Ewald sums for one dimension

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We derive analytic solutions for the potential and field in a one-dimensional system of masses or charges with periodic boundary conditions, in other words, Ewald sums for one dimension. We also provide a set of tools for exploring the system evolution and show that it is possible to construct an efficient algorithm for carrying out simulations. In the cosmological setting we show that two approaches for satisfying periodic boundary conditions—one overly specified and the other completely general—provide a nearly identical clustering evolution until the number of clusters becomes small, at which time the influence of any size-dependent boundary cannot be ignored. Finally, we compare the results with other recent work with the hope to provide clarification over differences these issues have induced.

I. INTRODUCTION

One-dimensional models play an important role in physics. While they are of intrinsic interest, they also provide important insights into higher-dimensional systems. One-dimensional plasma and gravitational systems were the first *N*-body systems simulated with early computers [1–4]. Plasma systems were used to investigate the Debye screening and thermodynamic equilibrium. In contrast, although the force law is similar, it was found that the evolution of gravitational systems toward equilibrium is extremely slow and still is not completely explained [5–9]. Recently, spin-offs of these models that, in some cases, are more amenable to computer simulation have been studied in great depth [10,11]. Three-dimensional dynamical simulations are an important component of modern cosmology. Starting from the precise initial conditions provided by observations of the cosmic background radiation [12], various model predictions can be compared with what we observe in "today's universe" [13]. It was shown by Rouet *et al.* that, in common with the observed positions of galaxies, a cosmological version of the one-dimensional gravitational system exhibits hierarchical clustering and fractal-like behavior [14,15]. Since then we, as well as others, have pursued different one-dimensional cosmological models, finding important attributes such as power-law behavior of both the density-fluctuation power spectra and two-body correlation function, in addition to the influence of dark energy [16–21]. In specific applications, for both plasma and gravity, it is preferable to adopt periodic boundary conditions because they avoid special treatment of the boundary and therefore best mimic a segment of the extended system [13,22–24]. However, since they act as a low-pass filter, no information supported on wavelengths larger than the system size is available. Therefore, in the context of plasma and gravitational systems, as well as in the Vlasov

limit [25], it is necessary to have a sufficiently large system that contains many Jeans' (or Debye) lengths [26].

In both plasma and gravitational physics, a large class of one-dimensional models is defined by a potential energy that satisfies Poisson's equation. In three dimensions they are represented by embedded systems of parallel sheets of mass or electric charge that are of infinite extent. From Gauss' law, the field from such an element is directed perpendicular to the surface and has a constant value, independent of the distance, and proportional to the mass or charge density (per unit area). In a linear array of sheets of equal mass or charge density, the force on a given sheet is then simply proportional to the difference between the number of sheets on the left and right. Problems with this formulation arise in specific applications where it is necessary to assume periodic boundary conditions, where the motion takes place on a torus. A particular case arises in constructing a 1+1-dimensional model of the expanding universe. In the cosmological setting, astrophysicists consider a segment of the universe that is following the average expansion rate. They assume that it is large enough to contain many clusters, but small enough that Newtonian dynamics is adequate to describe the evolution [27]. Comoving coordinates, in which the average density remains fixed, are employed, and it is assumed that the system obeys periodic boundary conditions [22,23]. In comoving coordinates fictitious forces appear, analogous to the Coriolis force in a rotating system. The source of the apparent gravitational field arises from the difference between the actual matter distribution and a negative background density. To compute the force on a particle in three-dimensional systems it is possible to carry out "Ewald" sums over the positions of all the other particles in both the system and all its periodic "replicas" [24,28]. In one dimension, because the field induced by a particle (mass or charge sheet) is constant, the solution is not obvious. At first glance it appears that the force is due to the difference between infinities and, at second glance, in the cosmological setting, that the negative background should exactly cancel with the force due to the particles in each replica. Thus, the problem

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is fraught with ambiguity. To get a different twist, consider the fact that, in a periodic system, we are describing motion on a torus, so that there is no clear distinction between left and right. In order to provide conclusive solutions to these problems, in the following pages we will follow the approach used by Kiessling in showing that the "so-called" Jeans swindle is, in fact, legitimate and not a swindle at all [29]. For clarity we will focus on the gravitational example.

