The velocity autocorrelation function (VAF) for a two-dimensional one-component plasma (OCP) is investigated by employing molecular dynamics techniques. The VAF exhibits well defined oscillations whose frequency is independent of the dimensionless coupling parameter $\Gamma$. However, the presence of a uniform perpendicular external magnetic field increases the height of the first peak. Molecular dynamics computer simulation results are presented for a two-dimensional OCP in a perpendicular magnetic field as a function of the Plasma parameter. Our simulation results clearly indicate that at high temperature, the magnetic field affects the VAF in a substantial way.

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I. INTRODUCTION

A great deal of effort has been devoted to gaining a better understanding of the optical and electron transport properties of one-component plasmas, which may be treated as two-dimensional electron gases (2DEG) or three-dimensional electron gases (3DEG) \cite{1-4}. This is due in part to 2DEG structures being used in models of semiconductor heterostructures. In contrast to its three-dimensional counterpart, the 2DEG is by far more challenging because of the quantum effects arising from the confinement. In studying static properties, both integral equation theory and Monte Carlo simulations have been developed. The hypernetted chain (HNC) approximation integral equation theory has been proved to be quite accurate compared to simulations based on phenomenological models \cite{3}, but it requires more elaborate numerical calculations due to the time consuming Frankel transform, i.e., the two-dimensional Fourier transform. Moreover, in the absence of a magnetic field,
dynamical properties have been investigated through molecular dynamics (MD) and Kubo-Greenwood short time expansions. Good agreement between these two approaches has been reported in the literature [5].

Fabrication of high mobility 2DEGs is desirable in the semiconductor industry. In these structures, electrons are confined in a layer between two carefully chosen semiconductor materials, such as GaAs and AlGaAs. These have found useful applications in semiconductor devices as a result of the unique electron transport properties at the interface. In low magnetic fields, applied perpendicular to the 2DEG, unusual transport properties have been observed. Apart from the well-known magnetoresistance oscillations which are due to commensurability effects in modulated 2D systems [6–10], a number of other low magnetic field anomalies appear at low temperature. For example, an observed anomaly is the positive magnetoresistance followed by a resistance drop at higher magnetic fields. Such behavior was observed in metallic single crystals [11, 12]. It has been successfully explained by the suppression of Bragg reflections due to the Lorentz force induced by the magnetic field, an effect known as magnetic breakdown [13].

A considerable amount of information is available for the electron transport and optical properties of the 2DEG [14–16] from both an experimental and theoretical point of view in the absence of a magnetic field. However, the effect of a perpendicular magnetic field could lead to novel behavior when the Coulomb interaction cannot be neglected [17]. Since an understanding of the physics of these systems in an applied magnetic field is helpful in device and metrological applications, there is much interest in their properties as a function of an applied field. For example, Cunningham, et al. [18] and Wright, et al. [19] have analyzed the effect of a perpendicular magnetic field on the plateaus of an acoustoelectric current in a narrow channel within a 2DEG. Their goal was to examine how the quantization of the acoustoelectric current was affected by magnetic field.

There has been a great deal of interest in the static, dynamic and thermodynamic properties of two-dimensional (2D) electron systems on Helium and other substrates [6]. More recently, there has been much effort regarding how a substrate affects the collective modes of graphene [20, 21]. The 2D system we are concerned with is described by the Coulomb potential which is the solution of Poisson’s equation, and is thus given by $U(r) = -\frac{e^2}{\log(r/L)}$, where $r$ is the distance between the two charges and $L$ is a scaling length which we choose as
the length of the simulation cell. Such a 2D one-component plasma (OCP) consists of identical point particles carrying a charge $-e$ and interacting through the Coulomb potential. To ensure charge neutrality, the particles are immersed in a uniform positive background of charge. The thermodynamic state of the OCP is completely defined by the dimensionless plasma coupling parameter $\Gamma = e^2/k_B T$, where $a$ is the radius of the Wigner-Seitz disk and $T$ is the temperature. Depending on the value of the coupling parameter, the system can be in the weakly correlated gaseous phase, strongly correlated liquid phase or in the crystalline Wigner lattice state. There is a reasonably good understanding theoretically for the 2D electron system \[7–10, 13\] in a magnetic field making use of various types of approximations to deal with the many-body effects. In this paper, we use molecular dynamics (MD) simulations.

