

SIMULATION OF MICROSCOPIC PROCESSES IN PLASMA

Viktor K. Decyk

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Invited paper presented at the 1987 International Conference on Plasma  
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University of California

Department of Physics

Los Angeles, CA 90024

Simulation of Microscopic Processes in Plasma

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Viktor K. Decyk

Physics Department

University of California, Los Angeles

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This talk is about how one can use particle simulations to study microscopic plasma phenomena, such as the behavior of test charges. In a particle simulation, one assumes some form for the force of interaction between particles, and then integrates on a computer the equations of motion of a large number of particles.<sup>1</sup>

This method is limited only by the validity of the known force law, and by the accuracy of the numerical integration scheme. Of course, if the number of particles followed on the computer is too small, then the result will not be described by plasma theories, that is, the model will not behave much like a plasma, but the results will still be valid. Particle simulation can be distinguished from other kinds of simulation by its independence from plasma theory, and thus it is meaningful to look at this kind of calculation as a computer experiment.

Most of this talk will be about test charges in plasmas. The concept of a test charge has proved to be an important tool in the theoretical development of plasma properties. It is, of course, unthinkable that one could ever measure in an experiment the effect by itself of a single test charge moving in a plasma. The purpose of this talk is to show how particle simulations can be used to perform computer experiments on just such single test charges. This gives us for the first time a "microscope" with which to look directly at how test charges interact with plasmas, and thus give us a possibility to evaluate some important theoretical concepts.

The method is based on the idea that computer experiments, unlike laboratory experiments, are absolutely reproducible. The essence of the method is to perform the simulation twice, first with a background plasma, and the second time with exactly the same initial conditions plus some small perturbing influence, such as an extra particle, a small current in an

antenna, etc. The results are subtracted, and what is left is the effect of the small perturbation.

The potential of a test charge is given in many plasma textbooks, such as Krall and Trivelpiece<sup>2</sup>, to be:

$$\phi(\underline{k}, \omega) = \frac{4\pi\rho_e(\underline{k}, \omega)}{k^2 \epsilon(\underline{k}, \omega)}$$

Where  $\rho_e(\underline{k}, \omega)$  represents an external charge, and

$$\epsilon(\underline{k}, \omega) = 1 - \frac{\omega_{pe}^2}{2k^2 v_t^2} Z^1\left(\frac{\omega}{\sqrt{2}kv_t}\right)$$

is the plasma dispersion relation for an electron plasma.

Therefore I will start with this equation, and in fact, much of this talk will be devoted to its meaning.

Suppose that we choose a test charge moving at constant velocity

$$\rho_e(\underline{x}, t) = q_t \delta(\underline{x} - \underline{x}_0 - \underline{v}t), \quad t > 0,$$

then

$$\rho_e(\underline{k}, \omega) = \frac{q_t e^{-i\underline{k} \cdot \underline{x}_0}}{i(\underline{k} \cdot \underline{v} - \omega)}$$

so that

$$\phi(\underline{k}, \omega) = \frac{4\pi q_t e^{-i\underline{k} \cdot \underline{x}_0}}{ik^2(\underline{k} \cdot \underline{v} - \omega)\epsilon(\underline{k}, \omega)}$$

To obtain the answer in  $(\underline{x}, t)$  space, one first inverts the Laplace transform in time:

$$\phi(\underline{k}, t) = \frac{4\pi q_t e^{-i\underline{k} \cdot \underline{x}_0}}{k^2} \int_{-\infty+ic}^{\infty+ic} \frac{d\omega e^{-i\omega t}}{2\pi i(\underline{k} \cdot \underline{v} - \omega)\epsilon(\underline{k}, \omega)}$$

+ initial value terms, which will vanish identically for the case in the simulation, since both runs are prepared identically except for the test charge.

The integrand has two poles, one at  $\omega = \underline{k} \cdot \underline{v}$  and another at  $\omega = \omega_j$ , where  $\omega_j$  are the roots of  $\epsilon$ . Applying Cauchy's theorem, this integral can be done by contour integration to give:

$$\phi(\underline{k}, t) = \frac{4\pi q t e^{-i\underline{k} \cdot (\underline{x}_0 + \underline{v}t)}}{k^2 \epsilon(\underline{k}, \underline{k} \cdot \underline{v})} - \sum_j \frac{4\pi q t e^{-i\underline{k} \cdot \underline{x}_0} e^{-i\omega_j t}}{k^2 (\underline{k} \cdot \underline{v} - \omega_j) \frac{\partial \epsilon(\underline{k}, \omega_j)}{\partial \omega}}, \quad t > 0$$

The two terms here are commonly called the Debye cloud term and the Cherenkov term, respectively. Performing the integral over  $\underline{k}$ , one can write the solution in real space as

$$\phi(\underline{x}, t) = \phi_D(\underline{x}, t) + \phi_C(\underline{x}, t),$$

where

$$\phi_D(\underline{x}, t) = 4\pi q t \int_{-\infty}^{\infty} \frac{dnk}{(2\pi)^n} \frac{e^{i\underline{k} \cdot (\underline{x} - \underline{x}_0 - \underline{v}t)}}{k^2 \epsilon(\underline{k}, \underline{k} \cdot \underline{v})}$$

$$\phi_C(\underline{x}, t) = -4\pi q t \sum_j \int_{-\infty}^{\infty} \frac{dnk}{(2\pi)^n} \frac{e^{i\underline{k} \cdot (\underline{x} - \underline{x}_0)} e^{-i\omega_j t}}{k^2 (\underline{k} \cdot \underline{v} - \omega_j) \frac{\partial \epsilon(\underline{k}, \omega_j)}{\partial \omega}},$$

where  $n$  is the spatial dimensionality.

Usually the second term is discarded, because  $\omega_j$  is always damped. However, in our case, this cannot be ignored because there are always some modes whose damping is small, and for those modes  $\phi_C$  is in fact much bigger than  $\phi_D$ .

For a stationary test charge,  $v = 0$ , the first term gives the well-known

Debye cloud:

$$\phi_D(\underline{x}) = \begin{cases} 2\pi q_t \lambda_D e^{-|\underline{x}-\underline{x}_0|/\lambda_D}, & \text{in 1D} \\ 2q_t K_0(|\underline{x}-\underline{x}_0|/\lambda_D), & \text{in 2D} \\ \frac{q_t e^{-|\underline{x}-\underline{x}_0|/\lambda_D}}{|\underline{x}-\underline{x}_0|}, & \text{in 3D} \end{cases}$$

where  $\lambda_D = v_t/\omega p$  is the Debye length. However, if  $v > 0$ , things are not so simple.

