Perfectly Translating Lattices on a Cylinder

Vishal Mehra and Jayme De Luca

Departamento de Física, Universidade Federal de São Carlos,
Rodovia Washington Luiz km 235, 13565-905, Caixa Postal 676, São Carlos, SP, Brazil

Abstract

We perform molecular dynamics simulations on an interacting electron gas confined to a cylindrical surface and subject to a radial magnetic field and the field of the positive background. In order to study the system at lowest energy states that still carry a current, initial configurations are obtained by a special quenching procedure. We observe the formation of a steady state in which the entire electron-lattice cycles with a common uniform velocity. Certain runs show an intermediate instability leading to lattice rearrangements. A Hall resistance can be defined and depends linearly on the magnetic field with an anomalous coefficient reflecting the manybody contributions peculiar to two dimensions.
I. INTRODUCTION

The advent of modern computers has made it possible to study many-dimensional dynamical systems in detail and to ferret out previously unsuspected characteristics. Phenomena such as relaxation to equilibrium [1], lack of ergodicity [2], and connection of dynamical to statistical properties [3] have been explored numerically. A category of models that continue to enjoy great attention is that of interacting-electron systems. In this paper we consider a particular member of this class: the classical dynamics of the confined two-dimensional electron gas (2DEG). While various aspects of 2DEG have been well-studied, it remains a convenient and relatively tractable system to understand dynamical properties of complex systems. It is well-known that at low temperatures the electron system freezes into an hexagonal Wigner lattice [4]. Extensive studies have been made of the possible conformations that result when this simple system is perturbed [5,6]. A simple example is provided by the inter-layer coupling between vertically separated 2DEGs which enhances the stability of the square lattice relative to the hexagonal [7]. The melting and structural transitions have also been well-studied [8]. The confinement is also a possible perturbation—ideal hexagonal lattice is obtained only for infinite system.

However, commonly used confining potentials preserve the hexagonal character with only slight edge distortions. Perturbed 2DEG models have relevance beyond electron systems: experiments on dusty plasmas [9] and ion plasmas [10] have been usefully explained in terms of formation of few layered and bi-layered Coulomb lattices.

The classical behavior of a confined 2DEG subject to an external magnetic field has been of some recent theoretical use [11–13]. In particular the magnetotransport phenomena in 2DEG have lead to important physical insights. New systems have been proposed in which the electron motion in 2DEG is nontrivially altered by a (possibly non-homogeneous) magnetic field [14]. Some possibilities have been realized by advances in the semiconductor technology [15]. Such systems are studied quantum mechanically for a full understanding but many features can already be appreciated within the classical theory. For example,
the classical chaos was found to control the low-field transport in systems with competing magnetic and electrostatic modulation \cite{16,18}. In this paper we analyze the structure and dynamics of 2DEG on a novel geometry. The electrons are constrained to the surface of a cylinder of radius $R_d$ and confined along the $z$ direction to a strip of width $W = 2\pi R_d$ by the potential of the uniform static positive background. We chose this geometry because it allows the electrons to carry a current along the $\phi$ direction. We apply the external electric and magnetic fields and observe the time-dependent response.

We have been motivated to this problem by certain reflections on usual textbook derivations of the classical 3-dimensional Hall effect \cite{19}. These derivations are based on free-electron Drude theory and consider independent electrons drifting with a common and constant drift velocity $V$. It is then easy to show that a constant transverse electric field, generated by excess boundary charge, can balance the magnetic force and bring a steady state. In the context of a classical 2-dimensional many degree-of-freedom interacting system this simple picture could be dynamically unstable. Here we conduct numerical experiments to see if a regime of interacting electrons drifting with a common uniform velocity can be attained in a 2D many-body system. A peculiarity of 2DEG is that the Coulomb field escapes from the surface; in 3D a constant transverse Hall field can be nicely produced by the boundary electrons only, while in 2D, because of Gauss’s law, these boundary electrons can only produce a $1/r$ field (the field of a charged wire). We see then that a global charge redistribution is called upon for to produce a constant field.