Our calculations are for a simplified model of electron layers such as those on a liquid helium surface. These systems have been generated by Grimes and Adams \[11\] as well as other related experiments \[12\], in which the thickness of the layers of the electrons trapped on the surface of liquid He is much less than the inter-particle spacing $a$, and we may thus treat the system as 2D. As a matter of fact, Ma, Girvin, and Rajaraman \[6\] have argued that even though the Coulomb potential in quasi-2D systems is really $1/r$, the effective potential is closer to $\log(r)$ for a layer with high dielectric constant surrounded by material with much smaller dielectric constant. The application of a uniform perpendicular magnetic field does not affect the classical nature of the system as long as the separation between Landau levels satisfies $\hbar \omega_c \ll k_B T$, where $\omega_c$ is the cyclotron frequency. The number density, $n$ has been varied over a wide range, i.e., $10^5 \leq n \leq 10^{10}$ cm$^{-2}$ with a Fermi energy of at most $10^{-3}$ K, for which the system may be treated classically. We have carried out calculations over a range of coupling parameters for which there is a variation of the velocity auto-correlation function (VAF) with magnetic field at finite temperature. Yamada and Ferry \[17\] have also investigated in detail the effect of magnetic field on some transport properties of 2D electron systems. Berne \[22\] has reported molecular dynamics calculations of the VAF of an OCP in a magnetic field for a limited number of values for the coupling parameter $\Gamma$. Additionally, Dzhumagulova et al. \[23\] have also investigated the effect due to a perpendicular magnetic field on the velocity autocorrelation function for a two-dimensional one-component system by employing a Yukawa potential and $\Gamma = 120$. 
In this paper, we will present a molecular dynamics study of a classical, interacting 2D electron system in the presence of a uniform magnetic field for a range of values of temperature, i.e., the coupling parameter $\Gamma$. Such systems have been used in the study of high-$T_c$ superconductors, where a logarithmic potential is seen to be appropriate for the vortices within a single layer. We have calculated the VAF, root mean square displacement and the self correlation correlation function as functions of magnetic field and plasma coupling parameter.

Hansen et al. [4], Kalia et al. [24] and de Leeuw et al. [25] have studied the VAF in a one-component plasma. Specifically, Hansen et al. [4] did their calculations in 3 D. Kalia et al. [24] employed a $1/r$ potential for selected values of the coupling parameter $\Gamma$. in the absence of magnetic field. de Leeuw et al. [25] considered a 2D one-component plasma using a $\ln(r)$ potential in the absence of magnetic field. for a coupling parameter $\Gamma = 72$. We have carried out extensive calculations and we present here new results, to see the effect of magnetic field. Agarwal and Pathak [26] reported results for the VAF of a 2D classical electron fluid using a short-time expansion in the absence of a magnetic field.

The rest of the paper is organized as follows. We first present details of the computational details of the simulations. Following this, we will present the result for the velocity correlation function root mean square displacement and single particle correlation function. We discuss these results with a summary in Sec. IV and highlights of our results.

### II. METHOD AND MODEL

The validity of the present calculations is examined by comparing the results in the absence and presence of magnetic field. The effect of the magnetic field is included through a Lorentz force. The advantage of our method enables us to watch the system evolving in real time, which in turn offers one various possibilities to calculate several time correlation functions required for comparison with experimental results.