II. PERIODIC BOUNDARY CONDITIONS

Let $\rho(x)$ be a periodic mass density (mass density per unit length) of the one-dimensional system with period $2L$ so that $\varrho(x+2L)=\rho(x)$. In addition write $\rho(x)=\rho_0+\sigma(x)$, where ϱ_0 represents the average of $\rho(x)$ over one period and $\sigma(x)$ is the periodic fluctuation. If, instead, the total mass was bounded, we could compute the potential in the usual way. The potential function for a unit mass located at x' is simply $2\pi G|x-x'|$ so we would normally write

$$\Phi(x) = 2\pi G \int |x-x'|\rho(x')dx', \qquad (1)$$

where the integration is over the whole line. Clearly, in the present situation, this will not converge. Following Kiessling [29] we introduce the screening function $\exp(-\kappa|x-x'|)$ and define Ψ by

$$\Psi(x,\kappa) = 2\pi G \int |x-x'|\exp(-\kappa|x-x'|)\rho(x')dx'. \qquad (2)$$

For mass densities of physical interest, for example, for both bounded functions as well as delta functions, Ψ clearly exists in the current case as long as $\kappa>0$. The contribution from the average, or background, term is quickly determined,

$$\Psi_0 = 2\pi G\left(-\frac{\partial}{\partial\kappa}\right)\int \exp(-\kappa|x-x'|)\rho_0 dx' = 4\pi G\rho_0/\kappa^2, \qquad (3)$$

and is independent of position. Therefore, although it blows up in the limit $\kappa\to0$, since ρ_0 is translation invariant, Ψ_0 makes no contribution to the gravitational field. On the other hand, we can formulate the contribution to Ψ from $\sigma(x)$, say Ψ_σ, and show that it is well behaved in this limit.

A. Fourier representation of the potential and field

Since the density fluctuation σ is a mass-neutral periodic function, we may represent $\sigma(x)$ as a Fourier series,

$$\sigma(x) = \sum_n{}' c_n \exp(i\pi nx/L), \qquad (4)$$

where the prime indicates that there is no contribution from $n=0$. Inserting into Eq. (2) we find

$$\Psi_\sigma(x,\kappa) = 2\pi G \sum_n{}' c_n b_n \exp(i\pi nx/L), \qquad (5)$$

where

$$b_n = \int |x-x'|\exp(-\kappa|x-x'|)\exp[in\pi(x'-x)/L]dx'$$

$$= \int |u|\exp(-\kappa|u|)\exp[(in\pi u)/L]du$$

$$= \int |u|\exp(-\kappa|u|)\cos(n\pi u/L)du$$

$$= 2\int_0^\infty u\exp(-\kappa u)\cos(n\pi u/L)du = 2\frac{\kappa^2-(\pi n/L)^2}{[\kappa^2+(\pi n/L)^2]^2}.$$

Now, taking the limit $\kappa\to0$, we find a general expression for the periodic potential $\phi(x)$,

$$\phi(x) = -4\pi G\sum_n{}' c_n(L/\pi n)^2\exp(i\pi nx/L) \qquad (6)$$

and for the gravitational field $E(x)$,

$$E(x) = -\frac{\partial\phi}{\partial x} = 4\pi Gi\sum_n{}' c_n(L/\pi n)\exp(i\pi nx/L). \qquad (7)$$

