 time-steps used in the simulation. The relative statistical error

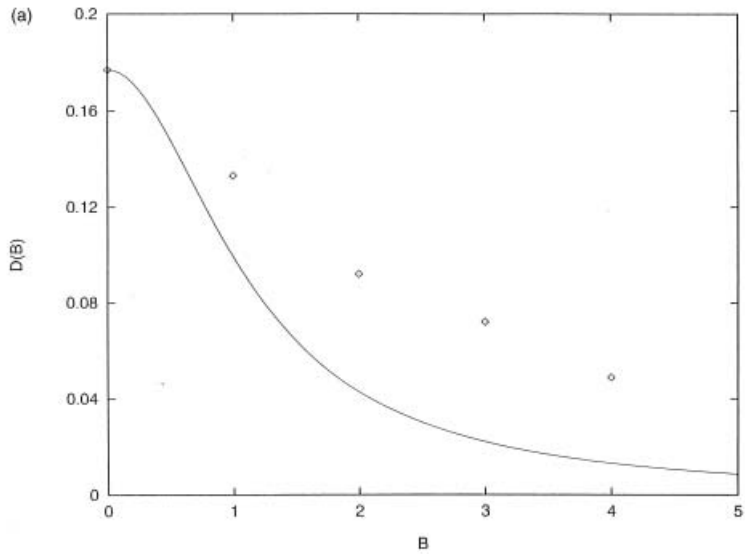
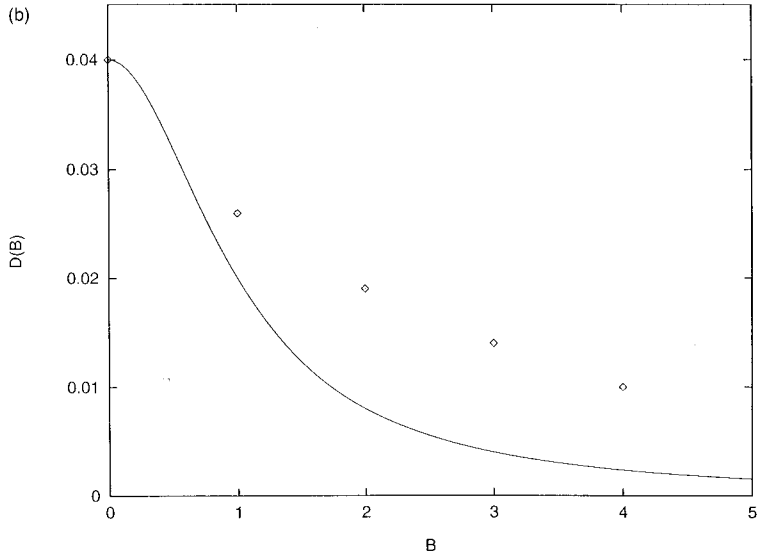


FIGURE 2 (a) Plot, for $\Gamma = 10$, of the diffusion coefficient as a function of the magnetic field strength, all in dimensionless units. MD results are indicated by diamonds and model results by solid line. (b) Same as (a), except for $\Gamma = 50$. (c) Same as (a), except for $\Gamma = 90$.



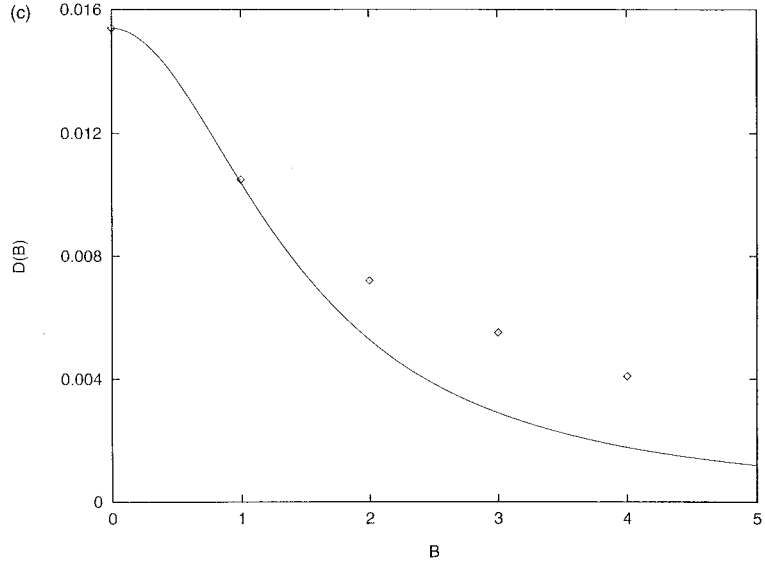


FIGURE 2 (Continued).

in our results on diffusion is estimated to be about 5%. In Fig. 2a, we have plotted the MD results (diamonds) and the model results (solid line) for $\Gamma = 10$, as a function of the magnetic field strength B. Similar plots are shown in Figs. 2b and 2c for $\Gamma = 50$ and 90, respectively. For comparison, we note that the diffusion coefficient, in the absence of a magnetic field, has been estimated at 0.014 [4] and 0.013 [5], for $\Gamma = 90$, while our result is 0.015.