In 2D, the Coulomb interaction between two particles of charge $e$ separated by a distance $r$ is given by $V(r) = -e^2 \ln r/L$, where $L$ is a scaling length chosen as the length of the simulation cell. Because of the long-range nature of the Coulomb interaction, we use the method of Ewald summations to take into account the interaction of an electron with an infinite array of periodic images of the other electrons and the uniform, positive background.
In computer simulation studies, one usually deals with systems composed of a few hundred particles in a rectangle of area $A$ under periodic boundary conditions. The energy of the system, composed of $N_0$ particles of charge $e$ embedded in a uniform neutralizing background, is given by

$$U = \frac{e^2}{2} \sum_n \sum_{i=1}^{N_0} \sum_{j=1}^{N_0} \left( \log |(\vec{r}_{ij} + \vec{n})| - \log |\vec{r}_{ij}| \right) + \frac{Ne^2}{A} \sum_{\vec{n}} \sum_{j=1}^{N} \int_A d\vec{r} \log |\vec{r}_j - \vec{r} + \vec{n}| - \frac{Ne^2}{A^2} \sum_{\vec{n}} \int_A d\vec{r} \int_A d\vec{r}' \log |\vec{r} - \vec{r}' + \vec{n}| , \quad (1)$$

where $\vec{r}_{ij}$ is the vector between particles $i$ and $j$, $\vec{n}$ is a vector whose components are $(n_xL, n_yL)$ and $n_x, n_y$ are integers. The first term on the right-hand side of Eq. (1) arises from the interactions between the particles. The sum over $n$ is carried out over all lattice vectors. The primes on the summation signs indicate that, when $n = 0$, the terms with $i = j$ have to be excluded. The second term arises from the interaction of particles with the background. The integral is to be taken over the rectangular cell of area $A = L_xL_y$. The third term represents the interaction of the background with itself. The sum in Eq. (1) is conditionally convergent and the energy $U$ depends on the shape of the macroscopically large periodic system. Adding the contributions of different cells of the system in circular annuli, Eq. (1) can be rewritten in the following form using the Ewald summation

$$U = \frac{e^2}{4} \sum_n \sum_{i=1}^{N_0} \sum_{j=1}^{N_0} E_1(\alpha^2(r_{ij}^2 + n^2)) + \frac{e^2}{4\pi A} \sum_k \exp\left(\frac{\pi^2 k^2}{\alpha^2}\right) \frac{\rho_k\rho_{-k}}{k^2} - \frac{Ne^2}{4} [C + \log(\alpha^2 A)] - \frac{N^2 e^2 \pi}{4\alpha^2 A} , \quad (2)$$

where the sum over the wave vector $k$ excludes the divergent term $k = 0$, as denoted by prime, $\alpha$ is a convergence parameter which controls the relative weights of the real space and reciprocal space sums, $\vec{k} = 2\pi \vec{n}/L$, and $C = 0.5772...$ is Euler’s constant. Also, in this notation, $E_1(x)$ denotes the exponential integral and the Fourier-component $\rho_k$ of the electron density is given by:

$$\rho_k = \sum_{j=1}^{N_0} \exp(2\pi i \vec{k} \cdot \vec{r}_j) . \quad (3)$$
From our numerical calculations, we have found that the value of $\alpha A^{1/2} = 6.5$ gives a satisfactory convergence rate for each of the two series in Eq. (2),

