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Quantum Hydrodynamic Description of Plasma

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Abstract: A quantum hydrodynamic description of plasma is a theoretical framework that attempts to describe the behaviour of a plasma at a macroscopic level, taking into account both quantum mechanics and the principles of fluid dynamics. In this framework, the plasma is treated as a collection of charged particles, such as ions and electrons, that interact with each other through the electromagnetic force. The behaviour of the plasma is described by a set of hydrodynamic equations, which describe the motion of the particles, their interactions, and the electromagnetic fields that they generate. At the quantum level, the particles are treated as wave functions, and the hydrodynamic equations are modified to include quantum effects such as wave-particle duality and uncertainty principle. One of the key advantages of a quantum hydrodynamic description of plasma is that it allows for a more accurate and comprehensive understanding of plasma behaviour than classical models. This can be particularly important in fields such as astrophysical plasmas.

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INTRODUCTION

Classical models work well for many aspects of plasma behaviour, but they have limitations in extreme conditions like astrophysical plasmas, where quantum mechanics plays a significant role. This project focuses on understanding astrophysical media through the quantum hydrodynamic description of plasma, using theoretical analysis and numerical simulations. The quantum hydrodynamic description of plasma is a valuable tool for understanding the properties of the universe's most abundant state of matter. During our literature survey, we undertook an exploration of classical plasma, quantum plasma, their inherent properties, and the formulation of quantum hydrodynamic equations and frameworks. We also understood in detail the Wigner Function and derived the Wigner-Poisson system. We also understood Fortran programming and its packages, particularly LCPFCT and CNVFCT, as these are used in numerically simulating our model and solving the equations in our model. We also used plotting tools like gnuplot that helped us to visualise our system.

THEORETICAL AND COMPUTATIONAL MODEL

For a one-dimensional case, the non-relativistic QHD equations are composed of the continuity equation, momentum equation and Poisson equation –

$$\frac{\partial n}{\partial t}+\frac{\partial (n v_x)}{\partial t}=0$$

$$\mathrm{mn}\,\frac{\partial\,\mathrm{u}}{\partial\,\mathrm{t}} + \mathrm{mn\,u}\,\frac{\partial\,\mathrm{u}}{\partial\,\mathrm{x}} = \mathrm{ne}\,\frac{\partial\,\phi}{\partial\,\mathrm{x}} - \frac{\partial\,\mathrm{P_{cl}}}{\partial\,\mathrm{x}} - \frac{\partial\,\mathrm{P_q}}{\partial\,\mathrm{x}}$$

$$\frac{\partial^2\phi}{\partial x^2}=\frac{e}{\epsilon_0}(n-n_o)$$

To represent the probability density of particles in both position and momentum space and capture the wave-particle duality inherent in quantum systems, we use the Wigner distribution function given by –

$$f(x,v,t)=\frac{m}{2\pi\hbar}\int_{-\infty}^{\infty} ds\ e^{\frac{imvs}{\hbar}}\psi^*\left(x+\frac{s}{2},t\right)\psi\left(x-\frac{s}{2},t\right)$$

N-particle Wigner function can be written as –

$$f^N(x_1,v_1,\ldots,x_N,v_N,t)=N\left(\frac{m}{2\pi\hbar}\right)^N\sum_{\alpha=1}^{M}\left(p_\alpha\int ds_1\ldots ds_N e^{\left(\frac{im}{\hbar}\sum_{i=1}^{N}v_i s_i\right)}\psi_\alpha^{*N}\left(x_1+\frac{s_1}{2},\ldots,x_N+\frac{s_N}{2},t\right)\psi_\alpha^N\left(x_1-\frac{s_1}{2},\ldots,x_N-\frac{s_N}{2},t\right)\right)$$

For electrostatic interactions in a quantum plasma, the Wigner-Poisson equations are given by –

$$\frac{\partial f}{\partial t}+v\frac{\partial f}{\partial x}=\frac{iem}{\hbar}\int\int dv' f(x,v',t)\frac{ds}{2\pi\hbar}e^{\frac{im(v'-v)s}{\hbar}}\left[\phi\left(x+\frac{s}{2},t\right)-\phi\left(x-\frac{s}{2},t\right)\right]$$

$$\frac{\partial^2\phi}{\partial x^2}=\frac{e}{\epsilon_0}\left(\int dv\ f(x,v,t)-z_i n_i\right)$$