Thus, for a periodic distribution of mass, the gravitational field is well defined. We can think of it as arising from both the mass in the primitive cell ($-L<x<L$) and the contribution from the infinite set of replicas or images. We see immediately that it is a solution of the Poisson equation, from which the result can also be obtained more directly from linear independence. For the sake of comparison, it is worth calculating the field contributed by the primitive cell alone. This is simply proportional to the difference in the mass on the right and left of the position x,

$$E_p(x) = 2\pi G\int_{-L}^L \sigma(x')[\Theta(x'-x)-\Theta(x-x')], \qquad (8)$$

where Θ is the usual step function. Substituting for $\sigma(x)$ we find

$$E_p(x) = 4\pi Gi\sum_n{}' c_n(L/\pi n)[\exp(i\pi nx/L)-(-1)^n]. \qquad (9)$$

While $E_p(x)$ and $E(x)$ are very similar, there is an important difference: the former is forced to vanish at the end points, $x=\pm L$, for all allowed mass distributions within the primitive cell. This result is expected since we only take into account the field of a neutral slice. Therefore, in the general case, $E_p(x)$ cannot represent the field on a circle (one torus).

So far, our treatment is quite general and applies to any one-dimensional periodic mass (or charge) distribution. To gain further insight and make contact with recent work, let us focus on the situation where the sources are $2N$ discrete equal-mass points (sheets) with positions x_j that live on the torus with the coordinate boundary points at $x=L$ and $-L$ identified. Then, in the primitive cell, the density fluctuation is

$$\sigma_p(x) = m\sum_{j=1}^{2N}\left[\delta(x-x_j)-\frac{1}{2L}\right], \qquad (10)$$

from which we may easily calculate the Fourier coefficients,

$$c_n = \frac{1}{2L} \int_{-L}^{L} \exp(-i\pi n x'/L) \sigma_p(x') dx'$$

$$= \frac{m}{2L} \sum_{j=1}^{2N} \exp(-i\pi n x_j/L), \qquad (11)$$

for $n \neq 0$. Then the gravitational potential and field consist of the contribution from the primitive cell and all the replicas. From Eqs. (6) and (7) they reduce to

$$\phi(x) = -4\pi m G L \sum_{j=1}^{2N} \sum_{n=1}^{\infty} (1/\pi n)^2 \cos[\pi n(x - x_j)/L], \qquad (12)$$

$$E(x) = -\frac{\partial \phi}{\partial x} = -4mG \sum_{j=1}^{2N} \sum_{n=1}^{\infty} (1/n) \sin[\pi n(x - x_j)/L]. \qquad (13)$$

Thus, the Fourier representations of the periodic potential and field are straightforward.

B. Direct summation over replicas

In the case of three dimensions one cannot do much better than Eqs. (12) and (13) since the Ewald sums cannot be represented as simple analytic functions [28]. Fortunately, in the present case, we can improve on this situation. Consider a single particle of mass m located at x_1. By summing over replicas, we can compute its contribution to the screened potential $\Psi(x, \kappa)$ directly,

$$\Psi(x, \kappa) = 2\pi m G \sum_{r=-\infty}^{\infty} |x - x_1 - 2rL| \exp(-\kappa|x - x_1 - 2rL|) \qquad (14)$$

$$= 2\pi m G \left(-\frac{\partial}{\partial \kappa}\right) \sum_{r=-\infty}^{\infty} \exp(-\kappa|y_1 - 2rL|), \qquad (15)$$

$$= 2\pi m G \left(-\frac{\partial}{\partial \kappa}\right) \sum_{r=-\infty}^{\infty} \{\exp[-\kappa(y_1 - 2rL)]\Theta(y_1 - 2rL) + \exp[\kappa(y_1 - 2rL)]\Theta(-y_1 + 2rL)\}, \qquad (16)$$

where $y_1 = x - x_1$. Choose integers $r_<(y_1)$ and $r_>(y_1)$ such that $r_< \leq y_1/2L \leq r_> = r_< + 1$, i.e., $y_1/2L$ is bounded from below and above by this pair of adjacent integers. Then,

