Classical molecular dynamics of two-dimensional electron gas

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1 Introduction

By carefully constructing layers of semiconductor, it is possible by subtly of quantum mechanics to create a two-dimensional electron gas. To be more precise, by band gap engineering (having different layer of semiconductor with different gap energies), it is possible to create a quantum well. Such a quantum well will trap the electrons in between the two layer of semiconductor, creating a two-dimensional environment composed of ionized electrons: a two-dimensional electron gas (2DEG).
At first look, we could think that such an environment is without any interest, but it is the exact opposite. For the physics point of view, 2DEG are a creative way to observe phenomena fundamentally dependent on the number of dimensions, Like the quantum hall effect and its more surprising fractional equivalent, In fact, 2DEG are the door to experimental investigations of statistical fractional mechanics. Furthermore, they also have multiple extremely important applications. They are a crucial element in multiple types of transistors. However, this is only a short overview of **some** of the application of 2DEG, there are used everywhere from the detectors to the topological insulators and quantum computers.

2 Motivation

With the constant shrinking of semiconductors, the 2DEG of each transistor will get increasingly closer to each other. However, each one of those transistor contains electronic machinery that produces some electric field. A crucial question arises from this situation: how close can they be from each other before problems arise due to mutual interference?
Even from a more physics point of view, multiple intriguing questions are associated to the 2DEG. Anyons quasi-particle with fractional spin only exist in the fractional quantum hall effect, but such

states are extremely sensitive. They can only exist in ultra-pure 2DEG with extremely high electron mobility. To avoid the degradation of 2DEG quality, some are using field effect electronics to analyze such a particles. It is based on the same principle as the field-effect transistor (MOSFET). The question then is how strong their electric field and how close the must electronics be from the 2DEG to have the desired effect on the it?

Those two questions can be grouped into one vital question, how do the electrons inside a 2DEG react to an external electrical field? We could instinctively think about analytically solving the Poisson equation, but this is not always possible. For example, the electronics used to investigate anyons necessitate complex interferometers, producing complicated electric fields which have no analytical solution. In addition, the fractional Hall effect only appears with the presence of magnetic fields, which is also not cover by the Poisson equation. In other words, a more general framework is necessary to investigate how the electrons react to an external electric field.

3 Methodology

Unfortunately, in the interest of time, our simulation of the molecular dynamics will be fully classical. The inter-electron interactions are implemented in a straightforward way via the Coulomb repulsion. In order to obtain a finite electric conductivity, the Drude model is implemented to simulate inelastic collisions between electrons and impurities (e.g. lattice sites, phonons, etc). Thus, the kinetic equation is given by

$$\frac{d\vec{p}}{dt} = \frac{-\vec{p}}{\tau} - |e|\vec{E}(t), \tag{1}$$

where τ is the mean-free-time (i.e. average time between electron-impurity collisions), and $\vec{E}(t)$ is the external driving electric field. In practice, τ controls the amount of damping applied to the electrons in each time step, and affects the amount of phase lag present when an external AC field is applied. The AC conductivity is given by

$$\sigma(\omega) = \frac{\sigma_0}{1 - i\omega\tau}, \tag{2}$$

where σ_0 is the DC conductivity of the material, and ω is the angular frequency of the external electric field. Some simple algebra shows that when written in polar representation, the phase of $\sigma(\omega)$ is given by $\phi = \arctan(\omega\tau)$. Thus, the Drude model predicts that, with a sinusoidal external driving field, the movement of electrons will also be the same form, but with a phase offset. It is noteworthy that the Drude model treats the electrons as non-interacting, and that this phase lag ϕ does not depend on electron density. It will be interesting to see whether this still holds with Coulomb interaction between

electrons (see section 5.1).