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+\phi(x)\psi$$

2.1 Derivation of Wigner-Poisson Equations System

The 1-particle Wigner function is given by:

$$f(x,v,t) = \frac{m}{2\pi\hbar}\int_{-\infty}^{\infty} ds\ e^{\frac{imvs}{\hbar}}\psi^*\left(x+\frac{s}{2},t\right)\psi\left(x-\frac{s}{2},t\right) \text{ ------------------(0)}$$

The Schrodinger equation is given by:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + e\phi(x)\psi \text{ ------------------(a)}$$

Let us take its complex conjugate:

$$-i\hbar\frac{\partial\psi^*}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi^*}{\partial x^2} + e\phi(x)\psi^* \text{ ------------------(b)}$$

Evaluating equation (a) at $\left(x-\frac{s}{2},t\right)$ and equation (b) at $\left(x+\frac{s}{2},t\right)$:

$$i\hbar\frac{\partial\psi\left(x-\frac{s}{2},t\right)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi\left(x-\frac{s}{2},t\right)}{\partial x^2} + e\phi\left(x-\frac{s}{2}\right)\psi\left(x-\frac{s}{2},t\right) \text{ ------------------(1)}$$

$$-i\hbar\frac{\partial\psi^*\left(x+\frac{s}{2},t\right)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi^*\left(x+\frac{s}{2},t\right)}{\partial x^2} + e\phi\left(x+\frac{s}{2}\right)\psi^*\left(x+\frac{s}{2},t\right) \text{ ------------------(2)}$$

Multiplying equation (1) with $\psi^*\left(x+\frac{s}{2},t\right)$ and multiplying equation (2) with $\psi\left(x-\frac{s}{2},t\right)$:

$$i\hbar\psi^*\left(x+\frac{s}{2},t\right)\frac{\partial\psi\left(x-\frac{s}{2},t\right)}{\partial t} = -\frac{\hbar^2}{2m}\psi^*\left(x+\frac{s}{2},t\right)\frac{\partial^2\psi\left(x-\frac{s}{2},t\right)}{\partial x^2} + e\phi\left(x-\frac{s}{2}\right)\psi^*\left(x+\frac{s}{2},t\right)\psi\left(x-\frac{s}{2},t\right) \text{ --------(3)}$$

$$-i\hbar\psi\left(x-\frac{s}{2},t\right)\frac{\partial\psi^*\left(x+\frac{s}{2},t\right)}{\partial t} = -\frac{\hbar^2}{2m}\psi\left(x-\frac{s}{2},t\right)\frac{\partial^2\psi^*\left(x+\frac{s}{2},t\right)}{\partial x^2} + e\phi\left(x+\frac{s}{2}\right)\psi\left(x-\frac{s}{2},t\right)\psi^*\left(x+\frac{s}{2},t\right) \text{ --------(4)}$$

Subtracting equation (4) from equation (3):

$$i\hbar\frac{\partial\psi^*\left(x+\frac{s}{2},t\right)\psi\left(x-\frac{s}{2},t\right)}{\partial t} = \frac{\hbar^2}{2m}\left[\psi\left(x-\frac{s}{2},t\right)\frac{\partial^2\psi^*\left(x+\frac{s}{2},t\right)}{\partial x^2} + \psi^*\left(x+\frac{s}{2},t\right)\frac{\partial^2\psi\left(x-\frac{s}{2},t\right)}{\partial x^2}\right] + e\psi^*\left(x+\frac{s}{2},t\right)\psi\left(x-\frac{s}{2},t\right)\left[\phi\left(x-\frac{s}{2}\right)-\phi\left(x+\frac{s}{2}\right)\right] \text{ --------(5)}$$

Now, we use the following identity:

$$\psi^*\left(x+\frac{s}{2},t\right)\frac{\partial^2\psi\left(x-\frac{s}{2},t\right)}{\partial x^2} - \psi\left(x-\frac{s}{2},t\right)\frac{\partial^2\psi^*\left(x+\frac{s}{2},t\right)}{\partial x^2} = -2\frac{\partial^2\psi^*\left(x+\frac{s}{2},t\right)\psi\left(x-\frac{s}{2},t\right)}{\partial x\,\partial s} \text{ ------(6)}$$

