Absorbing Boundary Conditions for the Finite-Difference Time Evolution of the Wigner Function using the Vlasov Equation

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ABSTRACT

Absorbing boundary conditions for the finite-difference time evolution of the Wigner function using a constant flux condition through the 2D region of calculation in phase space are presented. Numerical results on the time evolution of a Gaussian wave packet in phase space will be presented and discussed. The conditions minimize undesirable reflections at the artificial boundaries of the computation.

BACKGROUND

Phase-space density holes are vortex-like nonlinear structures that have been observed in the magnetosphere. To study the time evolution of these structures we evolve the Wigner function in time by solving the Vlasov equation using finite-differences. Wigner function is a quasi-probability density function in phase space.

EQUATIONS

In one-dimensional case, the Wigner Function is:

$$W(x,v,t)=\int_{-\infty}^{\infty}(e^{\frac{-imv\Delta}{\hbar}})\psi^*(x-\frac{\Delta}{2},t)\psi(x+\frac{\Delta}{2},t)d\Delta \qquad (1)$$

It satisfies the **Vlasov equation**

$$\frac{\partial W}{\partial t}-v\frac{\partial W}{\partial x}+\frac{eE}{m}\frac{\partial W}{\partial v}=0 \qquad (2)$$

CALCULATIONS

- Initial Conditions:

  We start from a Gauss function which is symmetric both with position and momentum

$$W(x,v,0)=e^{\frac{(x-x')^2}{2\sigma x^2}}e^{\frac{(v-v')^2}{2\sigma v^2}} \qquad (3)$$

- Calculations:

  By using finite difference approximation, the Wigner function can be evolved step by step in time.

$$\frac{\partial W(x,v,t)}{\partial t}=\frac{W(x,v,t+\Delta t)-W(x,v,t)}{\Delta t} \qquad (4)$$

$$\frac{\partial W(x,v,t)}{\partial x}=\frac{W(x+\Delta x,v,t)-W(x-\Delta x,v,t)}{2\Delta x} \qquad (5)$$

$$\frac{\partial W(x,v,t)}{\partial v}=\frac{W(x,v+\Delta x,t)-W(x,v-\Delta v,t)}{2\Delta v} \qquad (6)$$

ABSORBING BOUNDARY CONDITIONS USING PLANE WAVE DISPERSION[1]

Given the one-dimensional Schrödinger equation :

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t)=[-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial^2 x}+U(x)]\Psi(x,t) \qquad (7)$$

we first consider plane wave solutions

$$\Psi(x,t)=e^{-i(wt-kx)} \qquad (8)$$

The dispersion relation of the solutions is

$$\hbar k=\pm[2m^*(\hbar w-U)]^{\frac{1}{2}} \qquad (9)$$

where plus and minus signs means the right-going and left-going waves, after a linear approximation:

$$\hbar k=\pm\sqrt{2m^*/a}(\hbar w-U) \qquad (10)$$

These two relations (9) and (10) intersect at $\hbar w-U=a$

by using $\frac{\partial}{\partial t}\Leftrightarrow -i\omega,\frac{\partial}{\partial x}\Leftrightarrow ik$, we can rewrite the linear relation as

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t)=(-i\hbar\sqrt{\frac{a}{2m^*}}\frac{\partial}{\partial x}+U)\Psi(x,t) \qquad (11)$$

substituting this to the Wigner function , we can get

$$\frac{\partial}{\partial t}W(x,v,t)=-\sqrt{\frac{a}{2m^*}}\frac{\partial}{\partial x}W(x,v,t) \qquad (12)$$

or we can write it as

$$\frac{\partial}{\partial t}W(x,v,t)=-V\frac{\partial}{\partial x}W(x,v,t) \qquad (13)$$

these are the absorbing boundary conditions for the x boundaries, similarly we can get absorbing boundary conditions for v boundaries.

$$\frac{\partial}{\partial t}W(x,v,t)=-A\frac{\partial}{\partial v}W(x,v,t) \qquad (14)$$

