Trapping oscillations, discrete particle effects and kinetic theory of collisionless plasma

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Effects induced by the finite number $N$ of particles on the evolution of a monochromatic electrostatic perturbation in a collisionless plasma are investigated. For growth as well as damping of a single wave, discrete particle numerical simulations show a $N$-dependent long time behavior which differs from the numerical errors incurred by vlasovian approaches and follows from the pulsating separatrix crossing dynamics of individual particles.

Keywords: plasma, kinetic theory, wave-particle interaction, self-consistent field, particle motions and dynamics

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I. INTRODUCTION

It is tempting to expect that kinetic equations and their numerical simulation provide a fair description of the time evolution of systems with long-range or ‘global’ interactions. A typical, fundamental example is offered by wave-particle interactions, which play a central role in plasmas. In this Letter we test this opinion explicitly.

Collisionless plasma dynamics is dominated by collective processes. Langmuir waves and their familiar Landau damping and growth\textsuperscript{6} are a good example of these processes, with many applications, e.g. plasma heating in fusion devices and laser-plasma interactions. For simplicity we focus on the one-dimensional electrostatic case, traditionally described by the (kinetic) coupled set of Vlasov-Poisson equations\textsuperscript{5, 6}. The current debate on the long-time evolution of this system shows that further insight in this fundamental process is still needed\textsuperscript{5}. The driving process (induced by the binary Coulomb interaction between particles) is the interaction of the electrostatic waves in the plasma with the particles at nearly resonant velocities, which one analyses canonically by partitioning the plasma in bulk and tail particles.

Langmuir modes are the collective oscillations of bulk particles, with slowly varying complex amplitudes in an envelope representation; their interaction with tail particles is described by a self-consistent set of hamiltonian equations\textsuperscript{7}. These equations already provided an efficient basis\textsuperscript{4} for investigating the cold beam plasma instability and exploring the nonlinear regime of the bump-on-tail instability\textsuperscript{6}. Analytically, they were used to give an intuitive and rigorous derivation of spontaneous emission and Landau damping of Langmuir waves\textsuperscript{3}. Besides, as it eliminates the rapid plasma oscillation scale $\omega_p^{-1}$, this self-consistent model offers a genuine tool to investigate long-time dynamics.

As we follow the motion of each particle, we can also address the influence of the finite number of particles in the long run. This question is discarded in the kinetic Vlasov-Poisson description, for which the finite-$N$ correction is the Balescu-Lenard equation\textsuperscript{9} formally derived from the accumulation of weak binary collisions, with small change of particle momenta. It implies a diffusion of momenta, driving the plasma towards equilibrium. However, when wave-particle coupling is dominant, the Balescu-Lenard equation is not a straightforward approach to finite-$N$ effects on the wave evolution.

Here we investigate direct finite-$N$ effects on the self-consistent wave-particle dynamics. It is proved\textsuperscript{10} that the kinetic limit $N \to \infty$ commutes with evolution over arbitrary times. As one might argue that finite $N$ be analogous to numerical discretisation in solving kinetic equations, we also integrate the kinetic system with a "noise-free" semi-lagrangian solver\textsuperscript{4}. In this Letter we compare finite grid effects of the kinetic solver and granular aspects of the $N$-particles system, whose evolution is computed with a symplectic scheme\textsuperscript{4}.

We discuss the case of one wave interacting with the particles. Though a broad spectrum of unstable waves is generally excited when tail particles form a warm beam, the single-wave situation can be realized experimentally\textsuperscript{11} and allows to leave aside the difficult problem of mode coupling mediated by resonant particles\textsuperscript{12}. 