For  $v > 0$ , most of the significance of the integrals can be understood by considering the simplest possible case, a one dimensional cold plasma, where

$$\epsilon(k, \omega) = 1 - \frac{\omega p^2}{\omega^2}$$

In this case the integrals can be done analytically. For the Debye term

$\epsilon(\underline{k}, \underline{k} \cdot \underline{v})$  has poles at  $k v = \pm \omega p$ , so that one obtains:

$$\phi_D(x, t) = \begin{cases} 0 & x > x_0 + vt \\ \frac{4\pi q_t v}{\omega p} \sin\left[\frac{\omega p}{v}(x - x_0 - vt)\right] & x < x_0 + vt \end{cases}$$

This is just a sine wave extending to infinity behind the particle. For the Cherenkov term, there is a pole at  $k = 0$ , which gives the potential of an unshielded test charge, and a pole at  $k v = \omega_j$  which gives a potential which exactly cancels the Debye term for  $x < x_0$ .

$$\phi_C(x,t) = -2\pi q_t |x - x_0| \cos \omega_p t$$

$$+ \begin{cases} \frac{-4\pi q_t v}{\omega_p} \sin \left[ \frac{\omega_p}{v} (x - x_0 - vt) \right] - \frac{2\pi q_t v}{\omega_p} \sin \omega_p t & x < x_0 \\ \frac{2\pi q_t v}{\omega_p} \sin \omega_p t & x > x_0 \end{cases}$$

Thus the total solution [Fig. 1] is

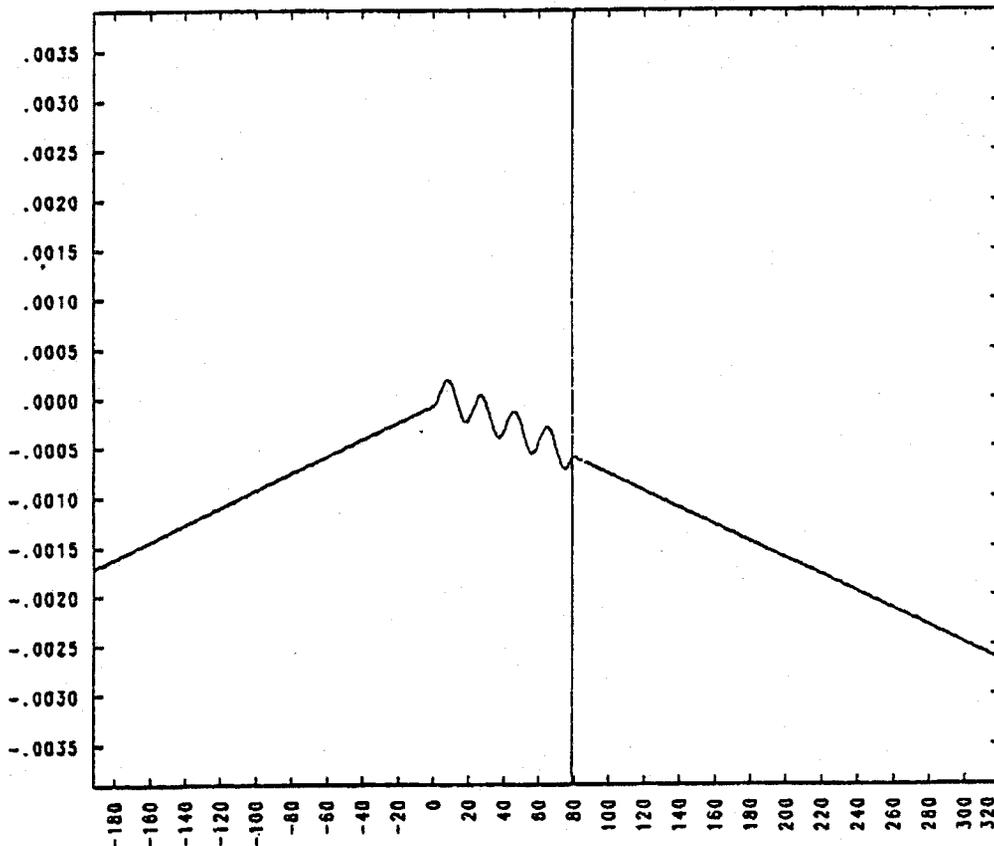
$$\phi(x,t) = -2\pi q_t |x - x_0| \cos \omega_p t$$

$$+ \begin{cases} \frac{-2\pi q_t v}{\omega_p} \sin \omega_p t & x < x_0 \\ \frac{4\pi q_t v}{\omega_p} \sin \left[ \frac{\omega_p}{v} (x - x_0 - vt) \right] + \frac{2\pi q_t v}{\omega_p} \sin \omega_p t, & x_0 < x < x_0 + vt \\ \frac{2\pi q_t v}{\omega_p} \sin \omega_p t & x > x_0 + vt \end{cases}$$

The unshielded potential  $2\pi q_t |x - x_0|$ , which oscillates at  $\omega = \omega_p$  is just the plasma response to the sudden creation at  $t = 0$  of a new charge. The oscillation at  $kv = \omega_p$  is the excitation of a plasma wake by the test charge. It moves with the particle. The Cherenkov term is necessary to produce the correct initial values: the oscillation cannot extend to infinity at  $t = 0$ , which the Debye term alone would predict.

The major features of the plasma response to a moving test charge are contained in the cold plasma model. The fully kinetic model introduces two new effects: damping and the excitation of waves not moving with the particle.

It turns out that the Debye term can be integrated analytically even in the fully kinetic case, for a one dimensional plasma. The result [Fig. 2] is:



POTENTIAL, SCALE= -8

T = 26.40000

Fig. 1 Plasma wake emitted by one dimensional test charge, as predicted by cold plasma model. Vertical bar shows location of test charge.