$$\sum_{r=-\infty}^{\infty} \exp[-\kappa(y_1 - 2rL)]\Theta(y_1 - 2rL)$$

$$= \exp[-\kappa(y_1 - 2r_< L)] \sum_{s=-\infty}^{0} \exp(\kappa 2Ls) \qquad (17)$$

and similarly for the second sum in Eq. (16). Therefore, each of the sums in Eq. (16) can be evaluated in terms of a geometric series to obtain the screened potential

$$\Psi_\sigma(x, \kappa) = 2\pi m G \left(-\frac{\partial}{\partial \kappa}\right) \{[\exp(-\kappa Y_<) + \exp(+\kappa Y_>)]/[1 - \exp(-2\kappa L)] - 1/\kappa L\}, \qquad (18)$$

where $Y_< = y_1 - 2r_< L$, etc., and we have subtracted the contribution from the average or background density, $m/2L$. Evaluating the derivative and then taking the limit $\kappa \to 0$, we obtain the gravitational potential ϕ_1 due to a single particle at x_1,

$$\phi_1(x) = -\frac{\pi m G}{2L}(Y_>^2 + Y_<^2). \qquad (19)$$

It is important to recognize that $\phi_1(x)$ is a periodic function of its argument and can be evaluated anywhere on the periodic extension of the torus, i.e., on the real line. As physicists we are typically interested in values of x and x_1 in the primitive cell, i.e., for $-L \leq x, x_1 < L$ with the points at $x = \pm L$ identified. Then we quickly find that for $y_1 \geq 0$, $0 \leq y_1/2L < 1$, whereas for $y_1 < 0$, $y_1/2L$ is sandwiched between $[-1, 0)$. Either way, the potential ϕ_1 and therefore the field E_1 can be represented as

$$\phi_1(x) = 2\pi m G \left[|x - x_1| - \frac{1}{2L}(x - x_1)^2\right], \qquad (20)$$

$$E_1(x) = -\frac{\partial \phi_1}{\partial x} = 2\pi m G \left[\frac{1}{L}(x - x_1) + \Theta(x_1 - x) - \Theta(x - x_1)\right]. \qquad (21)$$

Thus, in addition to the direct contribution from the mass located at x_1, there is an additional quadratic term in the potential and linear term in the field. Although these contributions are simple, care must be taken in their interpretation. They are not, respectively, equal to the potential and field contributed by the component of the background located between the point of application x and the location of the source x_1 but rather twice as large.

A number of observations are in order. First of all, it is obvious that these functions reproduce exactly the Fourier series derived above for the case of a single particle. Second, in the limit $L \to \infty$, they reduce to the familiar results on the line. Third, they are strictly functions of the displacement $x - x_1$. This is important as all points on the torus are equivalent: there are no special positions or intervals. Fourth, it is not necessary to distinguish which direction the distance between the points x and x_1 is measured. Going in either direction around the torus yields the same value of ϕ_1. Fifth, defining $\Theta(0) = \frac{1}{2}$, the field vanishes at both $x = x_1$ and at $x = x_1 - L \mod(2L)$, i.e., half way around the torus. Finally, when x_1 traverses the point at L and reappears at $-L$ or vice versa, there is no change in the field at x as we would expect from the physics.

C. Symmetry-based derivation

In the above we have employed the machinery of a screening function to obtain the desired result. While it has all the right properties, it is worth asking if we could have

obtained it from a simpler route. We seek a solution of Poisson's equation for a single mass located at x_1,

$$\frac{\partial^2 \phi}{\partial x^2} = 4\pi G \sigma(x), \qquad (22)$$

where, in the primitive cell,

$$\sigma = \sigma_p(x) = m \left[\delta(x - x_1) - \left(\frac{1}{2L} \right) \right]. \qquad (23)$$