The electron dynamics is simulated in a straightforward way. First, the electric field at the position of each electron is computed, this electric field includes the impact of the external electric field, but also the electric field generate by the electron inside the 2DEG. Form this, we can easily find the force acting on each particle. Using this value for acceleration, the velocity and position of each electron is evolved in time via forward Euler. This method is chosen mainly for its simplicity and low computational cost. It is important to note that since we are trying to simulate as many particles as possible (2DEG normally have a high electron density), the computational aspect is absolutely crucial. Also, we choose forward Euler because we are interested in the transient behavior (e.g. when applying a time-varying external electric field to observe phase lag) as well as the steady state. It will be interesting, however, to compare this against an semi-implicit method such as the Leapfrog method. Such a comparison will let us see how the stability of the code varies with the different methods and decide whether having a more computationally expensive method like the Leapfrog method is more advantageous for its higher stability (e.g bigger time-step).

Periodic boundary condition is chosen in cases where the bulk property is the point of interest, and is implemented in such a way that the electric field line emanating from an electron would, for example, cross the boundary on the right and loop back from the left. For some external electric fields, such as one radiating outward from the center of the simulation field, a reflective boundary condition is implemented. This reflection is chosen to conserve the momentum of the particle.

At each time step in the simulation, the momentum of an electron is damped according to the kinematic equation given by the Drude model to simulate collisions between electrons and impurities. It is important to note that it is a very crude approximation of the Drude model. The Drude model is not adapted to directly simulate the formation of structure, since it assumes that the electrons act as an ideal gas. So, we only take this small part of the theory to do our simulation. Furthermore, this will not affect on the steady state, since the damping is only significant when the electrons move.

Also, since then density of electrons inside a 2DEG is high and thus simulating each one of them would be hard, if not impossible to do on a normal computer, we do not directly simulate each electron. Instead, our particles are a cluster of multiple electrons, where the charge of each one of those super-particles are chosen such that the charge density of 2DEG stays realistic.

4 Testing

4.1 Molecular dynamics

To see that the implementation of molecular dynamics works, the first test is to look at the steady state with no external electric field and using periodic boundary conditions. Unsurprisingly, the electrons stabilize themselves into some form a sort of lattice, shown in figure 1. The lattice looks like a simple square lattice. We know that the force between the electron is purely repulsive, thus they will want to be as far away as possible within the limited space given. Since our simulation space is a square (the formation of lattice is purely due to finite size effect and will be strongly correlated to the form and size of the simulation), then the positions that let them maximize their distance between each other will be a square lattice.

Interestingly, we can see that there is some defect within the lattice in the second figure. To be more precise, we can see some kind of grain boundary: interface between lattices with different orientations. It is important to note that these are transient. After some time, the different lattices rearrange themselves to form a larger, cohesive lattice, like we see in the first figure. However, it is crucial to note that it take of lot of time for those defects to disappear, which is also the case for real life materials, thus it is likely not due to some kind of anomaly in the simulation. Note that some simulations were terminated before reaching this final steady state due to the sheer amount of time the simulations would take.

4.2 ODE Solver

We simulate some of the previous cases with a Leapfrog algorithm to see if there is any change in the final structure and to see if we could increase the time step size with this method, which would make it more efficient that the forward Euler method.

As shown in figure 1, the steady state for the case without any external electric field is the same as forward Euler. This confirms the validity of the numerical scheme of forward Euler. However, it is interesting to note that with this method, we can use time steps 15 times bigger than that of forward Euler before the simulation become unstable. This could give the impression that the Leapfrog algorithms is clearly more efficient than Euler, but it is not exactly the case in our implementation. For the Leapfrog method, we need to calculate the acceleration twice and this is done with a for-loop (looping over each electron), which is notoriously inefficient in python. As long as the calculation of the acceleration is not vectorized (again, due to time constraints), it is hard to says that the Leapfrog

algorithm is more efficient than forward Euler.

4.3 Boundary conditions

Results from testing our implementation of boundary conditions agree with expectations. We applied an constants electric field in the x direction. We expect to see drastic difference between the periodic boundary condition and the reflective one. An animation of the simulation labelled "Linear movement" can be found in the repository as supplemental material.