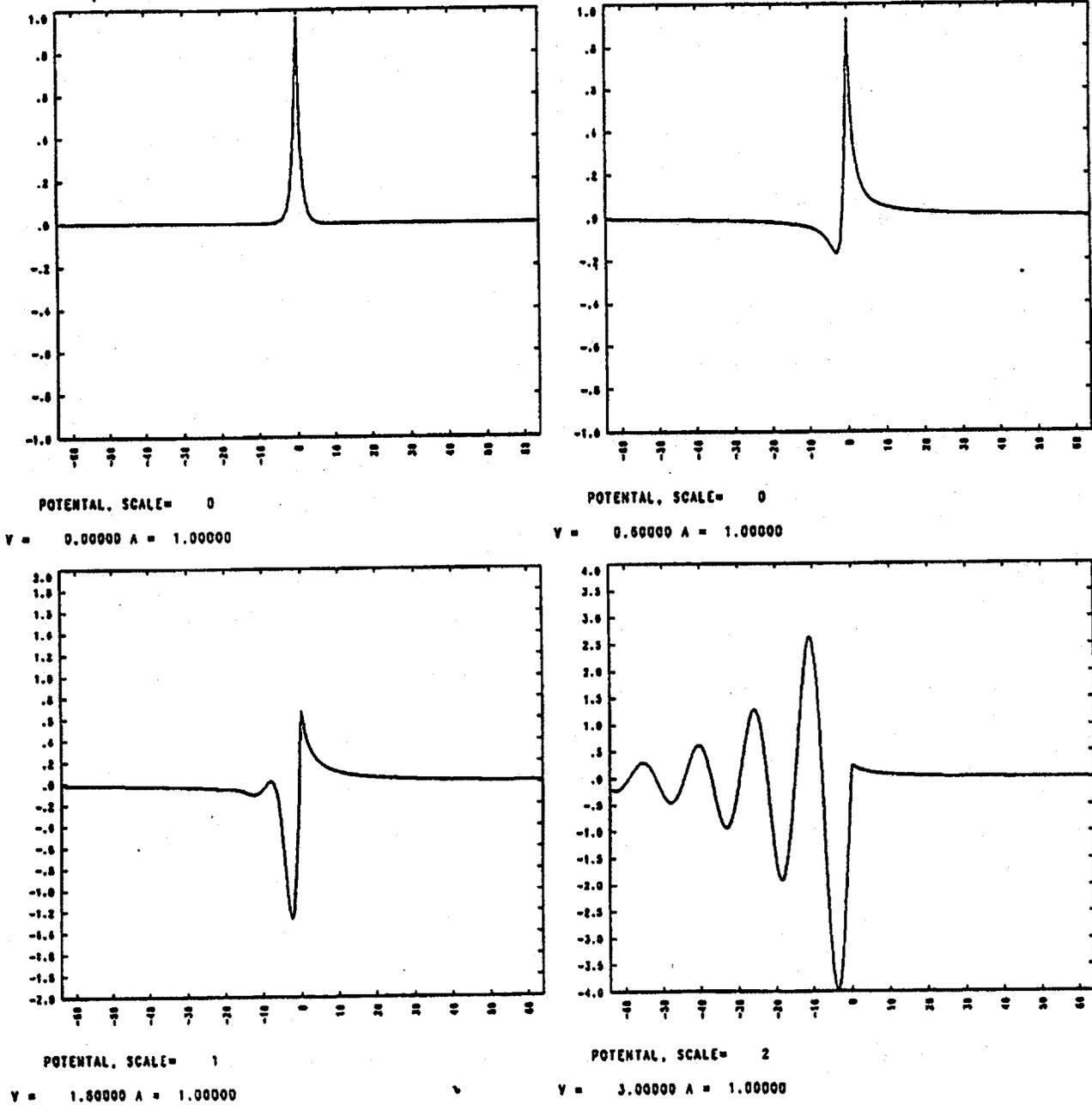


Fig. 2 Theoretical prediction of Debye shielding and wake behind a one dimensional test charge, for various velocities. Test charge is located at center and is moving to the right.

$$\phi_D(x, t) = \begin{cases} 4q_t \lambda_D \operatorname{Im} f\left(\frac{\kappa_0 |x - x_0 - vt|}{\lambda_D}\right), & x > x_0 + vt \\ -4q_t \lambda_D \operatorname{Im} f\left(\frac{\kappa_0 |x - x_0 - vt|}{\lambda_D}\right) + 4\pi q_t \lambda_D \operatorname{Im} \frac{e^{i\kappa_0(x - x_0 - vt)/\lambda_D}}{\kappa_0}, & x < x_0 + vt \end{cases}$$

where  $f(z)$  is a combination of complex sine and cosine integrals:

$$f(z) = \operatorname{Ci}(z) \sin z - \operatorname{Si}(z) \cos z,$$

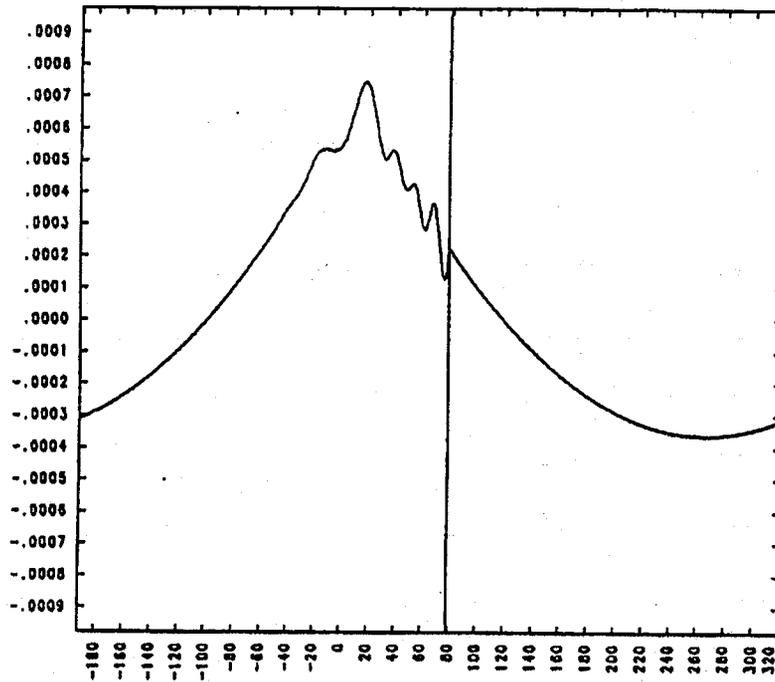
$$\kappa_0^2 = \frac{k^2}{k_D^2} [1 - \epsilon(\underline{k}, \underline{k} \cdot \underline{v})] = -1 + \frac{\sqrt{2}v}{v_t} D\left(\frac{v}{\sqrt{2}v_t}\right) - i\sqrt{\frac{\pi}{2}} \frac{v}{v_t} e^{-v^2/2v_t^2},$$

$$D(x) \equiv e^{-x^2} \int_0^x e^{t^2} dt \text{ is Dawson's integral.}$$

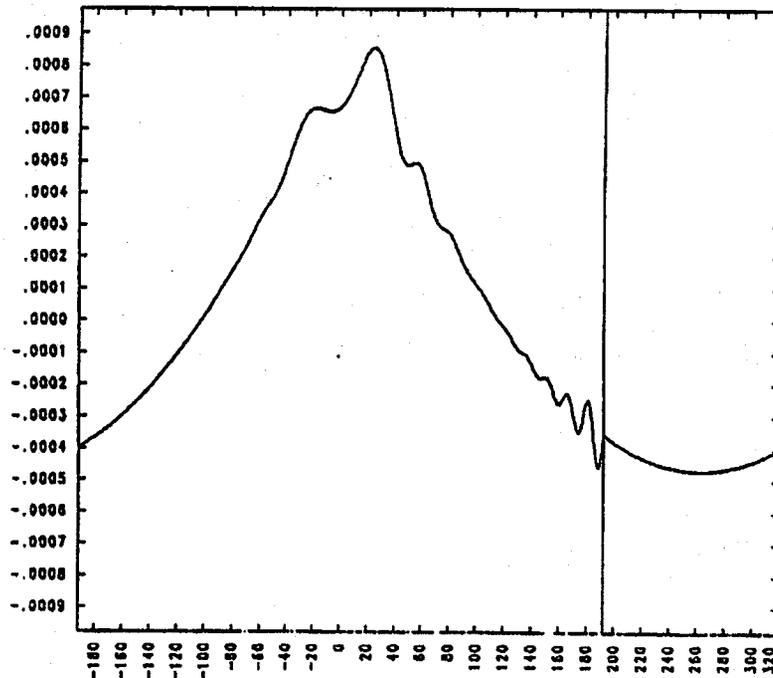
The imaginary part of the sine and cosine integrals gives a shielding around the test charge. The complex exponential term gives the wake behind the particle, and also contributes to the shielding.

This Debye term is in reality an asymptotic solution. To get the correct time evolution one needs to also consider the Cherenkov term. This I have not been able to do analytically but only numerically.