**III. NUMERICAL RESULTS**

We now report the results of our calculations for molecular dynamics simulation experiments for the 2D Coulomb system with magnetic field. The calculations were carried out for 256 particles and five values of the plasma parameter $\Gamma = e^2/k_B T$. We chose $\Gamma = 20$, 36, 50, 90 and 130 and the range of magnetic field was $0 \leq B^* \leq 20$ T, in a rectangular cell with periodic boundary conditions. A predictor-corrector method involving up to five time derivatives of the positions was employed to integrate Newton’s equation of motion. The total force $F_T$ on an electron is the sum of the forces arising from the Coulomb interaction and the Lorentz force so that $F_T = F(U) - \frac{e}{c}(v \times B)$, where $v$ is the velocity of the electron. We used the following dimensionless variables for length and time: $x^* = x/a$, $t^* = t/\tau$, where $\tau = \sqrt{ma^2/e^2}$ and $m$ is the mass of the particle. The reduced density is $n^* = na^2$ and we chose the electron density as $n = 1.477 \times 10^8$/cm$^2$ and five values of temperature ranging from $T = 7$ mK to 50 mK. The runs for the collection of data presented here for 256 electrons extended over $30 \times 10^5$ time steps, after an initial $10^6$ time steps for the system to reach equilibrium. During our simulations, the energy of the system remained constant to within one part in $10^5$. The equations of motion were integrated with a time step of $\delta t = 0.00123\tau$.

For convenience, we have used dimensionless units for space and time as follows: $r^* = r/a$, $t^* = t/\tau$, where $\tau = 0.1$ (in units of $\sqrt{ma^2/e^2}$). and $\Gamma = e^2/k_B T$. The reduced density $n^* = na^2$, which corresponds to the value $1.477 \times 10^8$ electron/cm$^2$ and at 20 values of temperature ranging from 0.19 to 1.0 K, corresponding to values of $\Gamma$ equal to 180.0 and 36.0, respectively. The runs for the collection of the data presented here for 256 electrons extended over $15 \times 10^4$ time steps, after an initial $10^5$ time steps for the system to reach equilibrium. We have done one set of calculations for $N_0 = 400$ particles to check the dependence on the value of $N_0$ for the system. It was found that this energy was independent of $N_0$ within the numerical accuracy of the calculations. During our simulations, the energy of the system remained constant to within 1 part in $10^4$. 
The velocity autocorrelation function, which is defined as

\[ Z(t) = \frac{\langle V_i(t) \cdot V_i(o) \rangle}{\langle V_i(o)^2 \rangle}. \]  

(4)

provides us with some insight into single particle dynamics.

In Fig. 1, we have presented our results for the velocity autocorrelation function when there is no external magnetic field as well as in the presence of a perpendicular magnetic field \( B^* = 1, 2, 5, 10 \) and \( 15 \) T and when the coupling constant \( \Gamma = 20 \). In Fig. 2, the magnetic field is chosen as \( 1 \) T and several values of \( \Gamma \) are used in our calculations. The results show a series of well defined oscillations, whose period is independent of the value of the dimensionless variable \( \Gamma \). This behavior is characteristic for one component charged fluids and has also been observed in the three dimensional OCP [2] and the classical 2D electron fluid. A comparison of the results shows that the frequency of the oscillation is independent of \( \Gamma \), but for a chosen time, \( Z(t) \) is decreased as \( \Gamma \) is increased. From Fig. 1, it is clear that the magnetic field has no effect on the VAF for the smaller values of \( \Gamma \). We have found that the effect is small if the value of \( \Gamma \) is increased. Furthermore, for large values of \( \Gamma \), the simulation results clearly show that in the presence of a magnetic field, the amplitudes of the oscillations are slightly changed, but as the time increases, after a few oscillations, their difference is negligible.

In Fig. 3, the root mean square (RMS) displacement is plotted as a function of time for various values magnetic field \( B^* \) for one coupling constant \( \Gamma = 20 \). The reason for plotting the RMS is to clearly see the effect of magnetic field on the diffusion constant. The simulation results clearly show that the diffusion constant does not decrease monotonically with magnetic field. Additionally, the RMS displacements at each magnetic field are investigated in order to determine what is the effect due to magnetic field on the diffusion. The mean square displacement is given by:

\[ \langle R^2(t) \rangle = \frac{1}{N} \left( \sum_{j=1}^{N} (r_j(t) - r_j(0))^2 \right). \]  