II. SIMULATION AND RESULTS

The Lagrangian for $N$ interacting electrons confined by the background potential $V_{\text{CON}}$ and subject to an external radial magnetic field $B$ is

$$\mathcal{L} = \sum_i \frac{1}{2} m \ddot{x}_i^2 - \sum_{i>j} \frac{e^2}{r_{ij}} - V_{\text{CON}}(z_i) - B R_d \sum_i z_i \dot{\phi}_i,$$  \hspace{1cm} (1)

where $\vec{x}_i$ is the coordinate of the $i$th electron and $r_{ij}$ is the distance between $i$th and $j$th electrons and $c$ is the speed of light. The electronic mass and charge are $m$ and $e$ respectively.
To remove any ambiguity we clarify that distances are not calculated along the surface but are ordinary three-dimensional distances: \( r_{ij}^2 = (z_i - z_j)^2 + 2R_d(1 - \cos(\phi_i - \phi_j)) \). The rotation symmetry possessed by \( \mathcal{L} \) implies the Noether’s constant:

\[
l_z = \sum_i mR_d^2 \dot{\phi}_i - BR_d \sum_i z_i.
\] (2)

The resulting equations of motion are

\[
m \frac{d^2 \vec{x}_i}{dt^2} = -\frac{\partial}{\partial \vec{x}_i} \left( V_{\text{CON}} + \sum_{i \neq j}^N \frac{e^2}{r_{ij}} \right) + \frac{e}{c} \vec{B} \times \frac{d\vec{x}_i}{dt},
\] (3)

where the confining potential \( V_{\text{CON}} \) of the positive background is taken to be either

\[
V_{\text{CON}} = -\left( \ln(z + W/2) + \ln(-z + W/2) \right),
\] (4)

or

\[
V_{\text{CON}} = ((2z + W) \ln(2z + W) + (-2z + W) \ln(-2z + W)),
\] (5)

the stripe being symmetrical about \( z = 0 \) and extending from \(-W/2\) to \(W/2\). The first potential is flat but rises steeply near the edges. The second potential has more parabolic character and is an approximation to the exact potential of a positive background: we found analytical solution for the potential of a positively charged flat rectangle with the same width and length of our cylindrical background, and the above second potential approximates this analytic form. The use of potentials with differing characters helps in distinguishing any peculiar effect of confinement from overall observations. These potentials are sketched in Fig.(1).

The form of equation (1) is simplified by using scaled units: lengths may be scaled by the average interelectronic distance \( R \): \( \vec{x} \to R \vec{x} \) and time is scaled as \( dt \to \omega^{-1} d\tau \) where \( \omega^2 \equiv e^2/mR^3 \). In these units the equations of motion are

\[
\frac{d^2 \vec{x}_i}{d\tau^2} = -\frac{\partial}{\partial \vec{x}_i} \left( \frac{R e^2}{c^2} V_{\text{CON}}(R \vec{x}_i) + \sum_{i \neq j} \frac{1}{r_{ij}} \right) + \hat{B} \times \frac{d\vec{x}_i}{d\tau},
\] (6)

where \( \hat{B} = n^{-3/4} B/\sqrt{(mc^2)} \) and \( n \) is the two-dimensional number density of the electron gas. For example at the experimentally attainable \( n = 10^{10} \text{ cm}^{-2} \) the above formula gives
$B = 0.284 \hat{B}$ Tesla. Because of the scale-invariance of the Coulomb interaction, $\frac{R}{\varepsilon^2} V_{CON}(R\vec{r}_i)$ is independent of $R$. Equation (4) has two components for each particle corresponding to $z$ and $\phi$ motions. We deliberately add an additionally force along the $\phi$ direction represented by a small electric field $E_\phi << 1$ and a weak damping so that the final equation for $\phi$ is

$$R_d^2 \ddot{\phi}_i = \hat{B} \dot{z} R_d + E_\phi (1 - \frac{R_d \dot{\phi}_i}{V}) + R_d^2 \sum_{j \neq i} \sin(\phi_i - \phi_j) \frac{1}{r_{ij}^3}.$$  

(7)

We chose this form of damping such that if all electrons cycle with a constant common velocity $V$, the damping force is balanced by $E_\phi$. The last term in the above equation is just the Coulomb repulsion between electrons. The equations of motion are integrated numerically using a 7/8 order embedded Runge-Kutta pair with self-adjusted step.