The total solution [Fig. 3] looks similar to the cold plasma result: there is a wake behind the particle superimposed on a much larger "ringing" of the unshielded test charge potential. There are two important differences. The first is that the sine wave behind the particle is damped, with the envelope given by the Landau damping result. Secondly, there are large oscillations in the vicinity of where the particle was created which get left behind, at least if the test charge velocity  $v > v_t$ .



T = 26.40000



T = 64.00000

Fig. 3 Plasma wake emitted by one dimensional test charge, moving at velocity  $3v_t$ , as predicted by Kinetic theory. Vertical bar shows location of test charge.

The "ringing" of the unshielded test charge which dominates the wake is not really of interest, and is an artifact of the way we initialized the system by suddenly creating a charge. If one wanted to see the wake more clearly, it would be better if one could find a more gentle way to initialize the system.

The answer is to do what nature does - create charges as a neutral pair. It turns out that the ringing is for the most part independent of the velocity of the test charge. So that if one creates an electron-positron pair, and shoots one of them off with a given velocity, the ringing due to each will cancel out, and one will be left with the plasma wave being excited by the test charge.

There is another thing we must consider if we are going to compare theory with simulation. In the simulation, one uses finite-size particles, which changes the wave properties somewhat. However, it is easy to fix the theory to take into account the finite size of the particles if aliasing effects can be neglected. One merely replaces:

$$q\delta(x - x^1) \rightarrow qS(x - x^1),$$

where  $S(x)$  is the particle shape function. In Fourier space this means replacing

$$q \rightarrow qS(k),$$

where  $S(k)$  is the transform of  $S(x)$ . The only place  $q$  enters in the equations is in the plasma frequency, so one has

$$\omega_p^2 \rightarrow \omega_p^2 |S(k)|^2,$$