Using equation (6) in equation (5):

$$i\hbar\frac{\partial}{\partial t}\left(\psi^*\left(x+\frac{s}{2},t\right)\psi\left(x-\frac{s}{2},t\right)\right)=\frac{\hbar^2}{m}\frac{\partial^2}{\partial x\,\partial s}\left(\psi^*\left(x+\frac{s}{2},t\right)\psi\left(x-\frac{s}{2},t\right)\right)+e\psi^*\left(x+\frac{s}{2},t\right)\psi\left(x-\frac{s}{2},t\right)\left[\phi\left(x-\frac{s}{2}\right)-\phi\left(x+\frac{s}{2}\right)\right] \text{--------(7)}$$

Multiplying each side by $\left(\frac{m}{2\pi\hbar}\right)e^{\frac{imvs}{\hbar}}$ and integration with respect to ds:

$$i\hbar\left(\frac{m}{2\pi\hbar}\right)\int_{-\infty}^{\infty}ds\ e^{\frac{imvs}{\hbar}}\frac{\partial}{\partial t}\left(\psi^*\left(x+\frac{s}{2},t\right)\psi\left(x-\frac{s}{2},t\right)\right)=\frac{\hbar^2}{m}\left(\frac{m}{2\pi\hbar}\right)\int_{-\infty}^{\infty}ds\ e^{\frac{imvs}{\hbar}}\frac{\partial^2}{\partial x\,\partial s}\left(\psi^*\left(x+\frac{s}{2},t\right)\psi\left(x-\frac{s}{2},t\right)\right)+e\left(\frac{m}{2\pi\hbar}\right)\int_{-\infty}^{\infty}ds\ e^{\frac{imvs}{\hbar}}\frac{\psi^*\left(x+\frac{s}{2},t\right)\psi\left(x-\frac{s}{2},t\right)}{\hbar}\left[\phi\left(x-\frac{s}{2}\right)-\phi\left(x+\frac{s}{2}\right)\right] \text{--------(8)}$$

Now using equation (0), we get:

$$i\hbar\frac{\partial f(x,v,t)}{\partial t}=\frac{\hbar^2}{m}\left(\frac{m}{2\pi\hbar}\right)\int_{-\infty}^{\infty}ds\ e^{\frac{imvs}{\hbar}}\frac{\partial^2}{\partial x\,\partial s}\left(\psi^*\left(x+\frac{s}{2},t\right)\psi\left(x-\frac{s}{2},t\right)\right)+e\left(\frac{m}{2\pi\hbar}\right)\int_{-\infty}^{\infty}ds\ e^{\frac{imvs}{\hbar}}\frac{\psi^*\left(x+\frac{s}{2},t\right)\psi\left(x-\frac{s}{2},t\right)}{\hbar}\left[\phi\left(x-\frac{s}{2}\right)-\phi\left(x+\frac{s}{2}\right)\right] \text{--------(9)}$$

Let us now evaluate the first term in equation (9) using integration by parts:

$$Term1\ =\left(\frac{m}{2\pi\hbar}\right)\left(\frac{\hbar^2}{m}\right)\int_{-\infty}^{\infty}ds\ e^{\frac{imvs}{\hbar}}\frac{\partial^2\psi^*\left(x+\frac{s}{2},t\right)\psi\left(x-\frac{s}{2},t\right)}{\partial x\,\partial s}$$

$$Term1=\left(\frac{m}{2\pi\hbar}\right)\left(\frac{\hbar^2}{m}\right)\frac{\partial}{\partial x}\left[\int_{-\infty}^{\infty}ds\ e^{\frac{imvs}{\hbar}}\frac{\partial}{\partial s}\left(\psi^*\left(x+\frac{s}{2},t\right)\psi\left(x-\frac{s}{2},t\right)\right)\right]$$