II. SELF-CONSISTENT WAVE-PARTICLE MODEL AND KINETIC MODEL

Consider a one-dimensional electrostatic potential perturbation $\tilde{\Phi}(z, \tau) = [\phi_k(\tau) \exp(i(kz - \omega_k \tau) + c.c.)$ (where $c.c.$ denotes complex conjugate), with complex envelope $\phi_k$, in a plasma of length $L$ with periodic boundary conditions (and neutralizing background). Wavenumber $k$ and frequency $\omega_k$ satisfy a dispersion relation $\epsilon(k, \omega_k) = 0$. The density of $N$ (quasi-)resonant electrons is $\sigma(z, \tau) = (nL/N) \sum_{l=1}^{N} \delta(z - z_l(\tau))$, where $n$ is the electron number density and $z_l$ is the position at time $\tau$ of electron labeled $l$ (with charge $e$ and mass $m$). Non-resonant electrons contribute only through the dielectric function $\epsilon$, so that $\phi_k$ and the $z_l$'s obey coupled equations \[ \frac{d\phi_k}{d\tau} = \frac{i ne}{\epsilon_0 k^2 N(\partial\epsilon/\partial\omega_k)} \sum_{l=1}^{N} \exp[-ikz_l + i\omega_k \tau] (1) \]
\[ \frac{d^2 z_l}{d\tau^2} = (iek/m) \phi_k \exp[i(kz_l - i\omega_k \tau)] + c.c. (2) \]
where $\epsilon_0$ is the vacuum dielectric constant. With $\alpha^3 = ne^2/(\epsilon_0 \epsilon_k(\partial\epsilon/\partial\omega_k))$, $\tau = \tau \epsilon$, $\epsilon = dV/dt$, $x = kz_l - \omega_k \tau$ and $V = (ek^2 \phi_k)/(\alpha^2 m)$, this system defines the self-consistent dynamics (with $N + 1$ degrees of freedom) \[ \dot{V} = iN^{-1} \sum_{l=1}^{N} \exp(-ix_l) \]  
\[ \dot{x}_l = iV \exp(ix_l) - iV^* \exp(-ix_l) \]  
for the coupled evolution of electrons and wave in dimensionless form. This system derives from hamiltonian $H(x, p, \zeta, \zeta^*) = \sum_{l=1}^{N} (p_l^2/2 - N^{-1/2} \zeta e^{ix_l} - N^{-1/2} \zeta^* e^{-ix_l})$, where a star means a complex conjugate and $\zeta = N^{1/2}V$. An efficient symplectic integration scheme is used to study this hamiltonian numerically \[ \tilde{\Phi}(z, \tau) = [\phi_k(\tau) \exp(i(kz - \omega_k \tau) + c.c.) \]

The system (3)-(4) is invariant under two continuous groups of symmetries. Invariance under time translations implies the conservation of the energy $H = H$. The phase $\theta$ of $\zeta = |\zeta| e^{-i\theta}$ plays the role of a position for the wave, and system (3)-(4) is also invariant under translations $\theta' = \theta + a$, $x'_l = x_l + a$. This translation invariance leads to the conservation of momentum $P = \sum_l p_l + |\zeta|^2$, where the contribution from the wave is analogous to the Poynting vector of electromagnetic waves (which is quadratic in the electromagnetic fields) \[ \text{Conservation of these invariants constrains the evolution of our system, and we checked that the numerical integration preserves them.} \]

In the kinetic limit $N \rightarrow \infty$, electrons are distributed with a density $f(x, p, t)$, and system (3)-(4) yields the Vlasov-wave system \[ \dot{V} = i \int e^{-ix} f(x, p, t) dxdp \]  
\[ \partial_t f + p \partial_x f + (iVe^{ix} - iV^*e^{-ix}) \partial_p f = 0 \]  
For initial data approaching a smooth function $f$ as $N \rightarrow \infty$, the solutions of (3)-(4) converge to those of the Vlasov-wave system over any finite time interval \[ \int. \]  
This kinetic model is integrated numerically by a semi-lagrangian solver, covering $(x, p)$ space with a rectangular mesh: the function $f$ (interpolated by cubic splines) is transported along the characteristic lines of the kinetic equation, i.e. along trajectories of the original particles \[ \text{Let us first study linear instabilities. One solution of (3)-(4) corresponds to vanishing field $V_0 = 0$, with particles evenly distributed on a finite set of beams with given velocities. Small perturbations of this solution have $\delta V = \delta V_0 e^{\gamma t}$, with rate $\gamma$ solving} \[ \gamma = \gamma_r + i\gamma_i = iN^{-1} \sum_{l=1}^{N} (\gamma + i\omega_l) \]  
\[ = iN^{-1} \sum_{l=1}^{N} \exp(-i\omega_l \tau) \]  

For a monokinetic beam with velocity $U$, (4) reads $\gamma = (\gamma + iU)^2 = i$; the most unstable solution occurs for $U = 0$ (with $\gamma = (\sqrt{3} + i)/2$). For a warm beam with smooth initial distribution $f(0)$ (normalized to $\int f dp = 1$), the continuous limit of (4) yields $\gamma = i f (\gamma + i\omega)^2 f dp$. For a sufficiently broad distribution ($|f'(0)| \ll 1$), we obtain $|\gamma_l| \approx \pi f''(0)$, where $f' = df/dp$, and $\gamma_l \approx \pi f''(0)$ for $|f''(0)| \ll 1$ and $\tau > 0$. Except for the trivial solution $\gamma = 0$, other solutions can only exist for a positive slope $f''(0)$. Then the perturbation is unstable as the evolution of $\delta V$ is controlled by the eigenvalue $\gamma$ with positive real part, i.e. with growth rate $\gamma_r \approx \gamma_\ell = \pi f''(0) > 0$. Negative slope leads to the linear Landau damping paradox: the observed decay rate $\gamma_l = \pi f''(0) < 0$ is not associated to genuine eigenvalues, but to phase mixing of eigenmodes \[ [11-13, as a direct consequence of the hamiltonian nature of the dynamics. \]

Now, this linear analysis generally fails to give the large time behavior. This is obvious for the unstable case as non-linear effects are no longer negligible when the wave intensity grows so that the trapping frequency $\omega_\ell(t) = \sqrt{2V(t)}$ becomes of the order of the linear rate $\gamma_r$. \[ \text{We used the monokinetic case as a testbed} \[ [18-19. \]

Finite- $N$ simulations show that the unstable solution grows as predicted and saturates to a limit-cycle-like behavior where the trapping frequency $\omega_\ell(t)$ oscillates between 1.2$\gamma_r$ and 2$\gamma_r$. In this regime, some of the initially monokinetic particles have been scattered rather uniformly over the chaotic domain, in and around the pulsating resonance, while others form a trapped bunch inside this resonance (away from the separatrix) \[ [9]. \]

This dynamics is quite well described by effective hamiltonians with few degrees of freedom \[ [18-20. \]

In this Letter, we discuss the large time behavior of the warm beam case, with $f'(0) \neq 0$ at the wave nominal velocity $p_0 = 0$. Fig. \[ \text{displays three distribution functions (in dimensionless form) with similar velocity width:} \]

\text{(i) a function (CD) giving the same decay rate for all}
phase velocities, \( (ii) \) a function (CG) giving a constant growth rate for all phase velocities \( \frac{d}{dt} \), \( (iii) \) a truncated Lorentzian (TL) with positive slope \( f'(0) > 0 \).

III. DAMPING CASE

For the damping case, the linear description introduces time secularities which ultimately may break linear theory down : the ultimate evolution is intrinsically nonlinear, not only if the initial field amplitude is large, as in O’Neill’s seminal picture \( \ref{fig:fig2} \), but also if one considers the evolution over time scales of the order of the trapping time (which is large for small initial wave amplitude). The question of the plasma wave long-time fate is thus far from trivial \( \ref{fig:fig2} \). Though some simulations \( \ref{fig:fig2} \) infer that nonlinear waves eventually approach a Bernstein-Greene-Kruskal steady state \( \ref{fig:fig2} \) instead of Landau vanishing field, the answer should rather strongly depend on initial conditions. Our \( N \)-particle, \( 1 \)-wave system is the simplest model to test these ideas.

A thermodynamical analysis \( \ref{fig:fig2} \) predicts that, for a warm beam and small enough initial wave amplitude, \( \omega_b \sim N^{-1/2} \) at equilibrium in the limit \( N \to \infty \). Fig. \( \ref{fig:fig2} \) shows the evolution of a small amplitude wave launched in the beam. The \( N \)-particle system (line N) and the kinetic system (line V) initially damp the wave exponentially as predicted by perturbation theory \( \ref{fig:fig2} \), for a time of the order of \( |\gamma_L|^{-1} \).

After that phase-mixing time, trapping induces nonlinear evolution and both systems evolve differently. For the \( N \)-particle system, the wave grows to a thermal level that scales as \( N^{-1/2} \), corresponding to a balance between damping and spontaneous emission \( \ref{fig:fig2} \). For the kinetic system, initial Landau damping is followed by slowly damped trapping oscillations around a mean value which also decays to zero, at a rate decreasing for refined mesh size. Fig. \( \ref{fig:fig2} \) reveals that finite-\( N \) and kinetic behaviors can considerably diverge as spontaneous emission is taken into account. The time \( \tau_N \) after which the finite-\( N \) effects force this divergence is found to diverge as \( N \to \infty \).

IV. UNSTABLE CASE

Now consider an unstable warm beam \( f'(0) > 0 \). Line N1 (resp. N2) of Fig. \( \ref{fig:fig2} \) displays \( \ln(\omega_b(t)/\gamma_r) \) versus time for \( \ref{fig:fig2} \). With a CG distribution with \( N = 128000 \) (resp. 512000) and \( \gamma_r = 0.08 \). Line V1 (resp. V2) shows \( \ln(\omega_b(t)/\gamma_r) \) versus \( \gamma_r t \) for the kinetic system and the same initial distribution with a \( 32 \times 128 \) (resp. \( 256 \times 1024 \)) grid in \((x,p)\) space. All four lines exhibit the same initial exponential growth of linear theory with less than 1\% error on the growth rate. Saturation occurs for \( \omega_b/\gamma_r \approx 3.1 \). Lines N1 and V1 do not superpose beyond the first trapping oscillation after saturation. Note that, in our system, oscillating saturation does not excite sideband Langmuir waves as our hamiltonian incorporates only a single wave, not a spectrum.

After the first trapping oscillation, kinetic simulations exhibit a second growth at a rate controlled by mesh size. Line V2 suggests that a kinetic approach would predict a level close to the trapping saturation level on a time scale awarded by reasonable integration time. This level is fairly higher than the trapping level \( \ref{fig:fig2} \) : such pathological relaxation properties in the \( N \to \infty \) limit seem common to mean-field long-range models \( \ref{fig:fig2} \). Both kinetic simulations also exhibit a strong damping of trapping oscillations, which disappear after a few oscillations, whereas finite-\( N \) simulations show persistent trapping oscillations.

One could expect that finite-\( N \) effects would mainly damp these oscillations, so that the wave amplitude reaches a plateau. Actually, we observe persistent oscillations for all \( N \), and the wave amplitude slowly grows further, whereas the velocity distribution function flattens over wider intervals of velocity.

This spreading of particles is due to separatrix crossings, i.e. successive trapping and detrapping by the wave \( \ref{fig:fig2} \). Indeed, when the wave amplitude grows (during its pulsation), it captures particles with nearby velocity, i.e. with a relative velocity \( \Delta v_{\text{in}} \approx \pm \sqrt{8|V|} \); the trapped particles start bouncing in the wave potential well. When the wave amplitude decreases, particles are released, but if they experienced only half a bouncing period, they are released with a relative velocity (with respect to the wave) opposite to their initial one, i.e. \( \Delta v_{\text{out}} \approx -\Delta v_{\text{in}} \). Now notice that a particle which has just been trapped would oscillate at a longer period than the nominal bouncing period (namely the one deep in the potential). Moreover, if the recently trapped particle had just adiabatic motion in the well, it would have to recross the separatrix when the resonance would enclose the same area as at its trapping \( \ref{fig:fig2} \). Thus one expects the particle to be unable to complete a full bounce, and the fraction of particles for which \( \Delta v_{\text{out}} \approx -\Delta v_{\text{in}} \) is significant.

During this particle spreading process in \((x,p)\) space, the wave pulsation is maintained by the bunch of particles which were initially trapped, and are deep enough in the potential well to remain trapped over a whole bouncing period. These particles form a macroparticle, as is best seen in the case of a cold beam \( \ref{fig:fig2} \). Note that, over long times, the macroparticle must slowly spread in the wave resonance, following two processes. One acts if the trapped particle motion is regular : the trapped motions are isochronous, i.e. have different periods (only the harmonic oscillator has isochronous oscillations). The other one works if the motion is chaotic : nearby trajectories diverge due to chaos. Both processes contribute to the smoothing of the particle distribution for long times,
but over much longer times than those over which we follow the system evolution and observe the wave modulation.