which changes the dispersion of waves somewhat. For long wavelength modes,

the first order correction with gaussian shaped particles gives

$$\omega^2 = \omega_{pe}^2 + [3 - a^2/\lambda_D^2] k^2 v_t^2$$

Usually  $a = \lambda_D$  is used, which changes the constant 3 to 2.

This correction also changes the Debye shielding and the plasma wake, [Fig. 4] primarily by eliminating sharp discontinuities and lengthening the wavelengths. But these corrections due to finite-size particles do not change things very much in the theory.

Thus we will use for the external charge, an electron-positron pair:

$$\rho_e(x,t) = q_t S(x - x_0) - q_t S(x - x_0 - vt), \quad t > 0$$

The resulting potential [Fig.5] will then clearly be the difference between the potentials obtained earlier, one with finite  $v$ , and one with  $v = 0$ .

Now that the prediction of theory is understandable, let us examine the results of a particle simulation. A usual particle-in-cell type of code was used, except that second order spline functions were used in the interpolation on the grid and 64 bit precision was used. Two runs are done. In the reference run, the electrons are distributed uniformly in space, with a Maxwellian velocity distribution from a gaussian random number generator. In addition, one extra test charge, with charge  $+e/10$ , is left at rest. The ions form a neutralizing background. The second run is prepared identically, except that the extra test charge moves with velocity  $v$ . The time history of the potential is recorded in each case, and the difference between the two is displayed. Both periodic boundary conditions and vacuum boundary conditions have been used.

The agreement between theory and simulation [Fig.6] is quite stunning, especially for early times. The figure shows the case of a test charge moving with velocity  $3v_t$ , and vacuum boundary conditions. There are 4000 particles

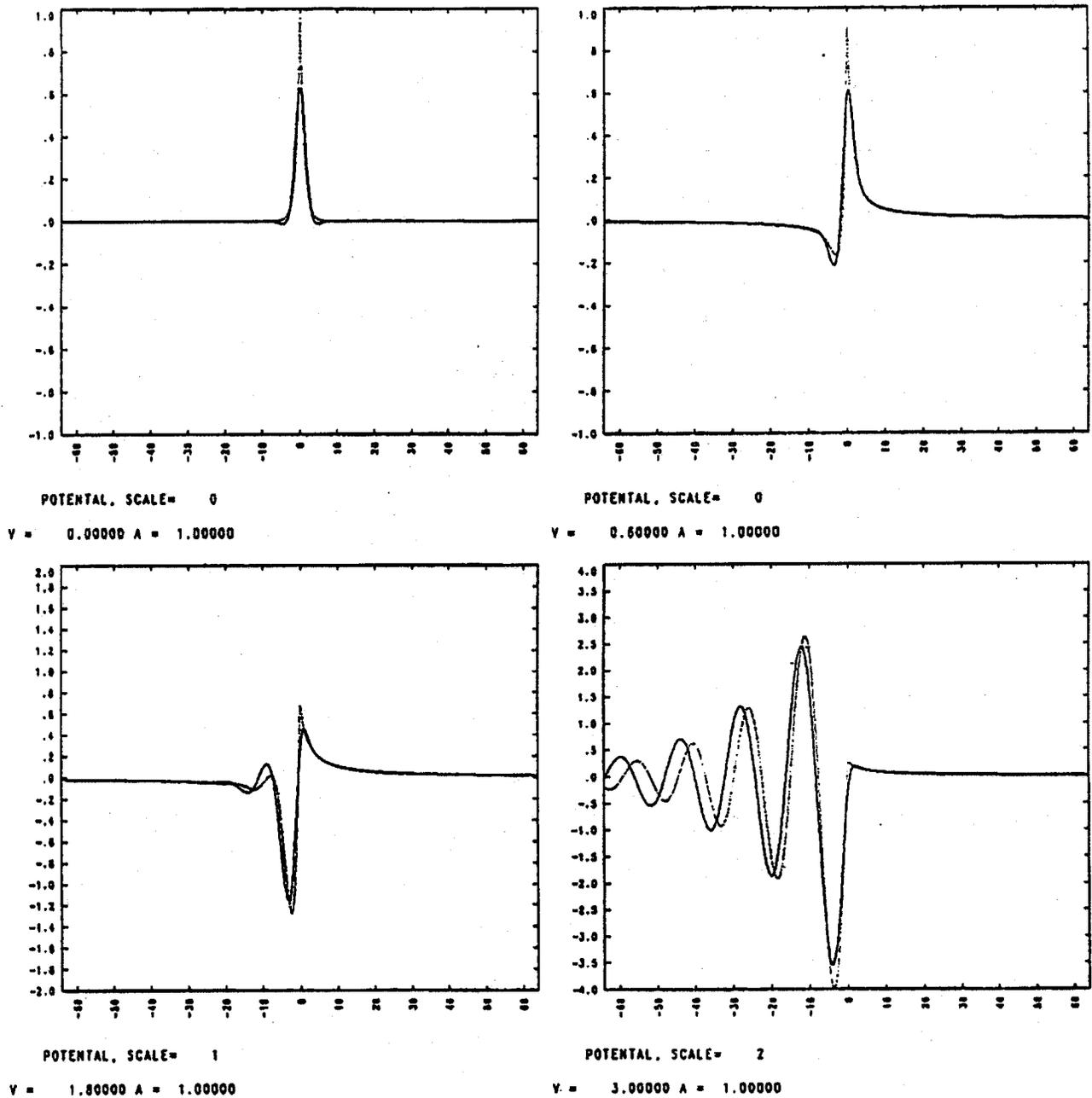
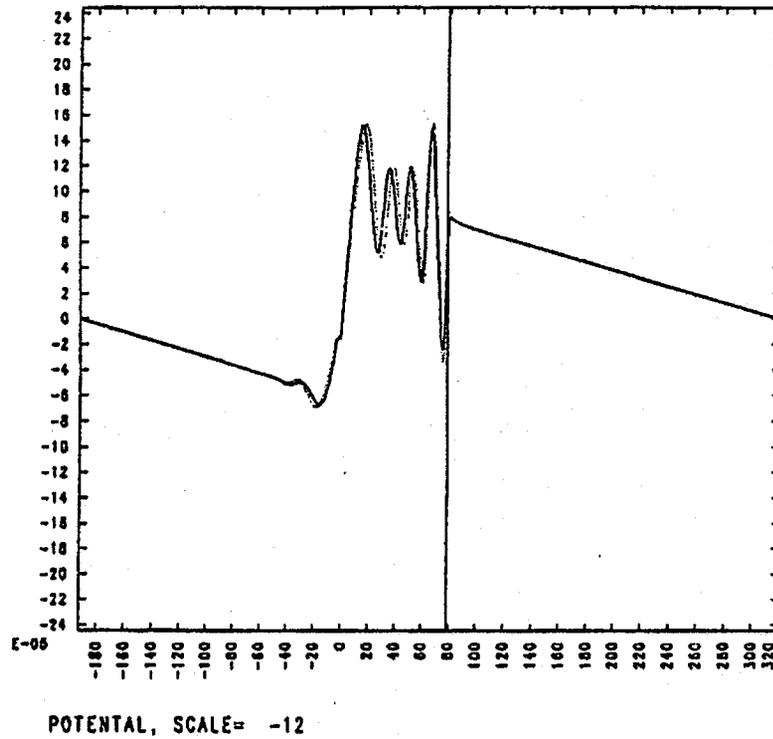
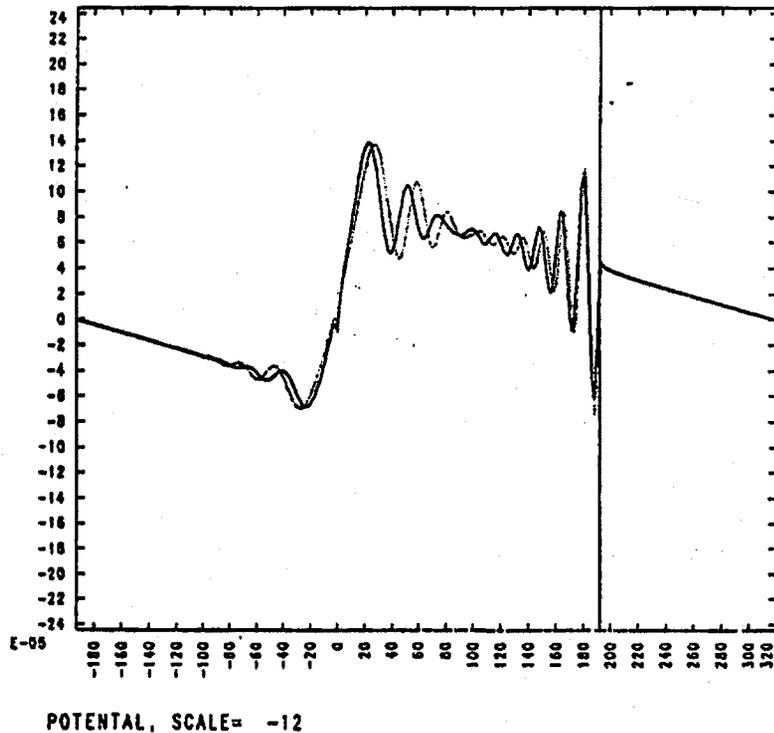