The general solution is

$$\phi(x) = 2\pi m G \left[|y_1| - \frac{1}{2L} y_1^2 + b y_1 \right], \qquad (24)$$

yielding

$$E(x) = -\frac{\partial \phi}{\partial x} = 2\pi m G \left[\frac{1}{L}(y_1) - \Theta(y_1) + \Theta(-y_1) + b \right], \qquad (25)$$

where b is an arbitrary constant, as before $y_1 = x - x_1$, and we have chosen the additive constant in the expression for ϕ such that $\phi(x=x_1)=0$. Symmetry requires that there is no preferred direction on the torus. Therefore, regardless of the location of the mass at x_1, the average of the field in $[-L,L)$ must vanish. Then we immediately obtain $b=0$ and the results given in Sec. II B. We could also have arrived at this conclusion by noting that, for the same reason, $\phi(x)$ can only depend on the distance between x and x_1. Finally, the requirement that $\phi(L)=\phi(-L)$ also demands the same conclusion. The fact that our limiting procedure, which is based on an exponential screening function, leads to a unique solution of the Poisson equation increases our confidence that the choice of a different screening function, e.g., a Gaussian, would not result in a different potential or field.

For the sake of comparison and to understand the connection with other recent work, it is worthwhile to consider $E_{1p}(x)$, the field generated solely by σ_p, the charge distribution in the primitive cell. This would be the correct field if the net contribution from each replica vanished. We quickly find

$$E_{1p}(x) = 2\pi m G \left[\frac{1}{L} x + \Theta(x_1 - x) - \Theta(x - x_1) \right]. \qquad (26)$$

Among other problems, note that it does not satisfy the symmetry requirements discussed above. We will return to this formulation in the ensuing discussion.

III. N-BODY SIMULATION

In carrying out a simulation, we need to know the field acting on each particle. Summing over all the contributions, the total field at x arising from the complete system of particles is then simply

$$E(x) = 4\pi m G \left[\frac{N}{L}(x - x_c) + \frac{1}{2}[N_R(x) - N_L(x)] \right], \qquad (27)$$

where, in Eq. (27), x_c is the center of mass of the $2N$ particles in $[-L,L)$ and $N_R(x)$, $N_L(x)$ are the number of particles to the right (left) of x counted on the segment $[-L,L)$. Since, from Eq. (21), the field from a single particle vanishes at its location, Eq. (27) gives the correct field acting on each particle, i.e., $E_j = E(x=x_j)$. The presence of the center of mass in Eq. (27) means that the instantaneous field experienced by each particle depends on the dipole moment of the system. The dependence on the center of mass is essential as it ensures that when a particle passes from $x=L$ to $x=-L$ or vice versa, there is no change in the field experienced by each particle. This was recognized as a basic problem in simulations of the one-dimensional single-component plasma some time ago (see [30] reprinted in [1]). Perhaps the correct mathematical form of the field was not known. In order to avoid discontinuous jumps in the field, a polarization charge was artificially induced at the system boundaries and was changed whenever a particle "switched sides." In this way the boundaries were seen as initially neutral reservoirs of particles. When a system particle enters one reservoir, another particle escapes from the other, so the boundaries are no longer neutral.

For systems of interest the equations of motion of the system of particles can frequently be cast in the form

$$\frac{dx_j}{dt} \equiv v_j, \quad \frac{dv_j}{dt} + \gamma v_j = E(x_j), \qquad (28)$$

where the value of the friction constant γ depends on the particular model [20,21]. In the cosmological setting the time has been rescaled to retain the simplicity of the equations of motion and increases exponentially with the comoving time coordinate [21,31]. By carefully summing over the index j we find that the velocity of the center of mass obeys the simple equation

$$\frac{dx_c}{dt} \equiv v_c, \quad \frac{dv_c}{dt} + \gamma v_c = 0. \qquad (29)$$

When a particle traverses the coordinate boundary at $x=L$ the center of mass changes discontinuously. However, the center-of-mass velocity is a smooth function of time so the first-order equation for $v_c(t)$ can be integrated immediately: $v_c(t)=v_c(0)\exp(-\gamma t)$. In particular, for the special case where the center of mass is initially at rest, its velocity maintains its initial value. On the other hand, $x_c(t)$ will change abruptly with each boundary traversal.