Following our theoretical expectations, the boundary conditions completely change the system. For the periodic boundary condition, the electrons simply move in the x direction *ad nauseam* and form a square lattice as before. In contrast, for the reflective boundary, the electron start to accumulate on the y boundary and form some kind of square lattice like seen in last case, but squish on the x direction, shown in figure 2. It is crucial to note that it will be very hard to find a steady state for this case. The electron at the reflective boundary will always be repel on the boundary and be reflected back, so they will always move a little bit. Thus, the steady state defined by the residue will never likely be achieved.

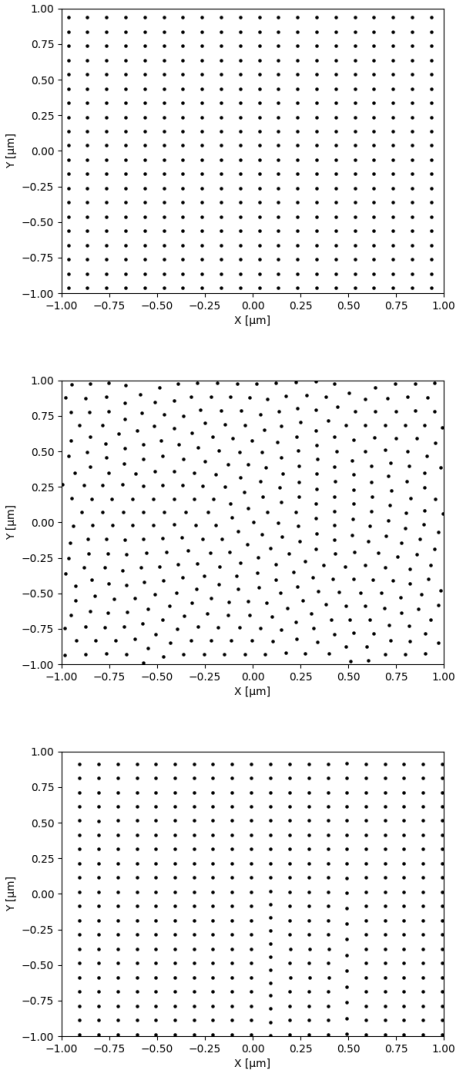

Figure 1: The steady state for no external electric field. The first one is the true steady state after a lot of iterations. The second is a very slow moving transient state. It is the steady state with some defects. The third one is the results with the Leapfrog method, it was stop a little bit before a perfect steady state.

Both those results make physical sense. The electron will still want to be as far away from possible, but now they also want to go to the right. If the periodic boundary is used, then nothing is stopping them to continue moving to the right for ever. So, if we would go to their reference frame associated to the their movement to the right, it will be the same mechanics as the case without any external electric field. For the reflective boundary, their movement will be stop by the boundary. Even, if the electron want to be on the right, their repulsion will stop them from all accumulating on the boundary. So, we

can think about this case as pushing the square lattice on the right side, so we should expect some kind of squish lattice on the right side. We precisely observe this phenomena.

4.4 Radial electric field

As a final test for expected behaviour, we used a positive electrical field in the radial direction. Again, we seen what we expect: the electrons cluster in the middle of the 2DEG, as shown in figure 3. It is noteworthy that the system does not reach a perfect steady state. The electron in the middle of the circle/lattice is unstable and always move a little bit. This means that the residue will always stay over the defined limit for steady state. The program will not automatically stop, hence the importance of implementing the maximum-iteration stopping condition. This problem can be avoided by choosing a lower mean-free-time to damp out these vibrations.

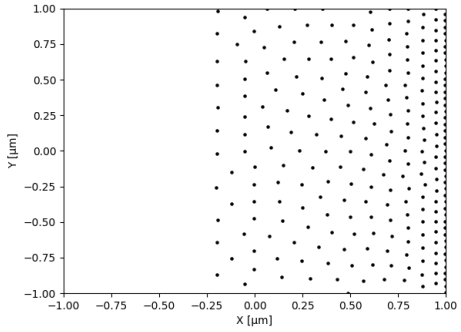

Figure 2: This is the resuls of the simulation for a constants electric field in x direction with reflective boundary condition

Again, this final steady state is expected. In this case, there is a balancing between the repulsion of the electron between each other and their attraction to the middle. It is the same logic as previously, but instead of being squish in the x direction, it will be squish in the radial direction. So, we should see some kind of circular cluster of electron with some kind of basic periodic lattice. Since, the cluster of electron is no longer in rectangular form, then the square lattice will not be the best way to keep the electron as far away as possible. Instead a lattice separated periodically in the radial and azimuthal direction will be prefer. All of this is seen in figure 3.