Fig. 4 Theoretical prediction of Debye shielding and wake behind a one dimensional test charge, for various velocities. Dashed line is the point particle result, solid line is the finite-size particle result. Test charge is located at center and is moving to the right.



T = 26.40000



T = 64.00000

Fig. 5 Plasma wake emitted by one dimensional electron-positron pair, positron moving at velocity  $3v_t$ , as predicted by Kinetic theory. Dashed line is the point particle result, Solid line is the finite-size particle result. Vertical bar shows location of moving test charge.

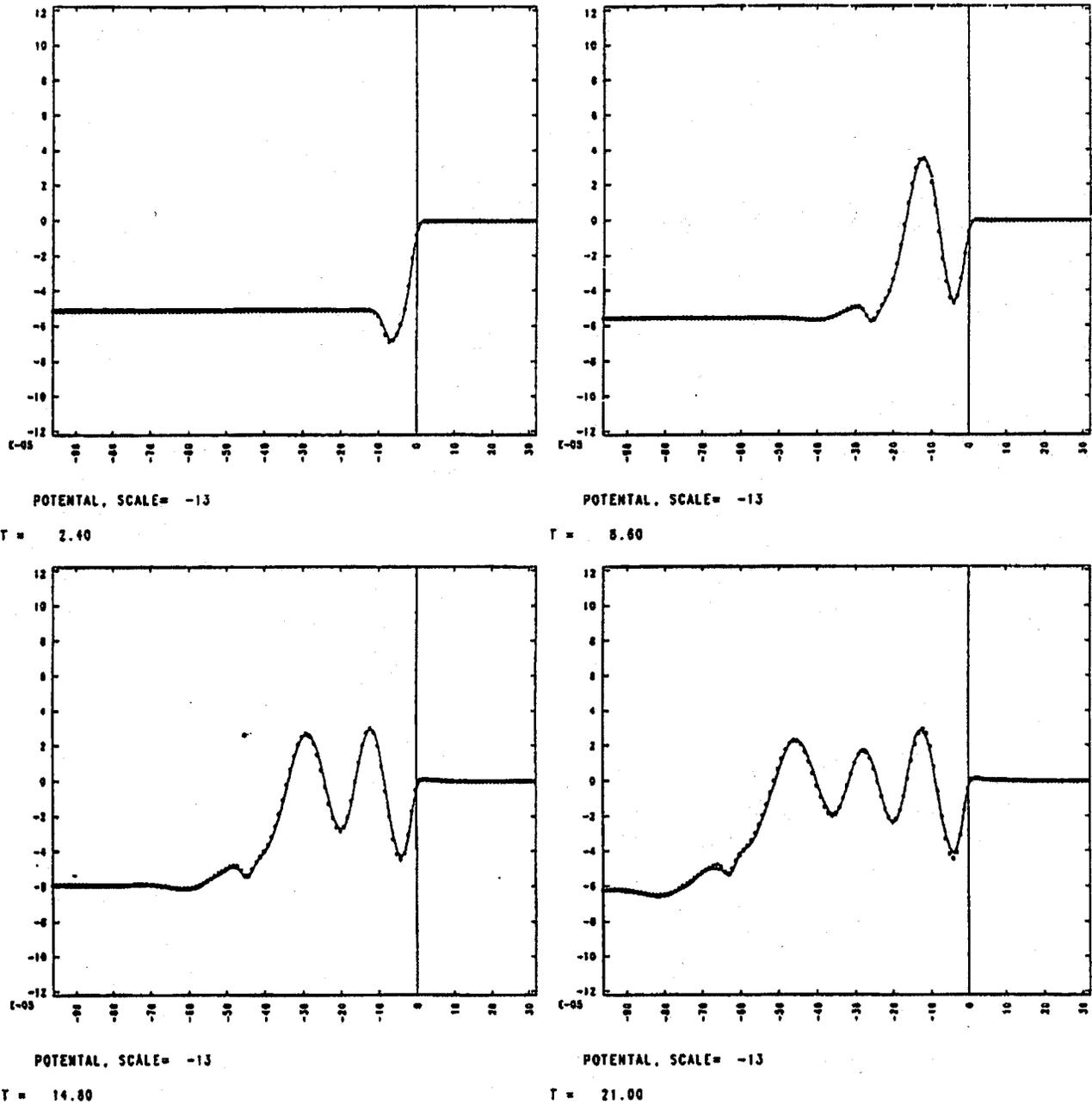


Fig. 6a Time evolution of the plasma wake behind test charge moving with velocity  $v = 3v_t$ . Dots represent prediction of plasma theory, lines represent simulation results. There is good agreement for early times, followed by the appearance of discreteness effects.

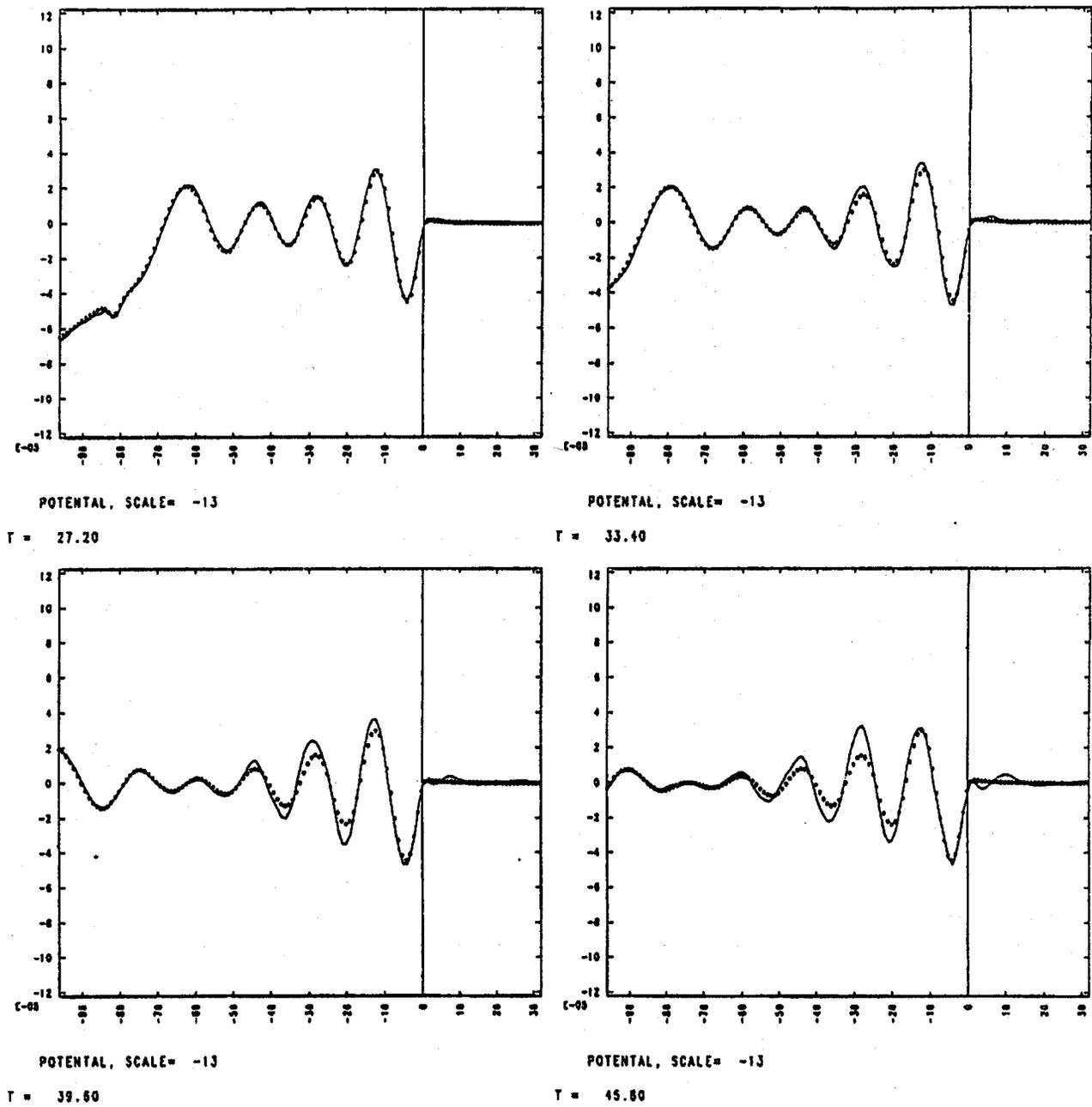
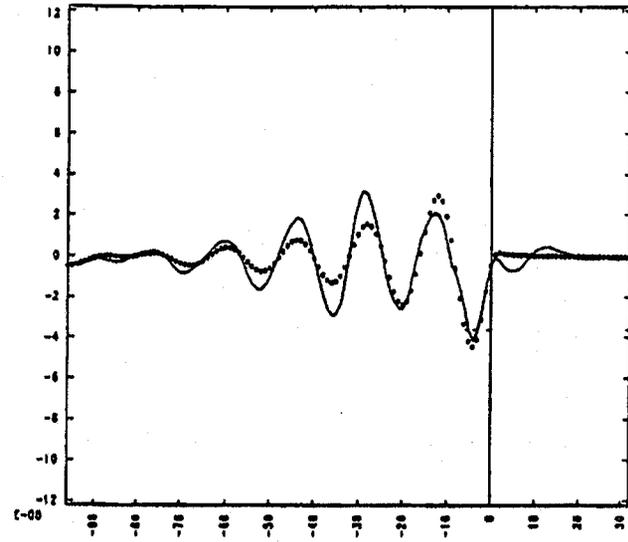
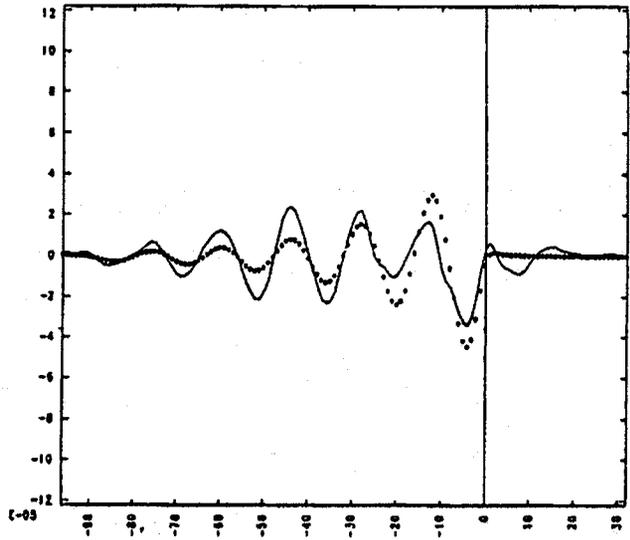