In carrying out a simulation it is necessary to obtain the crossing times of adjacent particles. Starting at $x=-L$, label the particles according to their order so that $x_{2N} > \cdots > x_{j+1} > x_j > \cdots > x_1$ and define $z_j = x_{j+1} - x_j$, the displacement between the adjacent particles. Then from Eqs. (27) and (28) we find that z_j obeys

$$w_j \equiv \frac{dz_j}{dt}, \quad \frac{dw_j}{dt} + \gamma w_j = 4\pi m G \left(\frac{N}{L} z_j - 1 \right) \qquad (30)$$

for $j=1,\ldots,2N-1$. To complete the ring we continue in the same sense and determine the rate of change of the displacement between x_{2N} and x_1, that is, $2L+x_1-x_{2N} \equiv z_{2N}$, and find that it too conveniently satisfies Eq. (30). Thus, by defining a positive direction or orientation on the torus, we can keep track of the all the relative positions between nearest-
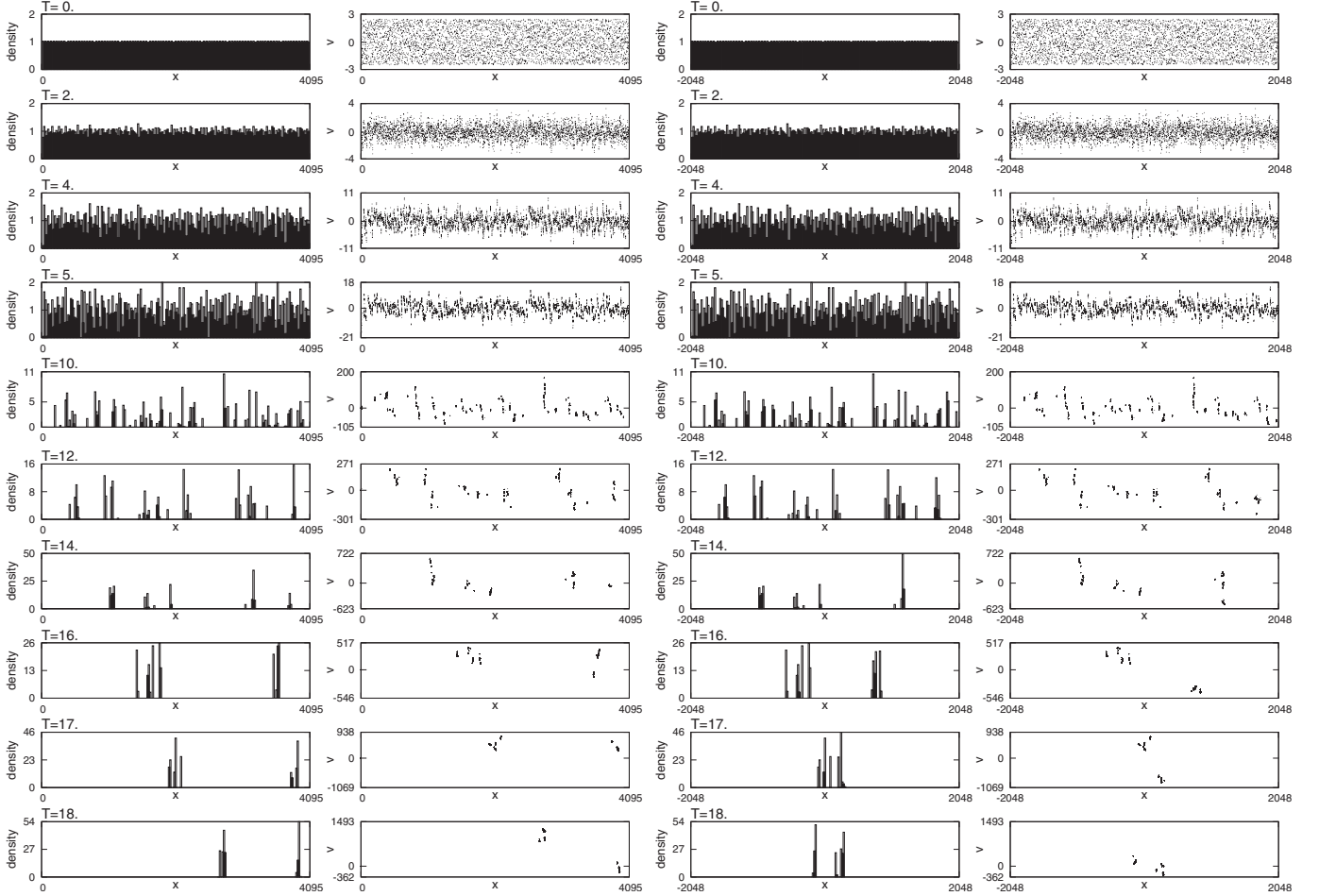
FIG. 1. Snapshots of the density and phase space at different times for a symmetric system (left) and a periodic system (right). The initial positions and velocities of all particles are the same for both simulations.