The initial states for the numerical integrations are generated in the following way: the energy of the confined Coulomb system is

$$E = \frac{1}{2} \sum_i v_i^2 + e^2 \sum_{i<j} \frac{1}{r_{ij}} + \sum_i V_{CON}(z_i).$$  

(8)

A naive candidate for a minimal-energy initial condition would be one which minimizes the above energy and with all electrons cycling with the same velocity $V$. It is straightforward to find this condition by steepest descent quenching and one obtains a translating lattice which approximates an ideal triangular lattice with some edge distortions. The problem with this condition is that in the presence of the external magnetic field $B$ (which does not appear explicitly in the energy), the translating electrons deflect upwards causing a lattice deformation. We observe, by integrating the equations of motion numerically from this condition with inclusion of the above defined weak dissipation, that the lattice shifts to a different configuration consistent with the presence of magnetic field and with a slightly higher steady state energy. (Notice that we are driving the system, so energy does not have to be constant). An equivalent way to accomplish this same final state is to seek minimum energy configurations with a certain property: they must describe a uniform motion of the entire system along the $\phi$ direction under a radial magnetic field $B \ (v_i = V \dot{\phi})$. What we are looking for is that the total force acting on each electron be zero.
\[ \nabla \Phi + BV = 0, \quad \Phi = \sum_{i \neq j} \frac{1}{r_{ij}} + V_{\text{CON}}. \quad (9) \]

This configuration can be obtained by a steepest descent procedure: we integrate the (modified) quenching equation

\[ \frac{d\vec{x}_i}{ds} = -\frac{\partial}{\partial x_i}(\Phi + BV \sum_i z_i/c), \quad (10) \]

\( s \) being the parameter along the quenching path.

The quenched configurations are obtained for various values of the parameter \( BV \) and then used as initial conditions for subsequent molecular dynamical runs. Fig.(2) shows a representative configuration obtained with the confinement of Eq.(2). The electrons arrange themselves in an hexagonal lattice slightly distorted by the confinement and magnetic field (notice that this is a global distortion, not a simple boundary perturbation of a perfect lattice). Electrons are projected out with an initial \( \phi \) velocity \( V/R_d \) plus small random components along \( \phi \) and \( z \) directions. Various quantities are calculated along the trajectory: the instantaneous rotation rate \( \sum_i \dot{\phi}_i/N \) which is related to the current \( I = \sum_i \dot{\phi}_i/2\pi \); the \( \phi \) averaged potential difference between the top and bottom edges : \( V_H \) (Hall voltage); and the Hall resistance \( R_H = V_H/I \). All these quantities are function of time and hence their time-development is likely to be informative. We also observe snapshots of the system at regular intervals. These snapshots could be folded to \( 0 - 2\pi \) or left unfolded to preserve information about angular motion.

We report the results of the simulations of \( N = 216 \) and 484 particles performed with the confining potential of Eqs (2) and (3). We distinguish between runs carried out with \( E_{\phi} \) zero and nonzero. Simulations with nonzero \( E_{\phi} \) reach a steady state after a brief transient which, is not attained by zero \( E_{\phi} \) runs. We henceforth call this state a Perfectly Translating Lattice (PTL). In the PTL state the electrons cycle with a common constant \( \phi \) velocity \( V/R_d \); motion along \( z \) being rapidly damped out. The resulting Hall resistance \( R_H \) should be a constant in such circumstances but we observe small fluctuations in \( R_H(t) \). The amplitude of these fluctuations is an irregular function of \( B \) generally varying between 0.1-1.0
percent. The presence of fluctuating $R_H$ is not disquieting however and can be understood as an artifact of the method employed to calculate Hall resistance of small finite number of electrons: Because we used a finite number of points to average the potential difference, small instantaneous fluctuations are generated if the number of electrons is small and we verify that the fluctuations become smaller for larger $N$ (number of electrons).

Two cases can be further differentiated with regard to the initial phase of the dynamics. Initial configuration for certain values of the external magnetic field $B$ turns out to be dynamically unstable. The system makes a transition to a new configuration through coordinated row-jumping of many electrons simultaneously. Such a transition is made possible by the existence of numerous local minima in the energy surface whose presence has been confirmed numerically by extensive quenching runs starting from distinct initial conditions. The instability only appears for scaled magnetic fields greater than 7.0 for $N = 216$ and 8.5 for $N = 484$ (for electron density of $10^{10}$ cm$^{-2}$ these fields correspond to 1.9 T and 2.3 T respectively). In a way, this result shows that the initial state found by minimization ceased to be stable and another extremum (not the minimum anymore) of the functional became an stable fixed point, a bifurcation. This instability is accompanied by slower relaxation to a PTL state and can be seen in Fig.(3) which plots the spread in the instantaneous rotation rate vs. time. Even more dramatically, velocity inhomogeneities are developed if all electrons are released with a common velocity $V$ with no random components. These inhomogeneities are not long lasting and ultimately a PTL is attained.