(5)

here, \( r_j(t) \) is the position of the \( j \)th electron at time \( t \), \( N \) the total number of electrons and \( < \cdots > \) stands for taking the time average of a quantity. In Fig. 3, we have presented results for the mean square displacement as a function of time for \( B^* = 0.0, 1.0, 2.0, 5.0, 10.0 \) and \( 15.0 \) T. Parabolic increments are applied for all magnetic fields. The slope of the linear
increments decreases with increasing magnetic field. Since one can obtain the diffusion constant from the slope of the curve, it is clear that for each value of $B^*$, the diffusion constant will be different. Therefore, magnetic field has some effect on the dynamics of the system. By making a comparison between three values of diffusion constant, it is apparent that by increasing the strength of the magnetic field, the diffusion constant is changing about 5%, we have run the system quite a long time, and the behavior will not change if one runs the computer program even longer.

In Fig. 4, we have plotted the self correlation function for $B^* = 1.0$ for $\Gamma = 20$, which is defined as

$$F_s(q, t) = \frac{1}{N} \sum_j \exp(iq \cdot (r_j(t) - r_j(o))) \tag{6}$$

The self correlation function is directly related to the diffusion constant. It is instructive to investigate whether the self correlation function also show in its behavior, the effect of magnetic field. We have plotted the self correlation function for various wave vectors for each of three values of magnetic field. We will make a comparison in two ways. First we will plot the self correlation function for each wavevector for three values of magnetic field, then chosen value of magnetic field and various wavevectors. Our calculations have shown that as the magnetic field is increased, the self correlation function is quickly reduced. This is consistent with the behavior of the mean square plots. In other words, the magnetic field has some clearly affects the dynamics of the single-particle motion of the system, as expected.

We conclude from our results for the pair correlation function that electrons have no preferred location. Since electrons cannot approach each other arbitrarily close due to the strong repulsive Coulomb force, they will preferably move to neighboring unit cells and the applied magnetic field has no control in determining which cells they would migrate into. This is the physical reason why magnetic field has virtually no effect on $g(r)$.

It is well known that relaxation times to equilibrium always favor shorter paths which correspond to smaller diffusion constant. This is clear from our results in Figs. 2 and 3 and are consistent with a semiclassical approach. In our classical formalism, electrons may move easily between potential minima and will never get trapped in potential well giving rise to some diffusion constant. However, in the presence of magnetic field, the diffusion
constant may be zero due to trapping in a potential minimum. However the applied magnetic field does not only change the electron dynamics, but also its energy. In summary, we have carried out molecular dynamics simulations for a Coulomb system in an external magnetic field. The simulation result clearly show the static properties are unchanged due to magnetic field.

IV. SUMMARY AND CONCLUSIONS

In Fig. 1, we have presented our results for the velocity autocorrelation function when there is no external magnetic field as well as in the presence of a perpendicular magnetic field $B^* = 1, 2, 5, 10$ and 15 T and when the coupling constant $\Gamma = 20$. In Fig. 2, the magnetic field is chosen as 1 T and several values of $\Gamma$ are used in our calculations. The results show a series of well-defined oscillations, whose period is independent of the value of the dimensionless variable $\Gamma$. This behavior is a characteristic for one component charged fluids and has also been observed in the 3D OCP \[27\] and the classical 2D electron fluid. A comparison of our results shows that the frequency of the oscillation is independent of $\Gamma$, but for a chosen time, $Z(t)$ is decreased as $\Gamma$ is increased. From Fig. 1, it is clear that the magnetic field has no effect on the VAF for the smaller values of $\Gamma$. We have found that the consequence of the applied magnetic field is not significant if the value of $\Gamma$ is increased. Furthermore, for large values of $\Gamma$, the simulation results clearly show that in the presence of a magnetic field, the amplitudes of the oscillations are slightly changed, but as the time increases, after a few oscillations, their difference is negligible.

Figs. 1 and 2 provide information about the dynamics of electrons over intervals of $\sim 10^{-13}$ sec which can be comparable with the time between particle collisions. This means that we are probing features of dynamical behavior mainly determined by electron-electron interactions.