Fig. 6b



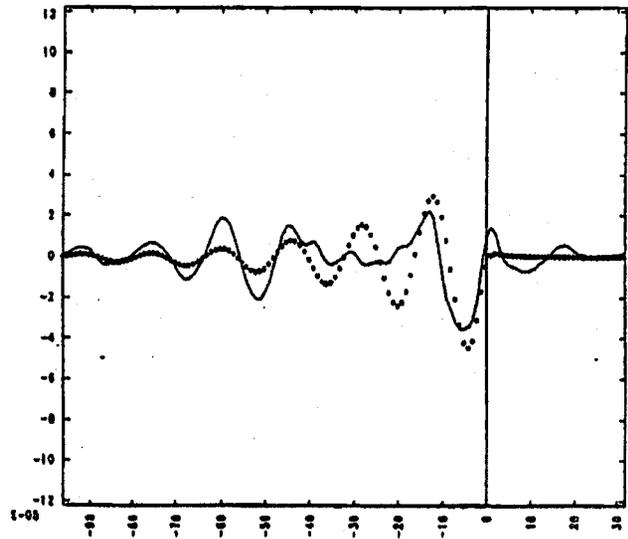
POTENTIAL, SCALE= -13

T = 52.00



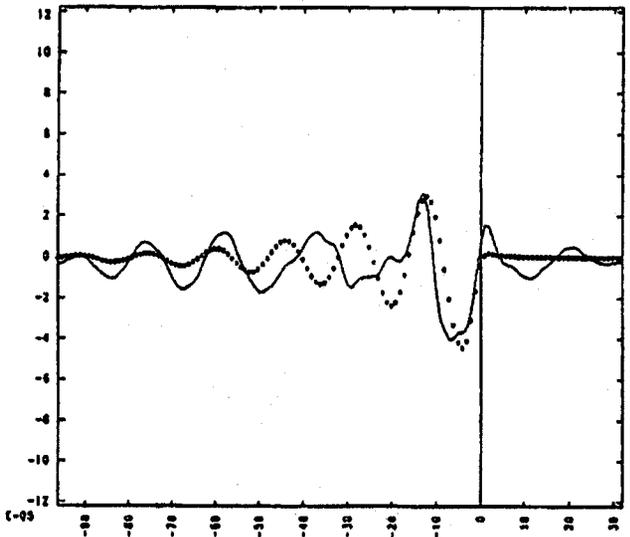
POTENTIAL, SCALE= -13

T = 58.20



POTENTIAL, SCALE= -13

T = 64.40



POTENTIAL, SCALE= -13

T = 70.60

Fig. 6c

n a Debye length here, so the plasma parameter  $g = (n\lambda_D)^{-1}$  is small enough to represent a real plasma.

As time goes on, however, disagreement between theory and simulation becomes evident. This disagreement is the result of particle discreteness, and indicates what the corrections to the first order theory are, which neglects particle discreteness.

Let's examine the major discreteness effects. The first thing which is evident is the occasional and local growth of the plasma wake, or parts of it, in time. A second effect is the evidence of an interference pattern in the wake, indicating secondary excitation of other modes. Thirdly, one can see the excitation of a precursor in front of the particle.

We have found that the discreteness effects depend on the random numbers used to initiate the system, but are exactly proportional to the charge of the test particle. The effects are more obvious when the test particle velocity is reduced, and when the plasma parameter is increased (that is, when  $n\lambda_D$  is reduced).

Although these effects are not entirely understood, we do have some clues as to their causes. The most important clue comes from examining the precursor in front of the test particle, as the test particle velocity changes, but for the same initial preparation of the plasma. One finds that this precursor does not depend very much on the test charge itself, and the leading edge propagates with a velocity about  $4v_t$ , which is just about the velocity of the fastest particle in the simulation. The conclusion is then that the precursor is caused by the background electrons which have traversed the wake behind the test charge, and finally overtake the test charge, and because of their long term memory, they propagate the disturbance in front of the test charge. This is reminiscent of a plasma echo, and needs further

investigation. Notice that the Cherenkov radiation left behind in the vicinity of where the test charge started, is also not strongly dependent on the test charge velocity, so that these fast electrons experience a fairly similar history.

One can conclude that a collision between two fast particles involves the excitation of other modes, i.e., electrostatic bremsstrahlung<sup>3</sup>. These modes turn out to enhance the high  $k$  part of the radiation (the wake), which begins to become somewhat turbulent [Fig.7]. If the test charge moves faster than any particle, then no precursor is observed, consistent with this picture [Fig. 8].

Finally, the sporadic growth in time of the wave is not well understood, but one can observe in the simulation that the growth rate is approximately given by

$$\gamma/\omega_p = 1/3 (n\lambda_D)^{-1/3}, \quad n\lambda_D \geq 100$$

and is independent of the charge on the test particle. This growth probably depends on the pre-existing fluctuation level of waves in the plasma.

The significance of this technique is that we now have a tool, a microscope if you will, for investigating such fundamental processes as the behavior of test charges. This gives us valuable clues for further theoretical developments in basic plasma properties, as well as an opportunity for theorists to directly test some of their hypotheses and assumptions. Note, for example, that the Fourier-Laplace transform of the potential created by a test charge, which we have been looking at, is a direct measurement of the full plasma  $\epsilon$ , discreteness effects included.

There are a lot of other applications of this subtraction technique. One can apply this to the study of the radiation pattern emanating from an antenna