$$Term1=\left(\frac{m}{2\pi\hbar}\right)\left(\frac{\hbar^2}{m}\right)\frac{\partial}{\partial x}\left[\ e^{\frac{imvs}{\hbar}}\psi^*\left(x+\frac{S}{2},t\right)\psi\left(x-\frac{s}{2},t\right)\Big|_{-\infty}^{\infty}-\int_{-\infty}^{\infty}\psi^*\left(x+\frac{S}{2},t\right)\psi\left(x-\frac{s}{2},t\right)\frac{imv}{\hbar}e^{\frac{imvs}{\hbar}}ds\right]$$

$$Term1=\left(\frac{m}{2\pi\hbar}\right)\left(\frac{\hbar^2}{m}\right)\frac{\partial}{\partial x}[0-2\pi ivf(x,v,t)]$$

$$Term1=\left(\frac{m}{2\pi\hbar}\right)\left(\frac{\hbar^2}{m}\right)\frac{\partial}{\partial x}[-2\pi ivf(x,v,t)]\ =\ -i\hbar v\frac{\partial f(x,v,t)}{\partial x}$$

Using the value of Term 1 in equation (9), we get:

$$i\hbar\frac{\partial f(x,v,t)}{\partial t}=-i\hbar v\frac{\partial f(x,v,t)}{\partial x}+\ e\left(\frac{m}{2\pi\hbar}\right)\int_{-\infty}^{\infty}ds\ e^{\frac{imvs}{\hbar}}\psi^*\left(x+\frac{s}{2},t\right)\psi\left(x-\frac{s}{2},t\right)\left[\phi\left(x-\frac{s}{2}\right)-\phi\left(x+\frac{s}{2}\right)\right] \text{----(10)}$$

Taking Inverse Fourier Transform of equation (0):

$$\psi^*\left(x+\frac{s}{2},t\right)\psi\left(x-\frac{s}{2},t\right)=\int_{-\infty}^{\infty}f(x,v',t)e^{-\frac{imv's}{\hbar}}\ dv' \text{ --------(11)}$$

Using equation (11) in equation (10), we get:

$$i\hbar\frac{\partial f(x,v,t)}{\partial t}=-i\hbar v\frac{\partial f(x,v,t)}{\partial x}+e\left(\frac{m}{2\pi\hbar}\right)\int_{-\infty}^{\infty}ds\ e^{\frac{imvs}{\hbar}}\left[\phi\left(x-\frac{s}{2}\right)-\phi\left(x+\frac{s}{2}\right)\right]\int_{-\infty}^{\infty}f(x,v',t)e^{-\frac{im\ 's}{\hbar}}\ dv' \text{ ----(12)}$$

Rearranging the terms:

$$i\hbar\frac{\partial f(x,v,t)}{\partial t}+i\hbar v\frac{\partial f(x,v,t)}{\partial x}=e\left(\frac{m}{2\pi\hbar}\right)\iint_{-\infty}^{\infty}dv'\ ds\, e^{\frac{im(v-v')s}{\hbar}}f(x,v,t)\left[\phi\left(x-\frac{s}{2}\right)-\phi\left(x+\frac{s}{2}\right)\right] \text{--------(13)}$$

Dividing the equation by $i\hbar$ and rearranging the constants:

$$\frac{\partial f(x,v,t)}{\partial t}+v\frac{\partial f(x,v,t)}{\partial x}=i\frac{me}{\hbar}\iint_{-\infty}^{\infty}dv'\ f(x,v,t)\ \frac{ds}{2\pi\hbar}e^{\frac{im(v-v')s}{\hbar}}\left[\phi\left(x+\frac{s}{2}\right)-\phi\left(x-\frac{s}{2}\right)\right] \text{--------(14)}$$

Equation (14) gives us the final evolution equation for the Wigner-Poisson system.

$$\boxed{\frac{\partial f(x,v,t)}{\partial t}+v\frac{\partial f(x,v,t)}{\partial x}=i\frac{me}{\hbar}\iint_{-\infty}^{\infty}dv'\ f(x,v,t)\ \frac{ds}{2\pi\hbar}e^{\frac{im(v-v')s}{\hbar}}\left[\phi\left(x+\frac{s}{2}\right)-\phi\left(x-\frac{s}{2}\right)\right]}$$

2.2 Computational Algorithm and Methodology

PIC (Particle in a Cell System)
In plasma physics, the PIC method is a numerical approach that simulates a collection of charged particles that interact via external and self-induced electromagnetic fields. A spatial grid is used to describe the field while the particles move in the continuous space. The field and the particle motion are solved concurrently.

In this section we describe the steps which will yield a self-consistent particle simulation model for a one-dimensional electrostatic plasma. Here we make the following assumptions:
1) There is no variation in the plasma and particle quantities (charge density, velocity, position, etc.) and in the electric field along the z-direction.
2) The magnetic field is zero in the x-axis in which the particles move.
3) We restrict our distances of the order of the Debye length. Since charge separation occurs over these distances the charge density is non-zero.
4) We restrict our interest to times of the order of the electron plasma frequency. Since average current densities over these times are zero, there is no self-magnetic field.
5) There are no collisions.

With these assumptions the Maxwell equations are reduced to the Poisson's equation which completely specifies the electric field distribution at a given time.

PIC Algorithm for the simulation of 1D electrostatic plasma simulation

1. Initialize *particle* data (position, velocity, perturbation distribution)
2. Initialize *grid* (field) data (Number of cells, length of grid, spacing between cells)
3. **while** $t < t_{max}$ **do**
4. Compute *particle* contributions to the *grid*
5. Calculate the fields (field is stored in grid points array in discretized form)
6. Update forces on *particle* positions
7. Move particles to new positions
8. $t \rightarrow t + t_{step}$
9. **end while**
10. Print *particles* and *grid* data
11. Print statistics

RESULTS AND DISCUSSION

In this simulation, ions are considered fixed in space and are therefore not represented in the simulation. First, an initial distribution of stationary electrons is defined. Standing waves are formed in the charge density when electrons are given a spatial perturbation of the form of a sinusoidal wave. In regions of higher charge density, electric fields accelerate the electrons to travel from their equilibrium positions. After the electrons are displaced, consecutive electric fields grow in the opposite direction to restore the neutrality of the plasma by pulling the electrons back to their original positions. Due to their inertia, the electrons will overshoot and oscillate around their equilibrium positions at the plasma frequency, ω_p.

Spatial input variables are as follows: L=100 cm, nt=500 s, dt=1 s, ng=100, where L is the length of the physical space represented by the simulation, nt is the number of time steps the particle motions and fields are updated, dt is the temporal length of each time step, and ng is the number of grid points.

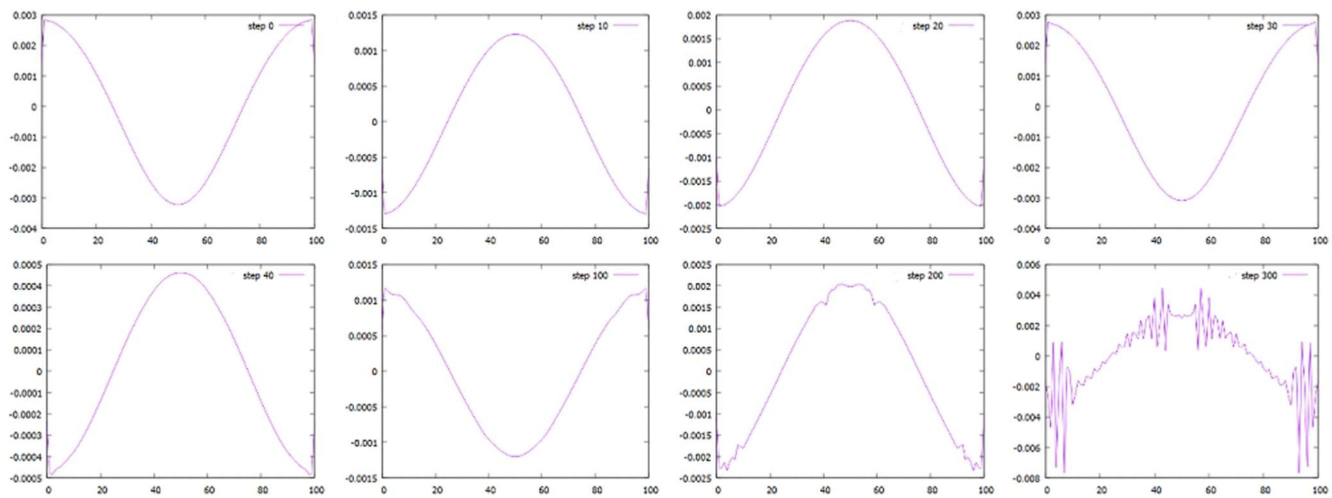


Figure 1: Plots showing charge density for different time steps
(Here x-axis represents grid points (cm) and y-axis represents charge density (stC/cm))

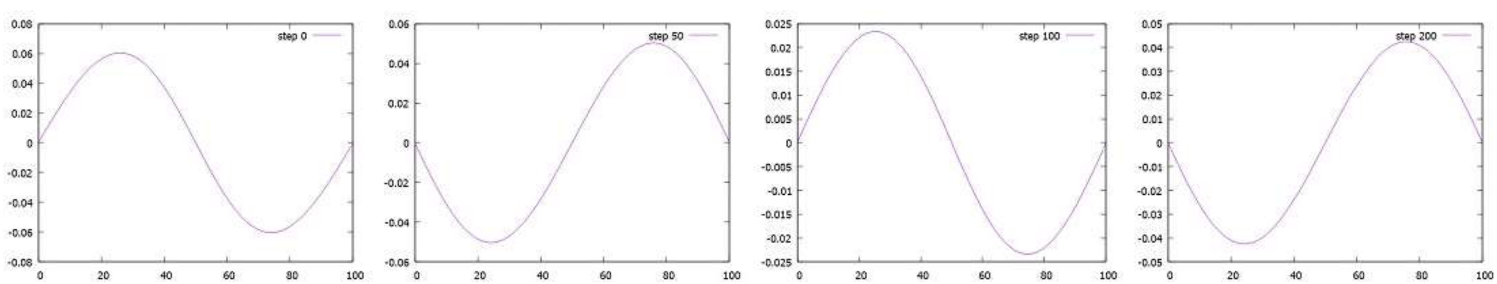


Figure 2: Plots showing Electric Field for different time steps
(Here x-axis represents grid points (cm) and y-axis represents Electric Field (stV/cm))

The Plasma initially possesses a sinusoidal charge density due to the spatial perturbation, then oscillates harmonically for the duration of the simulation. Figures 1 and 2 show the charge densities and electric fields (respectively) of a plasma through time. The non-uniform charge distribution seeks net neutrality, but once the electrons are evenly spread, their new non-zero velocities push the particles to oscillate at the plasma frequency. The electric field oscillation behaves similar to the charge density oscillation, as the electrostatic model means that the electric field is merely the negative of the charge density's derivative in space. The fluctuations introduced in the charge density plots at later time steps is due to instabilities in the numerical methods as they discretize continuous processes, introducing errors and approximations that can accumulate over time. As the simulation progresses, these errors may amplify, leading to deviations from the expected behaviour and the onset of numerical instabilities.

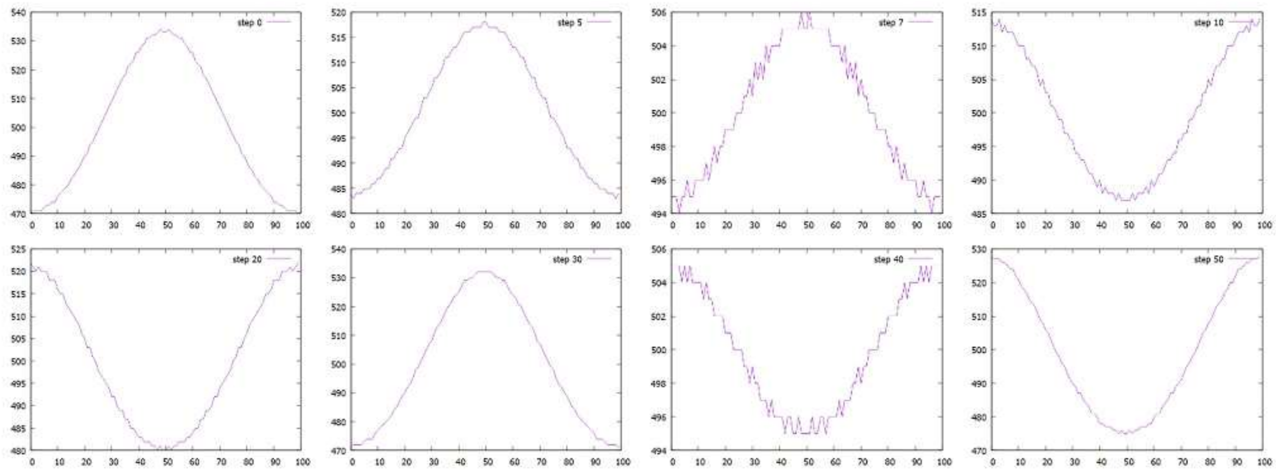


Figure 3: Plots showing particle position distribution for different time steps
(Here x-axis represents grid points (cm) and y-axis represents particle density (cm^{-1}))

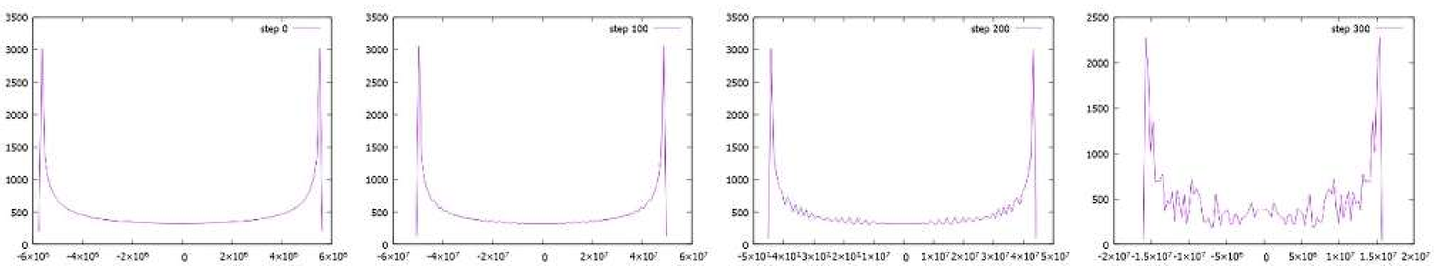


Figure 4(a): Plots showing particle velocity distribution for different time steps
(Here x-axis represents velocity (cm/s) and y-axis represents particle density within each velocity range (cm^{-1}))

Figure 3 and 4(a) show position and velocity distribution for different time steps respectively. These plots are very important and tell us about the number of particles present within a particular position and range of velocities. These can further be used to calculate quantities like square of mean velocity and mean of velocity squared (shown in Figure 4(b)), which give us information about the temperature, thermal spread and kinetic energy distribution within a plasma.

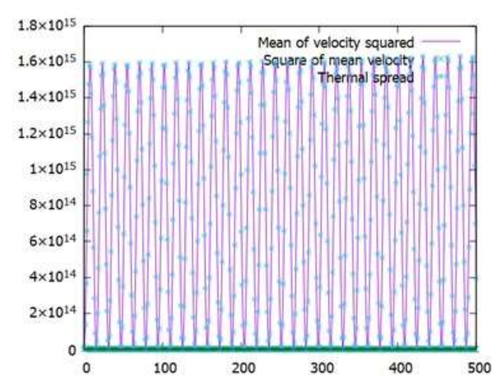
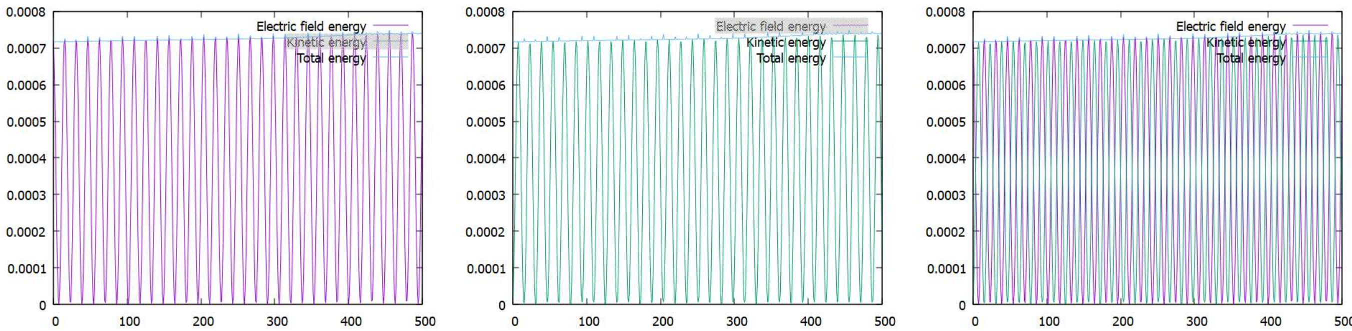


Figure 4(b): Time history plot for mean of velocity squared, square of mean velocity and thermal spread
(Here x-axis time steps (s) and y-axis represents velocity square $(cm/s)^2$)

In the later time steps of the simulation, the emergence of instabilities and errors may be attributed to the phenomenon of Landau damping in plasma simulation. Landau damping involves the resonant interaction between plasma waves and charged particles, particularly electrons, leading to energy exchange and wave damping. In numerical simulations, challenges arise when capturing these resonant interactions accurately, especially as the simulation progresses. If the simulation lacks sufficient resolution to represent Landau damping, it may result in deviations from expected physical behaviour, contributing to the observed instabilities and errors in later time steps.



(a) (b) (c)

Figure 5: Time history plots of (a) Electric field energy, (b) Kinetic energy , (c) Combined plot (Here x-axis represents time step (s) and y-axis represents energy of system (erg))

Figure 5 shows the time evolution of the kinetic, electric potential, and total energies. At t = 0, the energy is stored entirely in the form of electric potential, since all particles possess velocities of zero. After the electrons are displaced from equilibrium, kinetic energy grows and exchanges with electric potential at a period dependent on ω_p. Plasma energies show a periodic exchange between the kinetic and potential energies, tracking the total energy demonstrates the non-conserving property of this simulation. The total energy as shown in the plots is fluctuating curve and hence doesn't stay constant throughout the simulation.

CONCLUSION

In this report, we summarise our understanding of the quantum hydrodynamic description of plasma, which uses hydrodynamic equations, fluid equations and quantum correction (uncertainty principle and wave-particle duality) to describe the behaviour of a plasma at a macroscopic level. In this framework, the plasma is treated as a collection of charged particles, such as ions and electrons, that interact with each other through the electromagnetic force. To represent the probability density of particles in both position and momentum space and capture the wave-particle duality inherent in quantum systems, we use the Wigner distribution function. Our report delves deep into the derivation of Wigner-Poisson system of equations. In electrostatic quantum plasmas, the Wigner–Poisson system plays the same role as the Vlasov–Poisson system in classical plasmas.

We then move on to simulate the Vlasov–Poisson system for classical plasmas, as a foundational step to simulate Wigner-Poisson system for quantum plasmas in the future. The code is a 1-D electrostatic Particle-in-Cell (PIC) simulation. It models the motion of electrons in a plasma along the x-axis, with ions being stationary. The simulation evolves through time steps, with each step involving particle motion, charge density deposition on mesh points, solving the Poisson equation to compute the electric potential, and calculating the electric field.
We save data at each time step, such as potential distribution, charge density distribution, electric field distribution, and particle distributions in velocity and position. Plotting this data helps us to visualize and validate our understanding of the classical plasma.

In summary, this comprehensive exploration of the quantum hydrodynamic model and its application through the Wigner-Poisson system, alongside the simulation of classical plasmas using the Vlasov-Poisson system, has provided invaluable insights into the interplay of quantum and classical effects in plasma behaviour. This experience has enhanced our understanding of theoretical concepts as well as computational simulations.

FUTURE STEPS

We aim to understand the quantum hydrodynamic description of plasma that describes the behaviour of charged particles in a plasma, incorporating quantum effects. While our current code forms the basis for simulating classical plasma using 1-D electrostatic Particle-in-Cell (PIC) simulation, we aim to incorporate quantum mechanical corrections effectively in our simulation. Our goal is to work towards achieving this objective and further optimizing the code.

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