The short-time behavior of the velocity autocorrelation function can be studied with the use of a Taylor series expansion, i.e.,

$$\mathbf{v}_i(t) = \mathbf{v}_i(0) + \mathbf{v}'_i(0)t + \frac{1}{2}\mathbf{v}''_i(0)t^2 + \cdots .$$  \hspace{1cm} (7)

Multiplying by $\mathbf{v}_i(0)$ and taking an ensemble average, we obtain
\[
\langle v_i(t) \cdot v_i(0) \rangle = \langle v_i^2 \rangle - \frac{1}{2} \langle v_i'^2 \rangle t^2 + \cdots = \langle v_i^2 \rangle \left( 1 - \frac{1}{2} \frac{\Omega_0^2 t^2}{t} + \cdots \right),
\]

where \( \Omega_0^2 = \langle |F|^2 \rangle / 2mk_B T \). Time reversal symmetry ensures that the odd terms in \( t \) vanish. The short-time behavior of the velocity autocorrelation function is related to the mean square acceleration (or mean square force \( \langle |F|^2 \rangle \)) and provides information about the interaction between the particles as well as the lattice structure.

The second term in the Taylor series expansion of the VAF arises from the combined effect due to the random force \( F \) and the single-particle velocity (see Eq. (8)). Our findings confirm the rapid decay and oscillatory behavior in the VAF due to a single binary collision between the tagged particle and the other particles. Also, the rapid oscillations indicate the strong coupling with the collective plasma excitations \[26\]. The Einstein frequency \( \Omega_0 \) is for small oscillations in the potential well formed from the electron-electron interaction. Since our calculations show that the VAF at intermediate times strongly depends on the electron coupling parameter \( \Gamma \), the electron-electron interaction clearly dominates over the Lorentz force and at small times, their combined effect is given by the second term in Eq. (8). As \( \Gamma \) is increased, the system becomes disordered due to the random force field. The correlations between the random force and the velocity which together produce the oscillations in the VAF become less important as \( \Gamma \) is increased and after a long time.

The Lorentz force on an electron causes it to move on a circular orbit between collisions. After each collision, which is assumed instantaneous, the electron again moves on a circular path with a different center but whose cyclotron radius is unchanged since the energy is conserved. Consequently, the motion of the electron is equivalent to that in a randomly applied time-dependent magnetic field that changes the center of the cyclotron orbit. This explains why the VAF, a dynamical quantity, depends on the fixed external magnetic field. Also, the mean force which is determined by correlations through the pair correlation function is affected by the value chosen for \( \Gamma \).

In summary, we have carried out molecular dynamics simulations for the VAF of a 2D OCP system in an external magnetic field. We presented numerical results for a range of values of the coupling parameter \( \Gamma \) and the magnetic field \( B^* \). Our simulation results show
how the period and amplitude of the oscillations of the VAF depend on these two variables; the period of the oscillations does not depend on $\Gamma$ but their amplitude does.

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Figure Captions

Fig. 1 The normalized velocity autocorrelation function $Z(t)$ defined in Eq. [4] for $\Gamma = 20$ and magnetic fields $B^*=0.0$ T. and $B^*= 1.0 , 2.0 , 5.0 , 10.0$ and $15.0$ T. The time is measured in units of $\tau$.

Fig. 2 The velocity autocorrelation function $Z(t)$ for $\Gamma = 20, 36, 50, 90$ and 130 and magnetic field $B^*= 1$ T.

Fig. 3 Plot of root mean square displacement for $\Gamma = 20$ and magnetic fields $B^*= 0$ and $B^*= 1, 2, 5, 10$ and 15 T.

Fig. 4 Plot of the self-correlation function $F_s(q,t)$ for five values of $q^*$ for $\Gamma = 20$ and $B^*=1.0$. 
FIG. 1:
FIG. 3:
