ARTIFICIAL COOLING DUE TO QUIET INJECTION IN BOUNDED PLASMA PARTICLE SIMULATIONS

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Artificial Cooling Due to Quiet Injection in Bounded Plasma Particle Simulations

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ABSTRACT

An explanation is proposed for an artificial cooling effect seen in electrostatic particle-in-cell plasma simulations. Further simulations are done which test and support the explanation.

Introduction

The system in which the effect was observed is meant to simulate a Q-machine. Electrons and ions are injected from a hot plate (the left side of the system, which is chosen as $x = 0$), and particles which strike either side of the system are absorbed. In this case, the end plates are electrically isolated (an open external circuit). The density of injected ions is chosen to be much larger than the density of injected electrons, so that a potential maximum is created near the hot plate, thus creating a trapping well for electrons. The simulation parameters are shown in Table 1.

Recent simulations of Q-machines [1] have shown a surprising effect: the cooling and increase in density of electrons which are trapped in the sheath near the emitting (hot) plate. Electrons which are trapped in this potential well are found to cool over long time scales to less than a third of the temperature at which they were emitted.

Initially the simulation region is empty of particles. At $t = 0$, ions and electrons begin entering the system, and within a few ion transit times establish a near-equilibrium which agrees with what Vlasov theory suggests the equilibrium state should be. The potential profile for this near-equilibrium (from the simulation) is shown in Fig. 1. The electron and ion phase spaces for this same time are shown in Fig. 2. Next, over a long time scale (tens of ion transit times), the number of electrons in the trapping well steadily increases, the temperature of the trapped electrons decreases, and the spatial width of the trapping well increases (see Figs. 3 and 4). This process has not saturated in any of the runs which will be shown here, but saturation does occur later, at a trapped electron temperature which is much smaller than the injection temperature and a trapping well width which spans most of the simulation region.

No simple model predicts this cooling. The Vlasov model (fully time-dependent) predicts that the phase space density $f(x, v, t)$ in the trapped well may be no higher than the largest value of $f(x, v, t)$ at the point of injection ($x = 0$ for our simulations). For the Q-machine, this is also the value of f on the separatrix which defines the trapping region of phase space. Alternatively, one might expect that the distribution in the trapping well would fill in through some scattering process (due to the discrete particle model) to a Maxwellian shape. In fact, the distribution fills in far past this point.

Some possible explanations for this effect are: numerical inaccuracy, enhanced fluctuations due to an instability, and collisions. None of these explanations seem capable of accounting for the observed effect. The consideration of fluctuations, however, led to what seems to be the correct explanation.

An enhanced level of fluctuations would be expected to increase particle diffusion in velocity space, but in such a way as to *heat* trapped electrons. In thermodynamic equilibrium, this heating effect is balanced by a drag on the particles, giving rise to the Maxwellian distribution. The level of fluctuations in thermodynamic equilibrium is not zero, so an abnormally low level of fluctuations can be expected to cool electrons. Such a depressed level of fluctuations is in fact specifically introduced in order to increase the signal-to-noise level of most simulations. This artificially low level of fluctuations appears to be the cause of the artificial cooling observed in the Q-machine simulations. In almost thirty years of periodic simulations, artificial cooling like this has not been reported. A reason for this effect going unnoticed will also be given.

Ruling Out Some Possible Causes

Three candidates for the cause of the cooling effect can be eliminated. These are numerical inaccuracy, fluctuations, and collisions.

Numerical inaccuracy was tested by changing the simulation parameters Δx and Δt, which represent the spatial grid spacing (which limits the spatial resolution), and the time step (which limits the temporal resolution). When one or both of these parameters was reduced (improving the resolution), the cooling effect remained with the same magnitude.

An enhanced level of fluctuations can be eliminated because they are a heating influence. Increasing the fluctuation level enhances diffusion in velocity in both directions, and so should create just as much flux out of the trapping well as into it. In fact, when the density of particles in phase space within the well is higher that outside it, one would expect more particles to leave the well than enter it.

Collisions are harder to eliminate. In three dimensions, a Fokker-Planck analysis (see Appendix A) shows that ions moving above a certain x-velocity (approximately $\sqrt{3}$ times the thermal speed of ions of the same temperature as the electrons) heat the electrons, while ions moving slower than this velocity cool them. (The Fokker-Planck model is of questionable validity here due to the short scale length of the trapping well, but it should be indicative.) Thus, while the ions between the hot plate and the center of the well should do some cooling, the ions on the other side of the center of the well should do just about as much heating. The electrons which are not trapped should also do some cooling throughout the well, but the effective temperature of the passing electrons is very close to the emission temperature, so the strong cooling of the trapped electrons cannot be explained by electron-electron collisions. The overall balance of these effects is difficult to predict, but is likely to be small, and the equilibrium state would clearly be much closer to the collisionless state than is observed in simulation.

In one dimension, however, the collision process is very different [2]. For instance, particles of the same species do not scatter when they collide, they either pass through each other, or exchange velocities. Thus, the passing electrons cannot be cooling the trapped electrons through collisions in this simulation. Particles of differing species do not collide in the usual sense of introducing a random change in velocity, either. Their collisions exchange energy in a very simple and much more predictable way — either by reflecting velocities in the center of mass frame, or passing through each other with unaltered velocities. This has the result of greatly diminishing the effects of collisions relative to the three dimensional case. Given these facts in combination it seems implausible that collisions could be responsible for the effect. This is admittedly a weak argument; the strongest evidence for collisions being unimportant is the simulation evidence presented here for the depressed level of fluctuations being the only process of importance.

Electric field fluctuations

Thermal energy may reside in one of two reservoirs in a plasma: disorganized particle motion and fluctuations of the electrostatic wave field. The word field is used here not in the sense of the electric field, but in the sense of the set of waves which are supported by a medium (as in Quantum Field Theory). It is necessary to consider the electrostatic wave field as being something separate from the electric field, since the *organized* motion of particles plays a role in the electrostatic waves in the plasma. At short wavelengths the distinction between wave fluctuations and particle fluctuations becomes blurry, but at long wavelengths the distinction is clear.

There is coupling between these reservoirs, and energy flows between the two. In thermodynamic equilibrium, the flow of energy from wave fluctuations to particles is exactly balanced by the flow of energy from particles to wave fluctuations. These flows are called respectively, Landau damping and Cerenkov emission, and the flow rates are proportional to the energy present in the reservoir which is losing energy (see Fig. 5). The balance between these flows in thermodynamic equilibrium gives rise to the Fluctuation-Dissipation Theorem, which relates the temperature to the level of electric field fluctuations in the plasma.

Quiet injection

In order to reduce the background noise level in particle simulations, particles are usually put into phase space (either loaded initially or injected over time) nearly uniformly. This has the effect of drastically reducing the amplitude of fluctuations in the electric field [3]. For computer runs of short duration, this is entirely beneficial. Even for long runs, if the boundary conditions are periodic, the worst that can happen is that the fluctuation level of the electric field ($\langle E^2 \rangle$) rises up to the natural level, and since the total heat content of the fluctuations is not large (*i.e.*, $\epsilon_0 \langle E^2 \rangle / nkT$ is small), and the system is closed, the particles do not cool appreciably (see fig. 6). This cooling of particles in periodic simulations has not been explicitly reported, but should be observable. (Simulation experts may be reminded of Gitomer and Adam [4], but the effect they noted was a *rapid* rise in the level of fluctuations due to a multibeam instability — a very different phenomenon from that described here.)

A bounded simulation is an open system, and the situation is quite different. Most particles are in the system only for one or two transit times. Only the particles which are trapped stay for long times. The wave fluctuations, however, are not trapped at all. Since they are collective modes, they move at their group velocities (which are strongly affected by the bulk motion of the plasma). Thus the wave fluctuations can and do leave the system, only to be replaced with the artificially reduced fluctuations in the newly injected particles. In other words, the trapped electrons can cool via Cerenkov emission of waves which then leave the system. The energy flow is now much more complicated than in the periodic case (see Fig. 7). This mechanism is completely physical; if the noise level of injected electrons could be reduced in the laboratory, this effect would occur.

Simulation evidence

Simulation offers many methods of testing the hypothesis that the quiet injection of particles is responsible for the cooling of the trapped electrons. Several of these were tried, and all supported the hypothesis.

Figure 8 shows the results of a quiet start run. Plotted are the electron velocity distribution function averaged over a narrow region near the potential maximum at the end of the run, and the time history of the total number of electrons in the system. Note the elevated electron density and the decreased temperature of the trapped electrons in the distribution function plot, and the steady increase in the total number of electrons.

The most obvious test of the hypothesis is to replace the quiet injection scheme with one which has full noise, meaning that the times of injection are random with a uniform distribution in time, and that the velocities of injection are random with a half-Maxwellian distribution. The result, shown in Fig. 9, is that the system settles down to an equilibrium very quickly, and the trapped electrons never cool below the temperature of injection.

One more piece of information can be inferred from this run. A valid objection to the support this run gives the hypothesis is that *any* source of noise will cause heating, and so it is not obvious that the correct source of noise has been found or that lack of noise is indeed responsible for the effect. This run shows, however, that the noise is of roughly the right magnitude. If the noise level were too high, then the trapped electrons in the noisy case would reach a Maxwellian profile sooner than the quiet case (which initially comes to the flat distribution predicted by Vlasov theory), since fluctuations enhance diffusion in *both* directions across the separatrix. If the noise level were too low, some residual cooling effect would be seen. That neither of these effects are seen lends support for the hypothesis.

To further test the hypothesis, some runs were made with four times as many particles. Since the physical parameters were kept constant, the charge and mass of each particle was decreased by a factor of four. In the quiet start case, since the electrons are injected quasi-regularly, the fluctuations in the charge density should vary inversely with the number of particles, in this case a factor of four. This in turn should result in a factor of four reduction in the RMS fluctuation of the electric field

$\langle (E - \bar{E})^2 \rangle^{1/2}$. The diffusion rate is proportional to $\langle (E - \bar{E})^2 \rangle$, so the rate at which each particle diffuses into the trapping well should be reduced by a factor of 16. (Since there are four times as many particles, the absolute *number* of particles diffusing into the trapping well should be reduced by a factor of four.)

In the case of full thermodynamic noise, the Fluctuation-Dissipation Theorem dictates that increasing the number of particles by a factor of four must result in the mean-square electric field fluctuation $\langle (E - \bar{E})^2 \rangle$ decreasing by a factor of four. This in turn should reduce the rate of diffusion by only a factor of four. (In this case, the absolute *number* of particles diffusing into the trapping well in a given time interval will not be reduced.) As Figs. 10 and 11 show, the quiet and noisy runs obey roughly the expected behavior. The electric field was also followed to see if it obeys the behavior described in the last paragraph, and as Fig. 12 shows, it does.

Conclusion

Simulations support the hypothesis that quiet loading in bounded plasma particle simulations causes artificial cooling of trapped electrons. This effect is very small, and therefore has not been reported, in periodic simulations because of the low heat capacity of the wave fluctuation field, but it will be a limitation on the accuracy of some bounded plasma simulations.

Acknowledgements

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Appendix A: Fokker-Planck Analysis of Heating

To find the heating effect of ions on the trapped electron distribution in the three-dimensional case, the Fokker-Planck equation can be used. I will consider a spherically symmetric electron distribution (later a Maxwellian), and a cold beam of ions with which the electrons will collide. (The solution to this problem can be used as a Green's function for more complicated ion distributions.) Since the electrons all by themselves should move toward a Maxwellian, the effect of collisions between electrons should not be of interest in the context of cooling. Naturally, with a beam of ions moving through it, a spherically symmetric distribution will not stay spherically symmetric for long, but the collisions among electrons, and the trapping well in which the electrons reside will tend to return the distribution function to being nearly spherical. Also, we are not interested in a complete analysis, but only whether the beam imparts energy to the electrons or takes it from them, *i.e.*, whether dT/dt is positive or negative.

The Fokker-Planck equation can be written [5]

$$\left.\frac{\partial f}{\partial t}\right|_{coll} = -\Gamma\nabla_v \cdot \left\{ f\nabla_v h - \frac{1}{2}\nabla_v \cdot (f\nabla_v\nabla_v g)\right\} \qquad (a1)$$

where

$$\nabla^2 h = -4\pi\frac{m}{\mu}f_f = -4\pi\frac{m}{\mu}\delta^3(\vec{v}-\vec{v}_0) \qquad (a2)$$

and

$$\nabla^2 g = \frac{2\mu}{m}h \qquad (a3)$$

with Γ being a constant whose magnitude is unimportant here, f_f representing the distribution function of the field particles (in this case a cold beam of ions), and μ representing the electron-ion reduced mass, *i.e.*,

$$\mu = \frac{mM}{m+M}$$

The equations for h and g can be solved to yield

$$h = \frac{m/\mu}{|\vec{v}-\vec{v}_0|}$$

and

$$g = |\vec{v}-\vec{v}_0|$$

but these expressions will not be needed in the following calculation.

From (a1), the time derivative of the kinetic energy due to collisions with ions is

$$\frac{\partial W}{\partial t} = \frac{\partial}{\partial t}\int \frac{m}{2}v^2 f(v)\, d^3v = -\Gamma m \int \frac{v^2}{2}\nabla_v \cdot \left\{ f\nabla_v h - \frac{1}{2}\nabla_v \cdot (f\nabla_v\nabla_v g)\right\} \tag{a4}$$

Integrating the right hand side by parts (once for the first term and twice for the secon term) gives

$$\begin{aligned}\frac{\partial W}{\partial t} &= \Gamma m \int \left\{ \vec{v}\cdot f\nabla_v h + \frac{1}{2} f\nabla_v^2 g\right\} d^3v \\ &= \Gamma\mu \int \left\{ -\frac{m}{\mu}\nabla_v \cdot (\vec{v}f) + f\right\} h\, d^3v\end{aligned} \tag{a5}$$

Now writing m/μ as $1 + m/M$,

$$\frac{\partial W}{\partial t} = -\Gamma\mu \int \left\{ \frac{m}{M}\nabla_v \cdot (\vec{v}f) + (2f + \vec{v}\cdot\nabla_v f)\right\} h\, d^3v \tag{a6}$$

It is now possible to avoid a lot of algebra by defining

$$p(\vec{v}) = \int_v^\infty v' f(v')\, dv' \tag{a7}$$

and

$$q(\vec{v}) = \frac{1}{v}\int_0^v v'^2 f(v')\, dv' \tag{a8}$$

(this is where the assumption of spherical symmetry is used). We then note that

$$\nabla_v p = -\vec{v} f \tag{a9}$$

and

$$\nabla_v^2 q = 2f + \vec{v}\cdot\nabla_v f \tag{a10}$$

Equation (a6) can then be rewritten as

$$\frac{\partial W}{\partial t} = \Gamma\mu \int \nabla_v^2 \left\{ \frac{m}{M}p - q\right\} h\, d^3v \tag{a11}$$

Two integrations by parts reduces this to

$$\begin{aligned}\frac{\partial W}{\partial t} &= \Gamma\mu \int \left\{ \frac{m}{M}p - q\right\} \nabla_v^2 h\, d^3v \\ &= 4\pi\Gamma m \int \left\{ q - \frac{m}{M}p\right\} \delta^3(\vec{v} - \vec{v}_0)\, d^3v \\ &= 4\pi\Gamma m \left\{ q(v_0) - \frac{m}{M}p(v_0)\right\}\end{aligned} \tag{a12}$$

When v_0 is small, p dominates since it goes to a positive-definite constant whereas q falls off as v_0^2. When v_0 is large, q dominates, since it falls off as $1/v_0$ and p falls off like f — typically exponentially. Thus the expected behavior is reproduced; slow particles cool a distribution, and fast ones heat it. The transition point is the solution of

$$q(v_0) = \frac{m}{M} p(v_0) \tag{a13}$$

Now let us confine ourselves to a Maxwellian distribution to find an approximation to the velocity which neither heats nor cools the distribution. Assuming m/M is reasonably small, v_0 should be small, so p and q can be expanded in a Taylor series. For a Maxwellian distribution, $p = v_e^2 f$, so for small v, $p \rightarrow v_e^2 f(0)$ to leading order. For any distribution at all,

$$q \rightarrow \frac{v^2}{3v_e^2} f(0)$$

Setting these equal gives

$$v_0^2 \approx 3\frac{m}{M} v_e^2 = 3v_i^2 \tag{a14}$$

This approximation is good to one percent even for mass ratios as high as 1/40.

References

[1] T. L. Crystal, P. Gray, Wm. S. Lawson, C. K. Birdsall, and S. Kuhn, "Trapped Electron Effects on Negative-Bias D. C. States of a Collisionless Single-Emitter Plasma Device: Theory and Simulation", to be submitted to *Phys. Fluids.*

[2] O. C. Eldridge and M. Feix, *Phys. Fluids* **6**(1962), 398

[3] C. K. Birdsall and A. B. Langdon, "Plasma Physics Via Computer Simulation" (see Chapter 16), McGraw-Hill Book Company, 1985

[4] S. J. Gitomer and J. C. Adam, *Phys. Fluids* **19**(1976),719

[5] G. Schmidt, "Physics of High Temperature Plasmas" second edition (see Chapter 11), Academic Press, Inc., 1979

Table 1

Simulation Parameters

System length	2
Number of grid cells	256
Time step	1/128
Number of time steps	20,000
ϵ_0	1
q_e/m_e	-1
q_i/q_e	-1
m_i/m_e	40
v_{te}	1
v_{ti}	$1/\sqrt{40}$
Injected electron current	-63.83
Injected ion current	40.36
Injected electron flux	1277
Injected ion flux	807.4

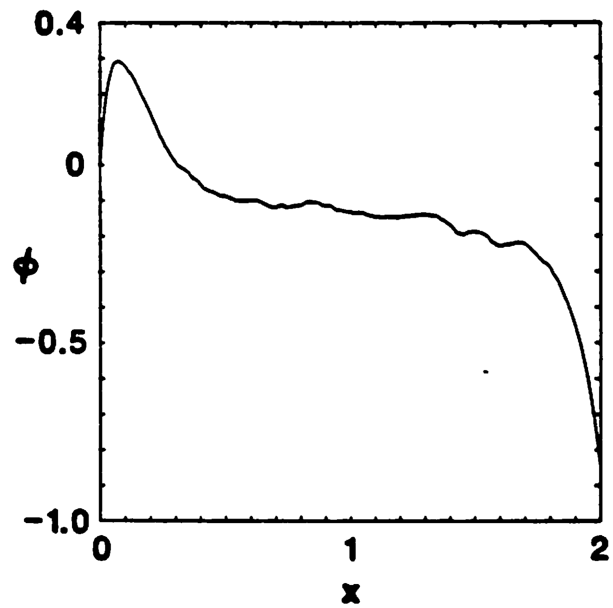

Fig. 1. Potential after initial transient, but before cooling of trapped electrons. This potential agrees with equilibrium theory.

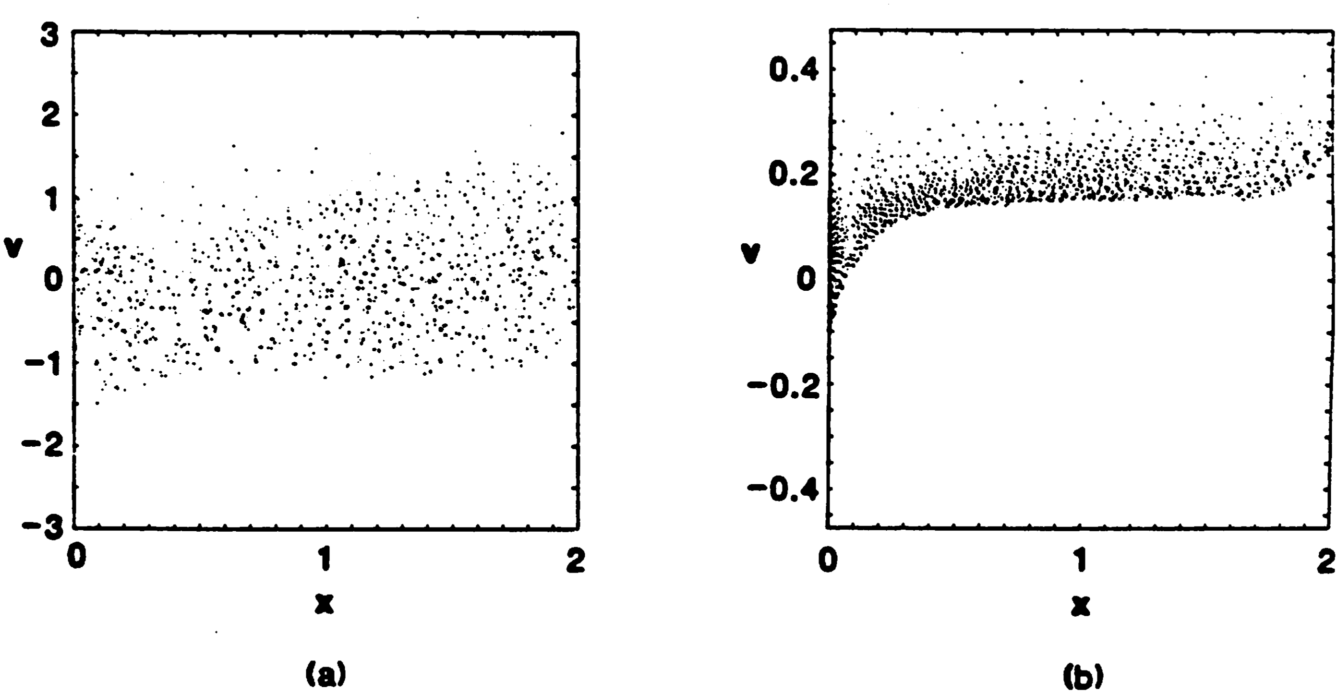

Fig. 2. Electron (a) and ion (b) phase spaces for potential in Fig. 1. Note smoothness and patterns due to quiet injection.

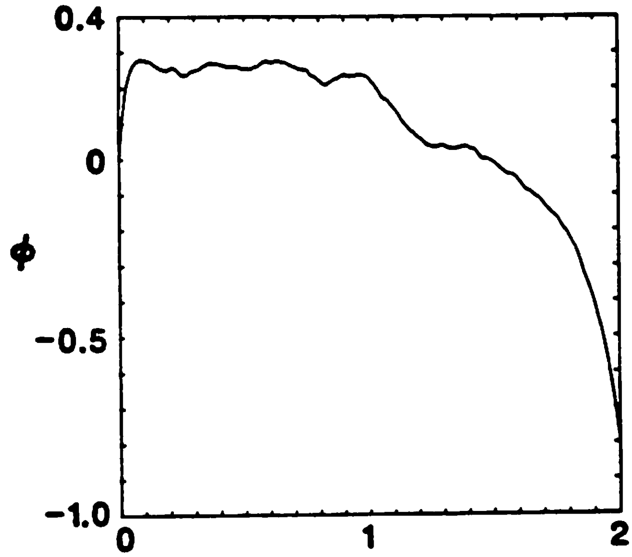

Fig. 3. Potential after some cooling of trapped electrons. Note elongation of trapping well.

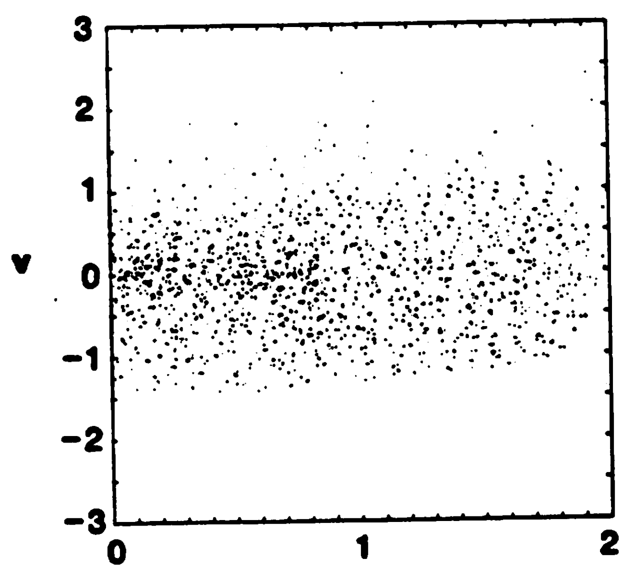

Fig. 4. Phase space for potential in Fig. 3. Note increased density of electrons in trapping well.

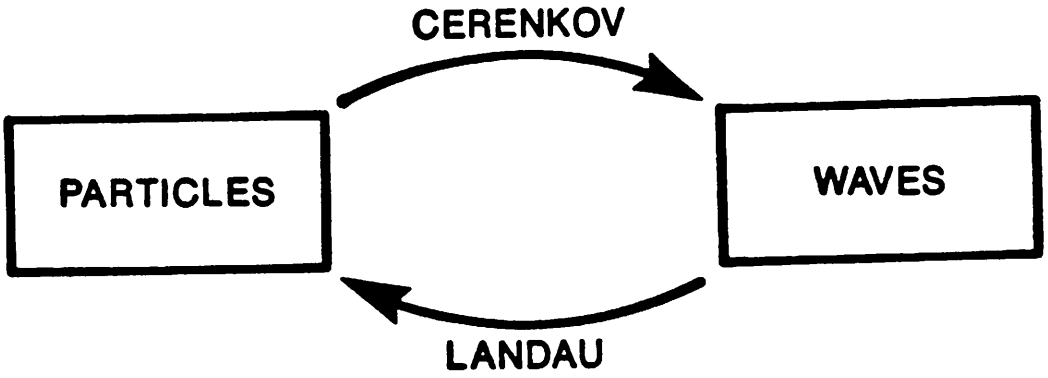

Fig. 5. Energy balance between particle thermal energy and wave fluctuations in periodic or infinite plasma.

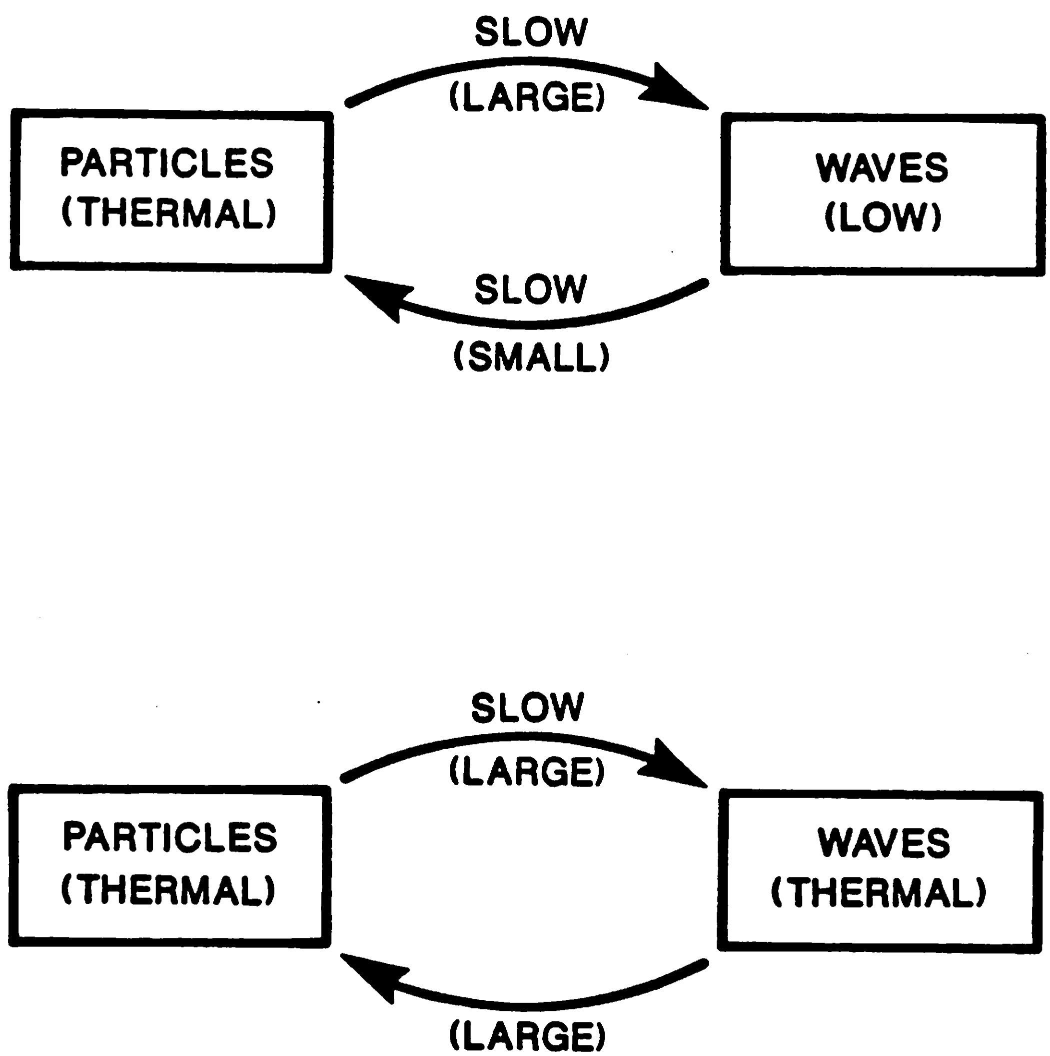

Fig. 6. Transition from initial quiet start (a) to final equilibrium (b) takes place on a slow time scale. The final energy content of the waves is much smaller than that of the particles.

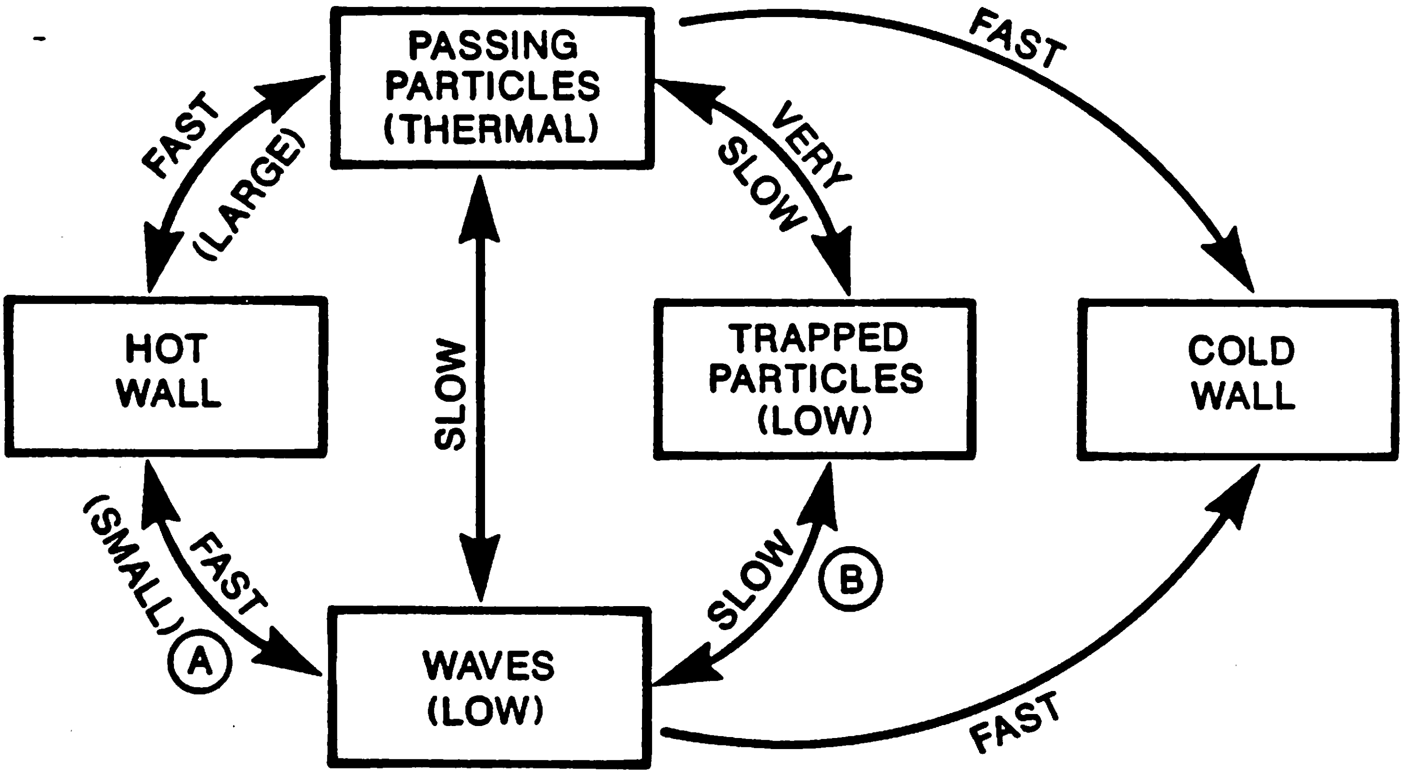

Fig. 7. Wave fluctuations equilibrate on a fast time scale to a low level (due to low level of injection noise) (A). Trapped electrons equilibrate on a slow time scale to low level by losing energy to low temperature fluctuations (B).

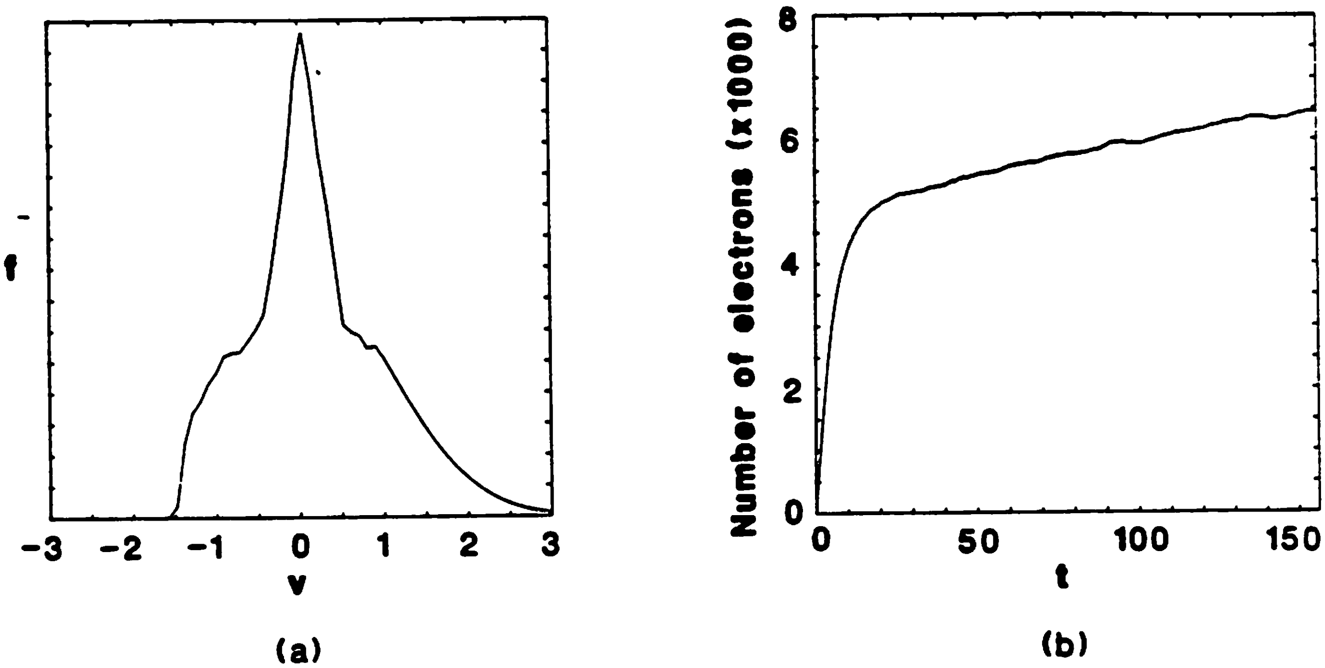

Fig. 8. Electron distribution at position of trapping well at end of run (a), and time history of the total number of electrons in the system (b) for quiet injection. The number of electrons grows as more electrons become trapped.

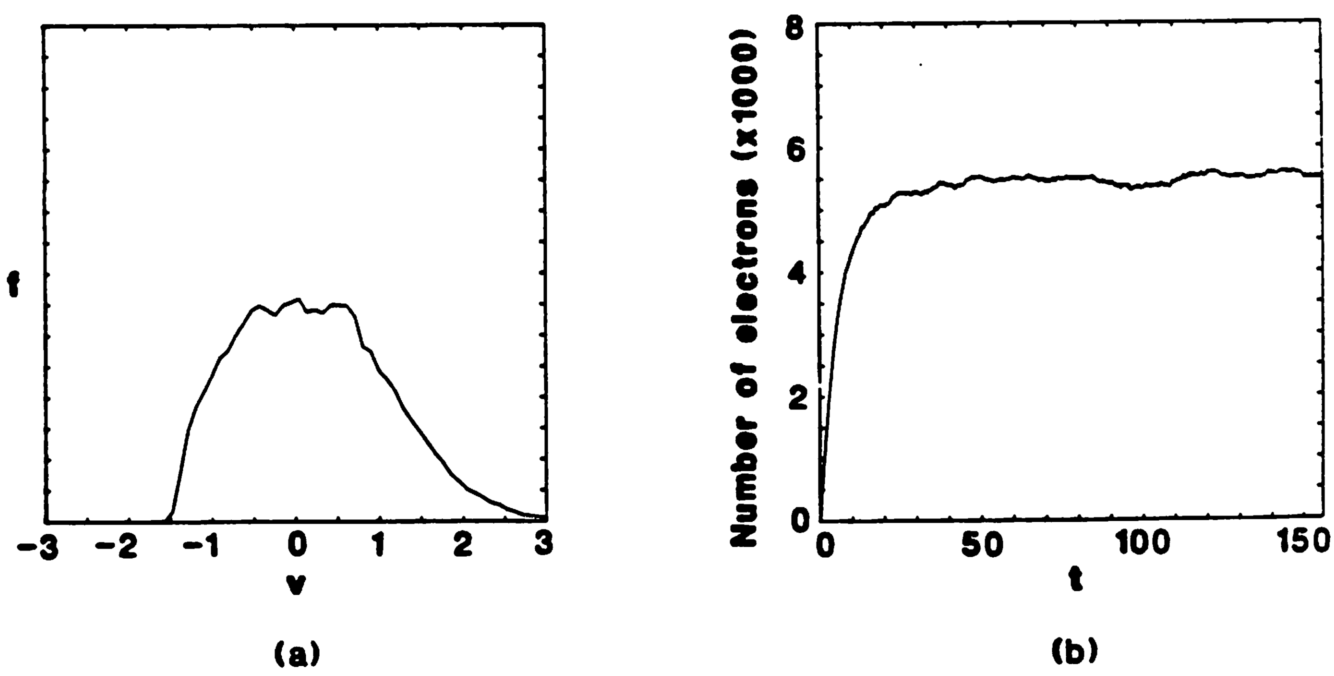

Fig. 9. Electron distribution at position of trapping well at end of run (a), and time history of the total number of electrons in the system (b) for noisy injection.

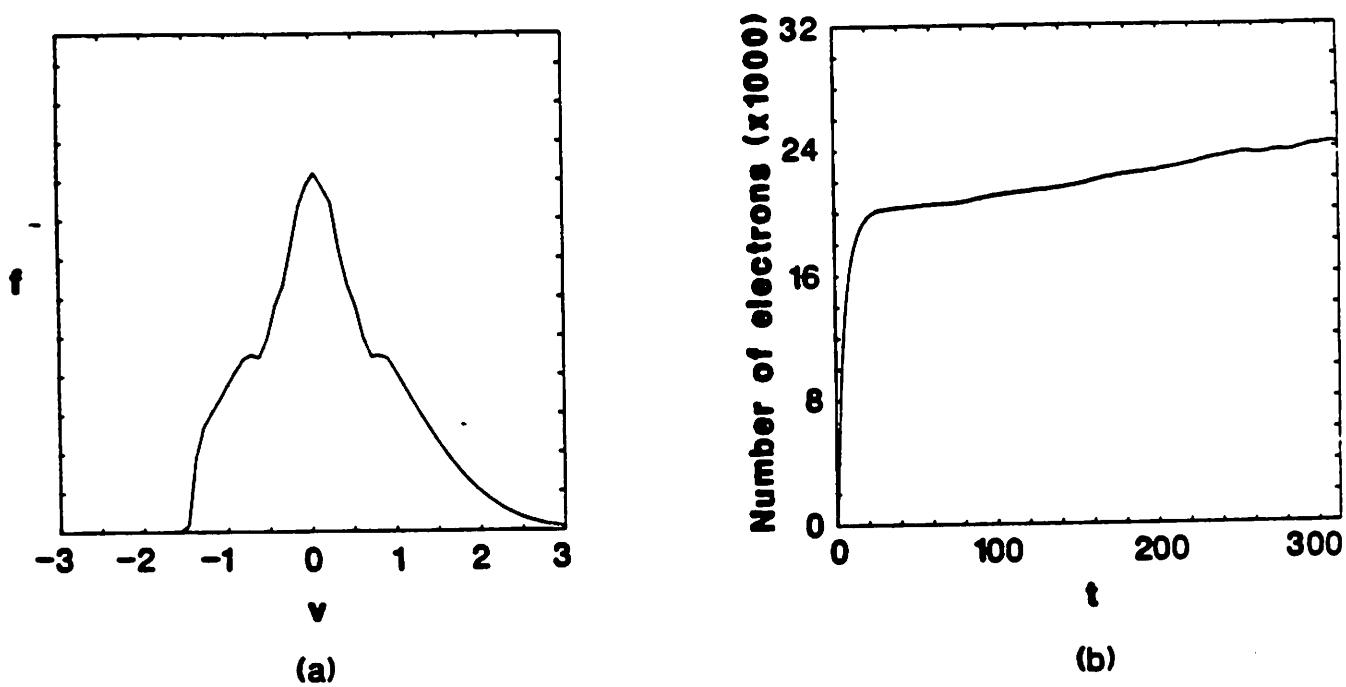

Fig. 10. Quiet injection results for electron distribution (a) and total number of electrons (b) with four times as many particles as in Fig. 8. (Note that this simulation was also run for twice as long as in Fig. 8.)

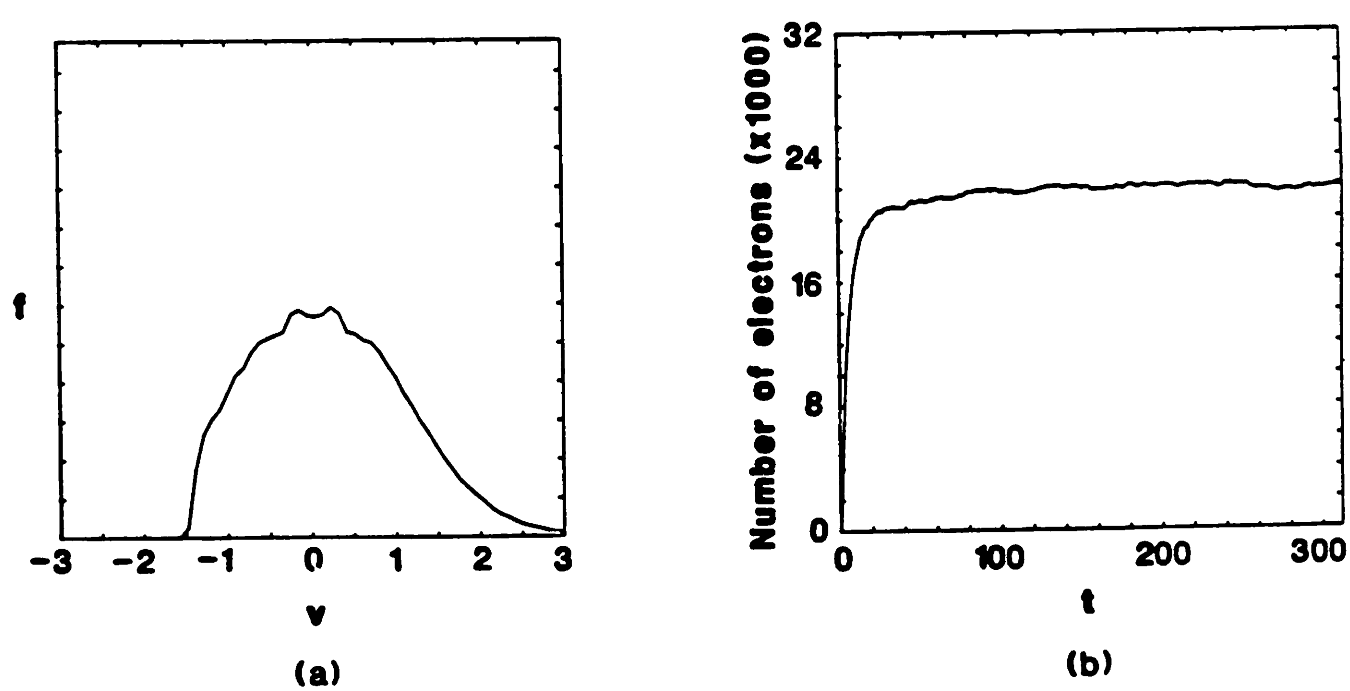

Fig. 11. Noisy injection results for electron distribution (a) and total number of electrons (b) with four times as many particles as in Fig. 8.

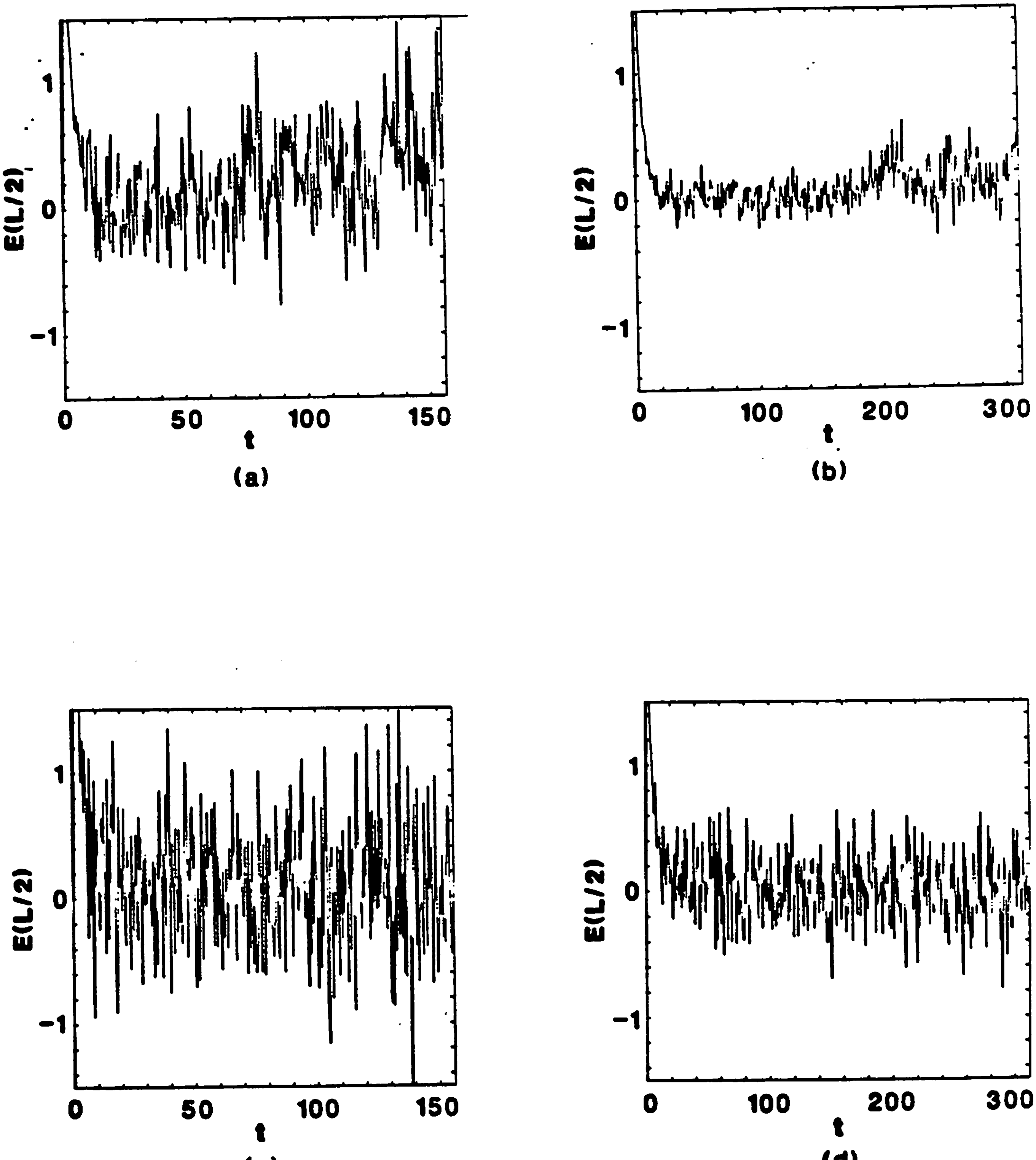

Fig. 12. Time histories of electric field in center of simulation region for four different runs. (a) and (b) are quiet injection runs with (b) having four times as many particles as (a), and (c) and (d) are noisy injection runs with (d) having four times as many particles as (c). RMS value of E in (b) should be 1/4 that of (a), and RMS value of E in (d) should be half that of (c).