ABSORBING BOUNDARY CONDITIONS USING CONSTANT FLUX

- We assume the flux f(t) that goes through the boundary $(N+1)\Delta x$ is the flux that went through $N\Delta x$ with a time shift T:

$$f(t)\big|_{x=(N+1)\Delta x}=f(t-T)\big|_{x=N\Delta x} \qquad (15)$$

  Where

$$T=\Delta x/V \qquad (16)$$

  In the case $\Delta x\rightarrow 0$, we can assume:

$$W((N+1)\Delta x,v,t)=W(N\Delta x,v,t-T) \qquad (17)$$

  we can rewrite it in another form:

$$\frac{W((N+1)\Delta x,v,t)-W((N+1)\Delta x,v,t-T)}{T}=\frac{\Delta x}{T}\frac{W(N\Delta x,v,t-T)-W((N+1)\Delta x,v,t-T)}{\Delta x} \qquad (18)$$

  which means

$$\frac{\partial W(x,v,t)}{\partial t}=-V\frac{\partial W(x,v,t)}{\partial x} \qquad (19)$$

  where V is the group velocity

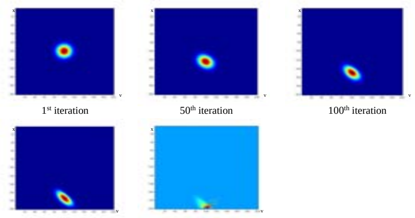
- Similarly we have:

$$\frac{\partial W(x,v,t)}{\partial t}=-A\frac{\partial W(x,v,t)}{\partial v} \qquad (20)$$

  at v boundary, where A is the group acceleration.

- Compare 13 and 14 to 19 and 20, we get the same absorbing boundary conditions using a dispersion relation for plane waves as using a constant flux assumption.

SIMULATIONS WITHOUT ABSORBING BOUNDARY CONDITIONS[2]

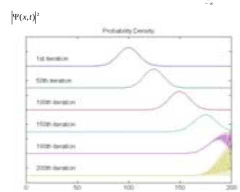


1st iteration — 50th iteration — 100th iteration — 150th iteration — 200th iteration

The figures above shows how Wigner function changes in time without applying absorbing boundary conditions, it reflects at the boundary and quickly diffuses to the whole space.

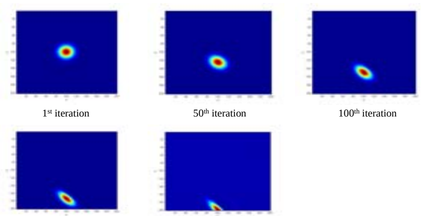
From Wigner function we can get x probability distributions:

$$|\Psi(x,t)|^2=\int_{-\infty}^{\infty}W(x,v,t)dv \qquad (21)$$



The graph left shows the temporal evolution of the Gaussian wave packet without absorbing boundary conditions, the wave package reflects and diffuses.

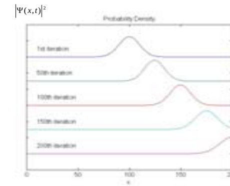
SIMULATIONS WITH ABSORBING BOUNDARY CONDITIONS



1st iteration — 50th iteration — 100th iteration — 150th iteration — 200th iteration

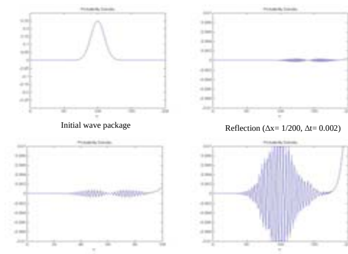
The figures above shows how the Wigner function changes in time by using the absorbing boundary conditions. Obviously, the wave package is absorbed at the boundary.

From the probability density graph we can see it more clearly



After using absorbing boundary conditions, the reflection is very small (less than 1%).

Small reflection still exists due to the use of first order finite difference approximation.



Initial wave package — Reflection (Δx= 1/200, Δt= 0.002) — Reflection (Δx= 1/100, Δt= 0.002) — Reflection (Δx= 1/200, Δt= 0.004)

By using smaller Δx and Δt, we can reduce the reflection significantly.

CONCLUSIONS

- It turns out we get the same absorbing boundary conditions using a dispersion relation for plane waves or using a constant flux assumption.
- The remaining small reflection is due to the first-order finite difference approximation, as we can reduce that by using higher resolution on x, v or t.

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