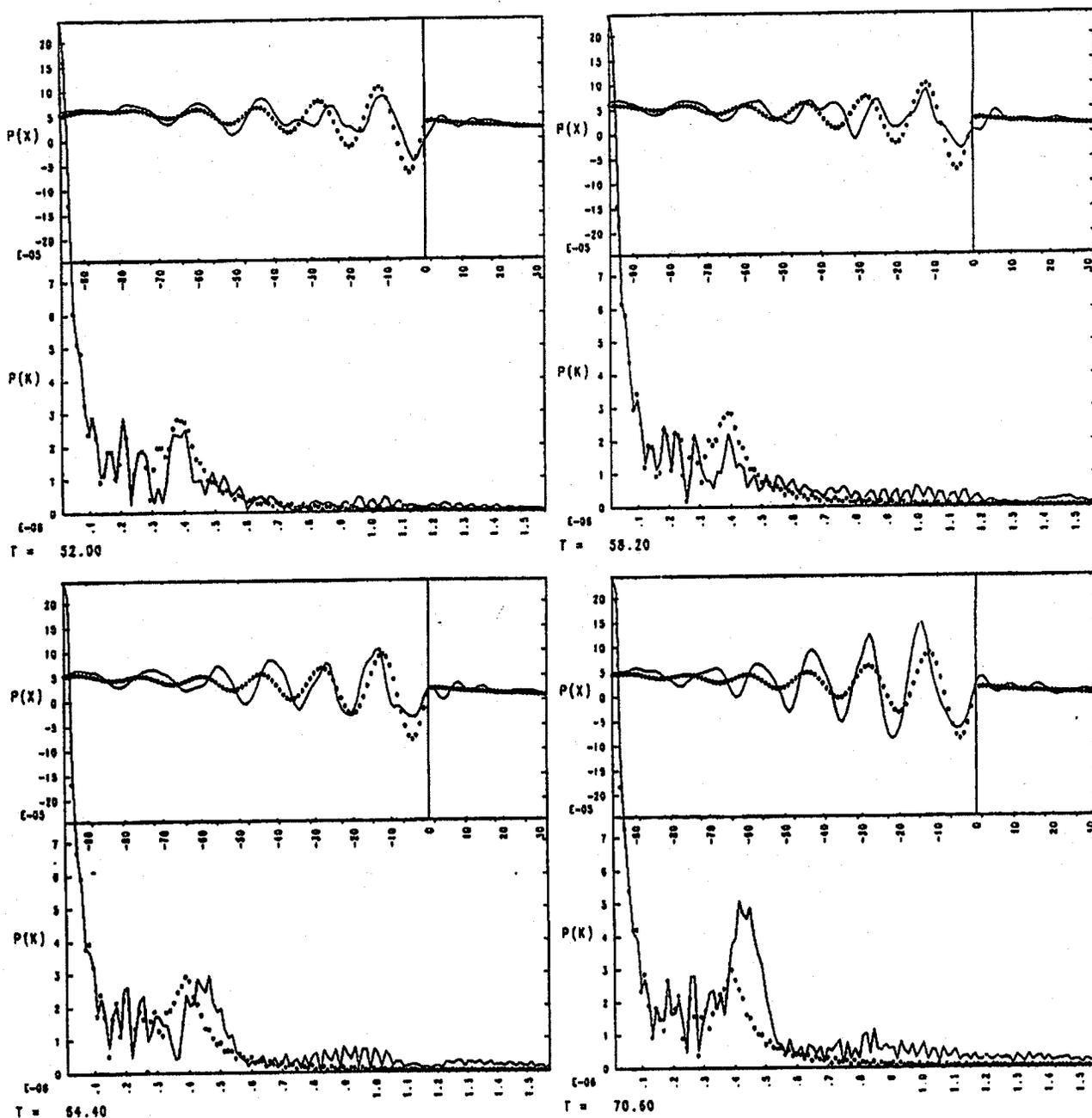


Fig. 7 Time evolution of plasma wake behind test charge moving with velocity  $v = 3v_t$ . Upper half shows potential in real space, lower half shows modulus of potential in Fourier space. Dots represent prediction of plasma theory, lines represent simulation results. High  $K$  part of spectrum is enhanced.

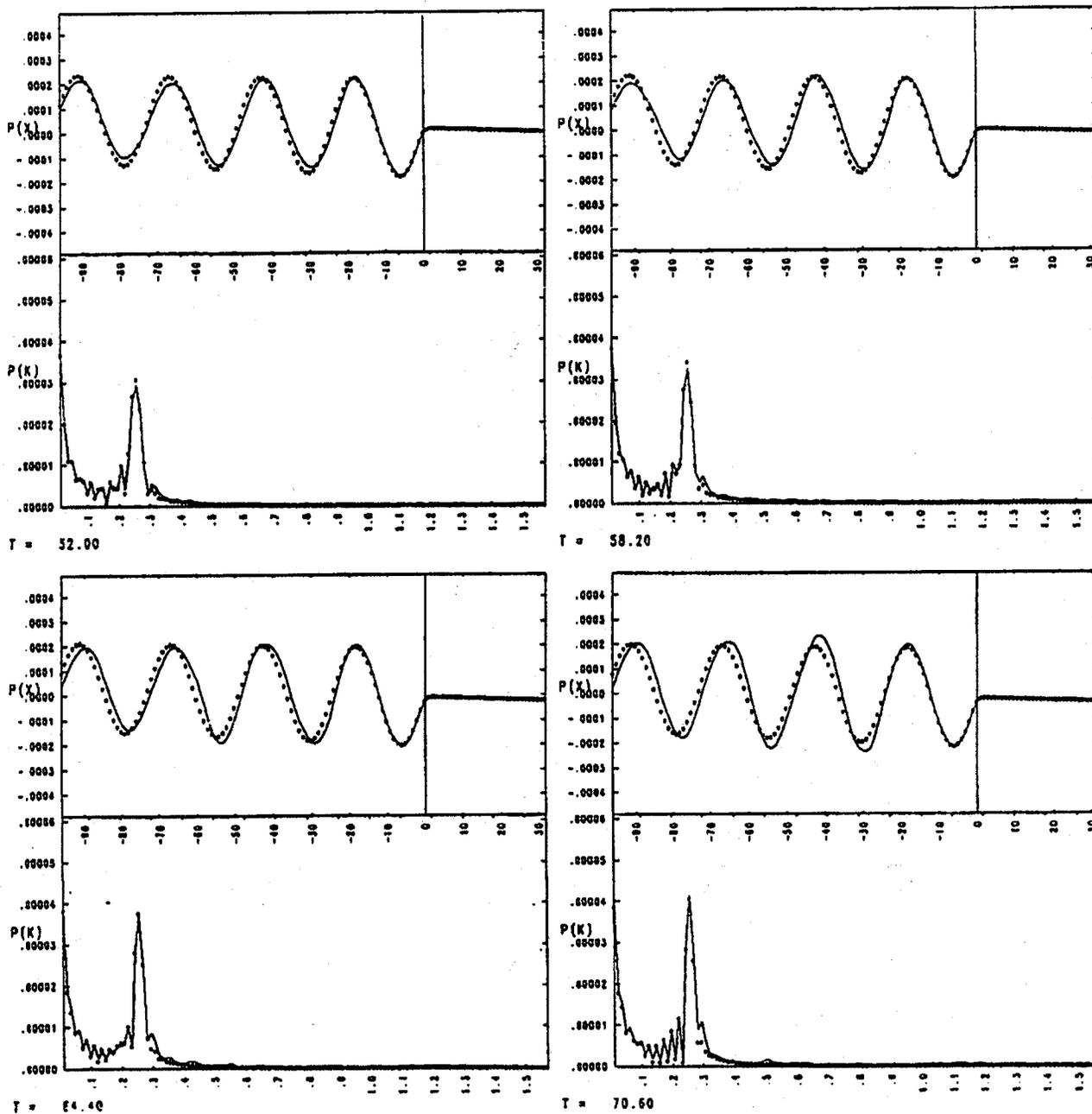


Fig. 8 Time evolution of plasma wake behind test charge moving with velocity  $v = 4.2v_t$ . Upper half shows potential in real space, lower half shows modulus of potential in Fourier space. Dots represent prediction of plasma theory, lines represent simulation results. High  $K$  part of spectrum not enhanced.

and we have already started this. One can imagine using other perturbations, a test wave for example, and examine its effect on the perturbed velocity distribution or on other waves. One does not need to limit the application of this technique to small effects. This technique is, in fact, a perfect filter, in the sense that all effects which are uncorrelated with the perturbation get subtracted out. Finally, this subtraction technique provides an extremely sensitive verification tool for new particle codes. If a new code can reproduce these results, one can have great confidence in its correctness. It can also be used to understand the physical behavior of computer models where the fundamental physical behavior is obscured by the mathematical approximations used, such as in some recent long time step (implicit) particle codes.

Acknowledgments

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