neighbor particle pairs subject to the constraints

$$\sum_{1}^{2N} z_j = 2L, \quad \sum_{1}^{2N} w_j = 0. \tag{31}$$

Since from Eq. (29) we already know the velocity of the center of mass v_c, we can invert the set $\{w_j\}$ and v_c to obtain the particle velocities v_j at any time using a matrix inversion given by Rybicki [32]. Conceptually, since the particles have equal mass, except for labels, they appear to experience elastic collisions with their neighbors. When the positions of a pair of particles cross, the particles exchange accelerations, but the velocities are continuous. At such an event the labels of the particle pair are exchanged to maintain the ordering in the given direction. As time progresses we see that, for this completely ordered system, when $z_j=0$, i.e., when the jth and $(j+1)$st particles cross, w_j changes sign. Moreover, since the particle labels have been exchanged, the velocities of the two neighboring pairs, z_{j-1} and z_{j+1}, also change discontinuously, i.e., $w_{j-1} \rightarrow w_{j-1}+w_j$ and $w_{j+1} \rightarrow w_{j+1}+w_j$ at the crossing time. This is all the information required to carry out a simulation. While we have focused on the gravitational system of equal masses, it is straightforward to extend the approach to

the case of unequal masses, as well as to the single and two-component plasmas.

In Fig. 1, we present a series of snapshots from two recent simulations of a one-dimensional model of the expanding universe in comoving coordinates in which only gravitational forces apply. The model used was the one introduced originally by Rouet *et al.* [14,15], i.e., Eq. (28) with $\gamma = \frac{1}{\sqrt{2}}$. Each simulation employs $2^{12}-1$ particles, and identical initial conditions were drawn from a uniform waterbag configuration in the μ space. The dimensionless, scaled, unit of time is expressed in terms of Jeans' period and the dimensionless length is simply the number of particles [20,21]. It is important to keep in mind that the scaled time is an exponentially increasing function of the comoving time coordinate [21,31]. The left sequence shows the evolution under the symmetric version of the system as it was originally employed (see the discussion below), while the sequence on the right exhibits the evolution obtained with Eq. (27). In each sequence, the left-hand column represents a histogram of positions, while the right-hand column shows the positions in the position-velocity plane, i.e., what statistical physicists call μ space and astrophysicists call phase space.