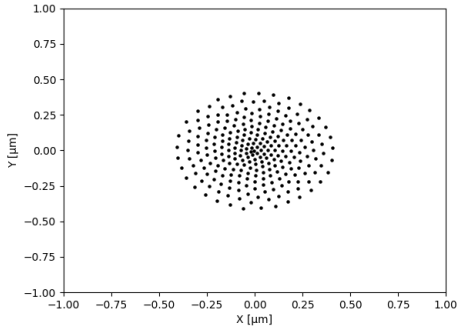

Figure 3: The is the steady state for electric field in the radial direction.

Everything is bold is to proof read and, there is one thing in red that it is comment of me, that I need to think about, you are welcome to give your opinion on the problem. Also, the red comment in the end/conclusion, I modify the sentence, what do you think ?

5 Results

5.1 Phase Lag

A quantitative and rigorous measurement of the phase lag between electron oscillation and the external field would require some time to implement. Due to time restriction, we will only look at limit cases qualitatively. From equation 2, we expect that the phase lag is large when $\omega\tau$ is large, and that the maximum phase lag is $\pi/2$. Beginning with a simulation using $\omega = 10^3$ THz and $\tau = 10^{-4}ps$, this gives $\omega\tau = 0.1$ and $\phi \approx 0.1rad$. Shown in figure 4, the external field is a plane wave travelling along the x-direction with polarization along the y-direction. This wave is illustrated via red arrows. Note that for illustrative convenience, the wavenumber of the field is manually fixed. The velocity of each electron is drawn by a small line, going away from the electron.

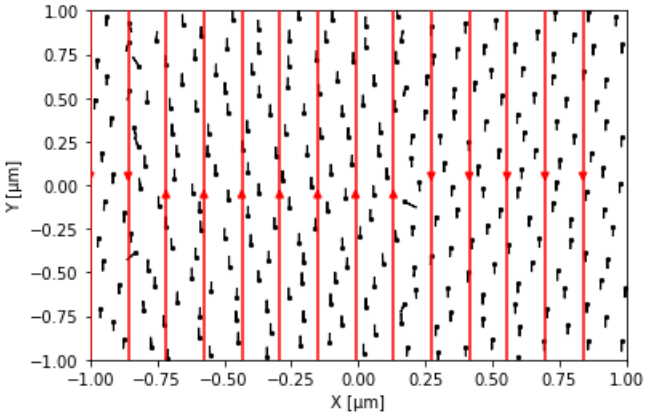

Figure 4: The little line represent the velocity of the electron and the red vector field is the external electric field. It is the case for no phase lag.

Looking at figure 4, we can see that the velocities of the electrons point in the same direction as the external field, with those near points where the external field is 0 having random-looking velocities (the charge of the electrons was taken to be $+|e|$ for convenience, hence the flipped direction of the force). The motion is thus in phase with the driving field. On the other end of the spectrum, using $\omega = 3 \times 10^4$ THz and $\tau = 10^{-3}ps$ gives $\omega\tau = 30$ and $\phi \approx 1.5rad$. From figure 5, we see that the electrons with random-looking velocities are not at places where the external electric field is 0. Instead, they are around 3 vertical red lines away from it. The half-wavelength of the external field is roughly 7 vertical red lines,