This second growth after the first trapping saturation depends on the shape of the initial distribution function. In Fig. 3(b), line N2 is the same as in Fig. 3(a), computed over a longer duration, and line N3 corresponds to $N = 64000$ with the TL distribution of Fig. 1. Although N3 corresponds to 8 times fewer particles than N2, the final level reached at the end of the simulation is lower. In the second growth, particles are transported further in velocity, so that the plateau in $\gamma_4$ is bound to depart from the analytic predictions of the kinetic theory. A basic property of the collisionless kinetic equation is that it transports the distribution function $f(x, p)$ along the particle trajectories (or characteristic lines in $(x, p)$ space). As long as the kinetic calculation of $f$ is accurate, one expects the kinetic scheme to follow closely the $N$-particle dynamics too. However, the kinetic scheme is bound to depart from the analytic predictions of the kinetic equation, because the (chaotic or anisochronous) separation of particle trajectories implies that constant-$f$ contours eventually evolve into complex, interleaved shapes. This filamentation is smoothed by numerical partial differential equation integrators, while $N$-body dynamics follows the particles more realistically, sustaining the trapping oscillations. Hence both types of dynamics will depart from each other when filamentation reaches scales below the semi-lagrangian kinetic code grid mesh.

The onset of filamentation is easily evidenced in kinetic simulations. Indeed, whereas the kinetic equation analytically preserves the 2-entropy $\int (1-f) f dxdp$, numerical schemes increase entropy significantly when constant-$f$ contours form filaments in $(x, p)$-space [25]. As this is also the time at which trapping oscillations are found to damp in our simulations, it appears that vlasovian simulations must be considered with caution from that time on – and it turns out that it is also the time from which the second growth starts.

In summary, discussing the basic propagation of a single electrostatic wave in a warm plasma, we presented finite-$N$ effects which do not merely result from numerical errors and elude a kinetic simulation approach. Their understanding depends crucially on the dynamics in phase space. The sensitive dependence of microscopic evolution to the fine structure of the initial particle distribution in phase space [15] implies that the interplay between limits $t \to \infty$ and $N \to \infty$ requires some caution. Somewhat paradoxically, refining the grid for the Vlasov simulations does not solve this problem.

The driving process in the system evolution is separatrix crossing, which requires a geometric approach to the system dynamics. Further work in this direction [24] will also shed new light on the foundations of common approximations, such as replacing original dynamics [1]-[2] by coupled stochastic equations, in which particles undergo noisy transport.

V. CONCLUSION

These observations clearly indicate that the kinetic models are an idealization and do not contain all the intricate behavior of a discrete particles system. Now, we must also admit that the kinetic simulation schemes do not exactly reproduce the analytic implications of the kinetic equation. It is then legitimate to ask whether the numerical implementation of the kinetic equations reproduce the difference between the finite-$N$ dynamics and the kinetic theory.

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[16] One can rewrite the hamiltonian dynamics (\ref{eq:hamiltonian}) using intensity-phase variables (I, θ) for the wave, with ζ = √T_e, where the total momentum P = ∑_l p_l + I is a linear function of the wave intensity and of the particle momenta, while the energy reads H = ∑_l p_l^2/2 − 2N^{1/2} ∑_l √Tcos(x_l − θ).
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FIG. 1. Initial velocity distributions.

FIG. 2. Time evolution of $\ln(\omega_b(t)/|\gamma_L|)$ for a CD velocity distribution and initial wave amplitude below thermal level: (N) $N$-particles system with $N = 32000$, (V) kinetic scheme with $32 \times 512 (x,p)$ grid. Inset: short-time evolution.

FIG. 3. Time evolution of $\ln(\omega_b(t)/|\gamma_L|)$. (a) CG initial distribution: kinetic scheme with (V1) $32 \times 128$, (V2) $256 \times 1024 (x,p)$ grid; $N$-particles system with (N1) $N = 128000$, (N2) $N = 512000$; (b) Comparison of CG (N2) with TL initial distribution for (N3) $N = 64000$, (N4) $N = 2048000$. 