The resultant of this temporarily existing velocity profile can be visualized most easily in Fig.(4) where the $\phi$ coordinates have not been folded to $(0 - 2\pi)$. This striking profile is not apparent after folding and the finally established PTLs do not differ from PTLs in cases where this instability is absent. We call this instability a shearing instability since it is visible as a shear in the velocity profile of the electrons. This shear is seen as a dispersion in unfolded lattice along $\phi$ coordinate.

We have carried out runs without forcing and dissipation i.e. $E_\phi = 0$ and these do not achieve a PTL state. They may or may not display the initial shearing instability but in
all cases the initial randomness in velocity distribution is magnified and the $z$ dynamics is not damped. An irregular velocity distribution develops even from a perfectly homogeneous initial velocity distribution. The instantaneous Hall resistance $R_H(t)$ is unsteady with large amplitude fluctuations and the system can not be said to be in a Hall regime.

From these simulations a plot of the Hall resistance $R_H$ vs. $B$ can be drawn. Only converged values of $R_H$ are used which rules out our undriven simulations ($E_\phi = 0$). In Fig.(5) results from unsheared and sheared states are displayed for $N = 216$ and 484. Data from the simulations employing confining potential of equation (3) has been plotted for $N = 216$ also. All are PTL configurations but the sheared states have experienced the shearing instability referred to earlier. We observe that $R_H$ from the unsheared states lie on straight lines though different slopes are obtained for the two confining potentials used: 1.07 and 1.05 for potential (1) and (2) respectively. Data for $N = 216$ and 484 overlap. Points from the sheared states are scattered haphazardly about this straight line.

How far do these data match our expectations? A plausible argument can be made for reasonableness of our simulation results: The Hall voltage $V_H$ is the difference between the top and the bottom edges of the stripe and may be expressed as

$$V_H = V(W/2) - V(-W/2) = \int_{-W/2}^{W/2} \nabla_0 \left( \sum_i \frac{1}{r_{i0}} + V_{CON} \right) .dl_0,$$

where $V = \sum_i 1/r_{i0} + V_{CON}$ and the integral is taken along a straight line from bottom to the top edge; $r_{i0}$ is the distance of the $i$th electron from integration element. Now the integrand may be split as

$$\nabla_0 \left( \sum_i \frac{1}{r_{i0}} + V_{CON} \right) \approx BV\hat{z} + \nabla \left( \frac{1}{r_{n0}} \right),$$

where $n$ labels the electron nearest to the integration element and $\hat{z}$ is the unit vector along $z$ direction. This follows from the assuming that the force-balance condition (Eq. 9) holds in a neighborhood of the electron nearest to 0:

$$\nabla \left( \sum_{i \neq j} \frac{1}{r_{ij}} + V_{CON} \right) = BV,$$
where $i, j$ label electrons. This equation holds only at the position of an electron and we use as an approximate equality in a neighborhood of the nearest point $0$. From the above it follows

$$V_H = \int B V \hat{z} \cdot dl_0 + \int \nabla \left( \frac{1}{r_{n0}} \right) \cdot dl_0. \quad (14)$$

The first term on the right yields the straight line dependence of $R_H$ vs. $B$ with a unit slope but the second term provides a correction. To evaluate this correction, we take an integration path passing through a column of electrons, avoiding each electrons by making a small semi-circle around it. If the distance between the $i$th and $(i + 1)$th electrons along this path is $d_i$, this correction evaluates to

$$2 \sum_i \left( \frac{d_{i+1} - d_i}{d_i} \right) \cdot \frac{1}{d_i}$$

Hence the correction to the unit slope depends on the degree of compression that the lattice undergoes under the external magnetic field. A 3D lattice does not suffer this kind of bulk squishing but only edge distortions. If the lattice rearrangement is global in the sense that lattice distances are affected throughout the bulk and not just at the edges then we can fairly expect a significant alteration of the slope of Hall resistance plot. This expectation is realized in our simulations as we have seen that the slopes of $R_H$ vs $B$ plot indeed differ from unity by a few percent. Lattices which are dynamically unstable and undergo rearrangement via the shearing instability would seem to require more correction according to this picture and in fact provide a needed check for the theory.