Our model involves a parameter $\hat{\gamma}(0)$, which is related to the diffusion coefficient in the absence of the magnetic field. We chose to obtain this parameter by matching the model diffusion coefficient to that of MD at $B = 0$. An exact microscopic expression for the friction coefficient $\gamma(t)$ is known, but since it is intractable, attempts have been made to model $\gamma(t)$. A simple phenomenological form assumes a Gaussian, given by

$$\gamma(t) = \alpha \exp(-\beta t^2) \tag{12}$$

The parameters α and β can be related to the coefficients appearing in the short-time expansion (or equivalently the frequency moments) of the velocity correlation function [10]. These frequency moments can be expressed in terms of integrals involving the pair and triplet distribution functions. Using published results [10] for $\Gamma = 90$, one gets a value of 0.018 for D_0. One can then use this value, to calculate $D(B)$ from (9). It is seen that though this D_0 is about 20% off the MD value, the resulting graph is not significantly different for values of B greater than 1. In other words, our model predicts that the diffusion coefficient as a function of magnetic field strength is not significantly affected by its initial value.

It is seen from the plots that while the model does follow the trend of the MD results, the agreement is better at larger values of Γ. An explanation lies in the fact that the Langevin equation works best when the particles undergo many collisions. Thus it is better suited for higher densities, and higher densities imply higher values of Γ, at a constant temperature. We can improve the model by incorporating a dependence of the friction coefficient $\gamma(t)$ on magnetic field. At higher densities, there are more inter-particle collisions and hence one may anticipate the dependence to be weaker. On the other hand, at low densities, the particles undergo fewer collisions since they would be cir-

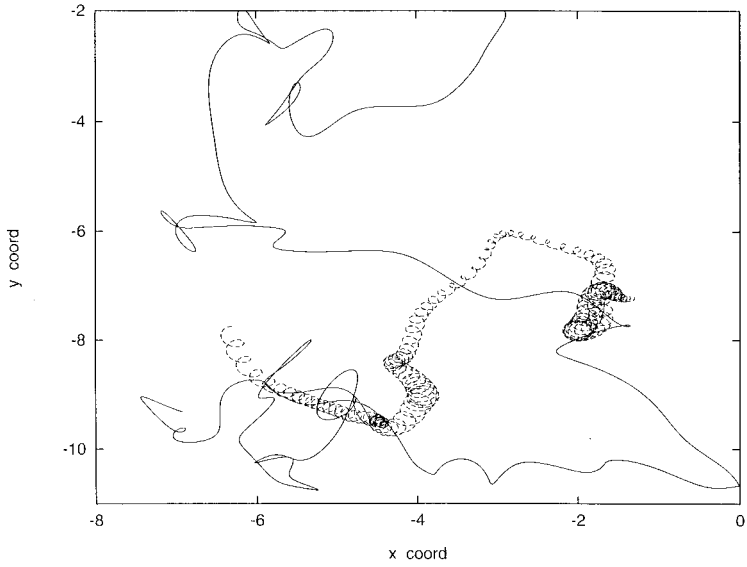


FIGURE 3 The motion of a typical electron for $\Gamma = 10$. Solid line is for $B = 0$ and the dashed line for $B = 4$.

culating about the magnetic field lines. Imagine, for example, the case of a high magnetic field, where each particle essentially circulates in small area and hardly undergoes a collision at all. In such a case, we would need to include an effective change in the friction coefficient as the magnetic field increases. We can improve the model by incorporating such a dependence, for example by introducing a term like $(1 + kB^2)$ in $\gamma(t)$, and obtaining the Γ-dependent (i.e. density dependent) parameter k by matching the diffusion coefficients at say $B = 1$.

In Fig. 3, we have plotted the motion of a typical electron for $\Gamma = 10$. The solid line represents $B = 0$ while the dashed line represents $B = 4$. One can see the formation of circular trajectories at the higher value of the magnetic field strength.

CONCLUSIONS

We have done extensive molecular dynamics simulation of a 2D electron gas interacting through the Coulomb potential, and subjected to a

uniform, constant and perpendicular magnetic field. A new algorithm, developed by us, has been used in the simulation. This algorithm treats the effects of the magnetic field exactly. MD results on diffusion clearly show a monotonic decrease as a function of magnetic field. We have also presented a simple model of diffusion, based on the generalized Langevin equation, for such a system. The results are in qualitative agreement with MD results.

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References

[1] H. Totsuji (1978). *Phys. Rev. A*, **17**, 399.
[2] R.C. Gann, S. Chakravarthy and G.V. Chester (1979). *Phys. Rev. B*, **20**, 326.
[3] H. Totsuji and H. Kakeya (1980). *Phys. Rev. A*, **22**, 1220.
[4] J.P. Hansen, D. Levesque and J.J. Weis (1979). *Phys. Rev. Lett*., **43**, 979.
[5] R.K. Kalia, P. Vashishta and S.W. deLeeuw (1981). *Phys. Rev. B*, **23**, 4794.
[6] B. Bernu (1981). *J. Physique-Lettres*, **42**, L-253.
[7] R.E. Johnson and S. Ranganathan (2002). *Phys. Chem. Liq.* (preceding paper).
[8] P.P. Ewald (1921). *Ann. Phys.* (*Leipzig*), **64**, 253.
[9] R.E. Johnson and S. Ranganathan (2001). *Phys. Rev. E*, **63**, 056703.
[10] G.K. Agarwal and K.N. Pathak (1983). *J. Phys. C: Solid State Phys*., **16**, 1887.