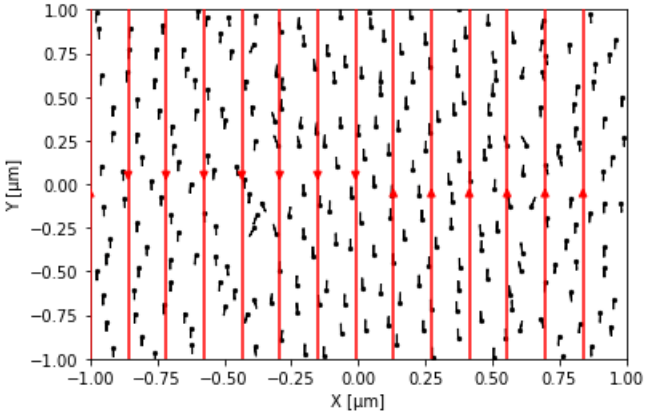

Figure 5: Following the same visualization method as 4, but in the case where the phase lag is large.

thus a phase-shift of around 3 lines corresponds to 1/4 of a cycle, agreeing with $\phi \approx \pi/2$.

Another indirect test of equation 2 is that the phase lag should depend only on the combination $\omega\tau$, and not the quantities separately. Looking at a simulation with $\omega = 1.5 \times 10^4$ THz and $\tau = 2 \times 10^{-3} ps$ ($\omega\tau = 30$), we see the same amount of phase lag as before. The animation is stored in a folder named "Phase lag animations" in the repository, labelled 3.

As mentioned in section 3, the Drude model neglects inter-electron interactions. With this simulation, we can roughly test whether the phase shift depends on the electron density. Note that in the simulation, the electron density is implemented by modulating the electric charge, so the number of electrons displayed in the animation does not change. An electron density of $10^3 \mu m^{-2}$ was used for the animations mentioned above, so we re-simulate the cases of large and small phase lags using an electron density 5 times higher ($n = 5 \times 10^3 \mu m^{-2}$). Looking at the animations (stored in the same folder and labelled 4 and 5 for small and large phase lags, respectively), we do not see a significant change on the amount of phase lag.

5.2 Field Effect Electronics

This objective is simple: we want to know how close a transistor, interferometer, or any object creating a electric field that is used for any field-effect electronics must be from the 2DEG to have the necessary effect. We know that the strength of the electric field diminishes according to the inverse square law, so we can take any electrical field and multiply it by $\frac{1}{z^2}$ to show the effect of the z distance on the magnitude of the field. To find the effect of the z distance on the lattice structure of the electron, we will launch the simulation at different z-values and see the final lattice structure formed.

Since the simulation can be slow to run for multiple z-values, if the quantity of particles is important, we instead run for a few z-values and do a three dimensional (x,y and z) spline of the electric potential. This method avoids having to rerun the simulation if we want to rapidly see whether the lattices stay similar. We know that when extremely close to the electron, the potential will spike compared to the general background. Thus we can say that roughly where the electric potential is one order of magnitude bigger than the average value (so mostly the background) is where there is an electron nearby. Such a method allows us to estimate the position of an electron from the spline, illustrated in figure 6.

We can see at 1.5 μm, we can see the classic radial structure previously mentioned. In fact, we can see that structure starts to diffuse away around 3 μm, and after 5 μm the structure is extremely close to the one observed without any electric field. This implies that a few millimeters of distance is

enough to have an important effect on the 2DEG. It is still important to mention that this conclusion is fundamentally related to strength of the external electric field, which we arbitrarily chose to be $5 \cdot 10^7 N/C$. If we would take a stronger electric field, the effect of distance would diminish. Similarly, an external field with a smaller magnitude will be decay more quickly compared to our present results. However, this still illustrates the power of this methodology to analyze the electrons in 2DEG. Note that strength of the electric field was chosen arbitrarily simply because such a value will be profoundly related to the type of application where the 2DEG is used and thus varies widely.

6 Discussion and further improvements

Like it was shown, this simulation is capable of simulating not only multiple steady states associated to various systems, but it can also be used to investigate some transient states like phase lag. There remain, however, various improvements which would make this implementation more versatile.