### III. DISCUSSION AND CONCLUSION

In conclusion we have performed dynamical simulations on a 2DEG constrained to a cylindrical stripe and subject to crossed electric and magnetic fields. The classical confined electron gas has a natural non-trivial minimal energy state and provides a convenient test bed to study many-body dynamics and long-range effects. In this work we included many-body effects on the dynamical picture used in the classical derivations of the Hall effect in...
two dimensional systems. We have analyzed the formation of the steady state presupposed in classical derivations. This state, which we refer to as a Perfectly Translating Lattice (PTL), in which all electrons cycle with a common constant velocity, is formed by a relaxation process. The initial configurations are obtained by a generalized quenching procedure. This initial configuration is liable to be dynamically unstable for magnetic fields above a threshold. The quenching procedure sometimes yields rather shallow local minima which readily allow further rearrangements to nearby wide basins. The inter-basin like motion is manifested in simultaneous jumping of many electrons and a slower relaxation to PTL state. The Hall resistance $R_H$ can be calculated and plotted as a function of external magnetic field $B$. Appropriately for PTL states $R_H$ is a linear function of $B$ except for sheared states. An explanation has been put forward based upon force-balance condition as it obtains for PTL states. If one repeated the same study for a confined 3D electron-gas, the minimal energy state would be a tridimensional Wigner lattice and inclusion of a drift velocity in the presence of an external magnetic field would produce only boundary charge rearrangement. The obtained PTL would be the same ideal Wigner lattice and there would be no many-body correction to the Hall coefficient. Our results are specific to 2D classical systems.

The present work evolved from our earlier attempts to study the same problem but with the electrons interacting via the Darwin Lagrangian, which is the first relativistic correction to the Coulomb interaction. We find that the relativistic corrections break the scale-invariance of the Coulomb interaction, even in the absence of a magnetic field, only by requiring a critical density of the electron gas $\rho_c$ [20]. Even though these is a much richer dynamical system, we did not continue the studies because the equations of motion are algebraic-differential and become impossible to integrate above the critical density even by use of the modern specialized integrators RADAU [21] and DASSL [22].
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FIGURES

FIG. 1. Confining potentials of Eq.4 (full line) and Eq.5 (dashed line) compared. On horizontal axis is scaled \( z/R \) and the vertical axis is \( V_{CON} \) in units of \( e^2/R \).

FIG. 2. Configuration of 2DEG obtained by the special quenching procedure detailed in the text. This particular state is arrived using confinement of Eq.4 with \( \hat{B} = 7.0 \) and \( V/c = 0.05 \). The horizontal and vertical axes denote \( \phi \) and \( z \) coordinates respectively.

FIG. 3. Relaxation to PTL as measured by variance of the instantaneous rotation rate: \( \Delta R = \sum_i (\dot{\phi}_i - \dot{\phi} >)^2 \). Three cases are plotted for \( N = 216 \). Slowly-decaying curves are obtained from \( \hat{B} = 7 \) trajectories which shear in the way discussed in the text; they differ in the distribution of initial velocities: all electrons are started with \( \dot{\phi}_i = V/R_d, \dot{z}_i = 0 \) (dotted curve) or small random components are added to \( \dot{\phi}_i = V/R_d, \dot{z}_i = 0 \) (full curve). The nondispersing trajectory (dashed curve) comes from a \( \hat{B} = 9 \) run and exhibits rapid decay. These behaviors are typical for dispersing and nondispersing trajectories respectively.

FIG. 4. The unfolded view of a sheared \( N = 484 \) run with confining potential 4 at \( \hat{B} = 13.5 \). Unfolding preserves some information about the past angular velocities by displaying the net angular motion. Individual electrons are marked with pluses.

FIG. 5. The Hall resistance \( R_H \) calculated from simulations as detailed in the text. \( R_H \) from unsheared \( N = 216 \) trajectories using \( V_{CON} \) of Eq.4 are shown with crosses; sheared ones with pluses. Points from \( N = 484 \) using potential 4 are marked as boxes; these runs were unsheared for \( \hat{B} < 8.5 \) and sheared for \( \hat{B} > 8.5 \). Data from runs using \( V_{CON} \) of Eq.5 is depicted with stars (\( N = 216 \)). The remnant fluctuations are much smaller than the symbol-size. Hall resistance \( R_H \) is in units of \( e/(\omega R) \) and the \( x \)-axis is the scaled magnetic field \( \hat{B} = n^{-3/4}B/(mc^2) \).