One major feature overlooked in this project is the electric current. In a 2DEG, there is normally some kind of electric source and drain where the electrons will enter and exit the system. By looking at the speed at which those particles are leaving the 2DEG, we could find the electric current that an external electric field would generate. In fact, this could be done by creating a mixed boundary condition, where a small section of reflective boundary is a pseudo-periodic boundary. With those modifications, we could possibly simulate the classical Hall effect.

We also mentioned in section 1 the interference of two transistors could cause on each other, if they are close enough. This could be simulated by coupling two simulations to each other, where the external electric field inputted into a system is the electric field generated by the electrons of the other simulation. Similarly, this would let us simulate some more complex heterostructures where the wafer has two quantum wells, thus two 2DEGs.

Another feature lacking in this project is the magnetic field generated by the electrons. We know from electrodynamics that moving charged particles should generate a magnetic field, but this aspect was completely ignored in this implementation.

7 Conclusion

In summary, we use classical molecular dynamics to simulate the structure formed by electrons in a 2DEG due to an external electric field and analyze one of the characteristic transient states, the phase lag phenomenon. Such phenomena can hardly be investigated with analytic model for realistic electric

fields, and various transient states associated with other forces acting on the electrons are not governed by the Poisson equation. This illustrates the reason we decided to utilize molecular dynamics for such a purpose. We develop the necessary methodology to observe how diminishing the magnitude of an external electric field, by increasing the distance between the difference electronic element of field effect machinery, will affect the lattice formed by the electrons in their steady state.

For future works, we could implement important aspects of 2DEG that were missing in this implementation. For example, the magnetic fields created by the electrons moving or the presence of a electronic source and drain. We could also push the simulation into more complex systems where multiple 2DEG are capacitively interconnected, such as heterostructure with two quantum wells.

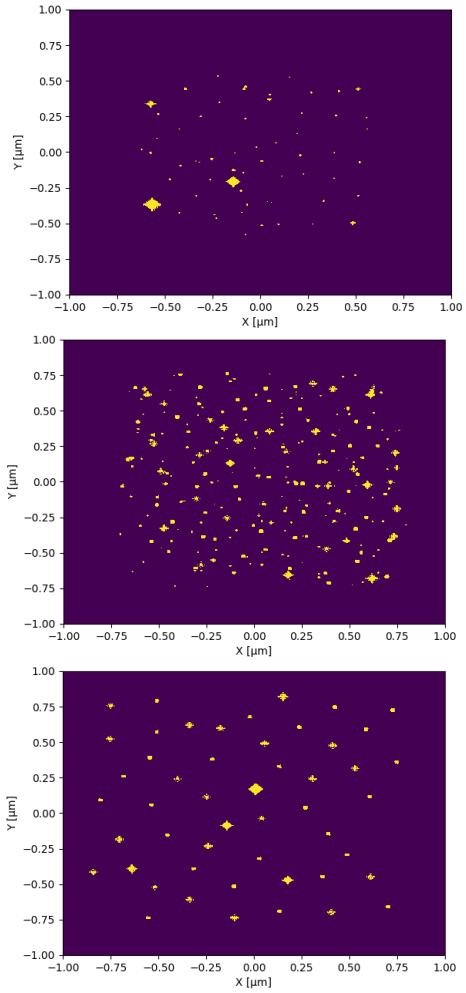

Figure 6: Different final results of the simulation estimated by the spline at different z values, 1.5, 3, 5 μm. The yellow zone is represent zone where the magnitude of the electric potential is more than 5 time bigger than the average electric potential. This indicated that probably a electron is there, beware it is a crude estimation of their positions.

8 Contribution

Justin Mainville: Coulomb interactions between electrons; the external electric field; calculation of the internal electric field and potential; the Z-sweep for field effect. He also did the code documentation and contributed to the report.

Zhongan Lin: Drude model damping; boundary conditions; external AC electric fields and the visualization (animation). He also helped during the writing of the report.

9 Reference

One general reference is used during this report, it is the book "Solid state physics" by Neil W. Ashcroft and N. David Mermin (1976).