We observe an initial shrinkage in the phase plane due to the friction constant, followed by the breakup of the system into many small clusters that results from the intrinsic gravi-
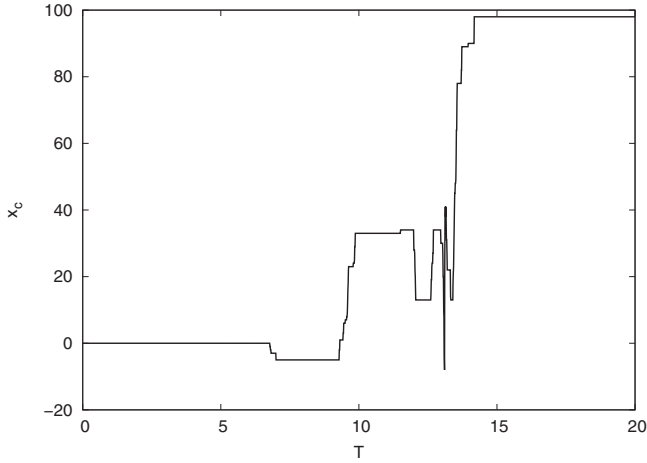
FIG. 2. Time evolution of the center of mass for a simulation containing 255 particles. Each time a particle crosses the coordinate system boundary there is a corresponding variation of unity.

tational instability [26]. As time progresses, in each case we observe the continual self-similar creation of larger clusters from smaller ones. Comparing the two snapshot sequences, we see that initially, and for some time, they are virtually identical. Before $T=10$ there is no discernable difference between the two runs in the location of cluster positions in the phase plane. Then, at $T \simeq 10$, we do notice a minute difference between them. Even at $T=12$ they are remarkably similar. Finally, at $T \simeq 14$, we observe a noticeable difference between the runs: in the first sequence the few remaining clusters are slowly gathering toward the right-hand coordinate boundary, whereas in the second, they remain evenly dispersed throughout the system. This occurs because there is a natural bias in the original implementation of the model. By forcing the system to be symmetric, the motion effectively takes place in a fixed external potential proportional to $-x^2$ (as explained below, for the symmetric system there is a "ghost" system of particles for $x<0$ that we do not display). Consequently, as the system loses "energy," matter naturally gathers near the right-hand coordinate boundary in the neighborhood of the potential minimum. In the second simulation the potential is translation invariant on the torus so there are no favored locations and the clusters remain uniformly dispersed. Notice that by the time we can see any significant differences, there are only about five clusters in the system so the boundaries are starting to play a role in the evolution. Thus, the simulation is no longer representative of the larger system. At earlier times, while the number of clusters was large, as we would intuitively anticipate, the boundaries had little effect. To illustrate the working of the algorithm, in Fig. 2 we plot the position of the center of mass for a small system (255 particles). We can see how x_c shifts in time. There are periods of little change, as well as periods of significant change, when a cluster or group encounters a coordinate boundary.

IV. DISCUSSION AND CONCLUSIONS

There is a long history of work on one-dimensional plasma models, both theoretical and computational, dating

back to the 1960s [1,2]. Some papers explicitly discuss the case of periodic boundary conditions. As we pointed out earlier, in simulations of the single-component plasma, Eldridge and Feix employed a polarization field at the boundaries to control the discontinuities in the electric field [30]. In a review paper Kunz gave an analytical expression for the potential, but there is no derivation [33]. Periodic boundary conditions are required for cosmological simulations [22–24]. The first one-dimensional cosmological simulations were carried out by Rouet *et al.* [14,15]. To avoid the problem of introducing a "polarization" field at the boundaries, they assumed that the system was perfectly symmetric at all times, i.e., for every particle at $x_j>0$ with velocity v_j there is an image or ghost particle at position $-x_j$ with velocity $-v_j$. When a particle reaches the coordinate boundary, the image particle is there to meet it. Thus, the $2N$-particle system is equivalent to an N-particle system with $0<x<L$ with reflecting boundaries. Notice that this construction forces the center-of-mass position and velocity to vanish, simplifying the equations of motion [see Eq. (27)].

In other one-dimensional simulations, Aurell *et al.* employed open boundaries [34,35]. In their studies an initially localized fluctuation interpenetrates a quiescent region. The field they employed is essentially given by Eq. (26). Yano and Gouda [17], as well as Tatekawa and Maeda [16], employed the Zeldovich approximation [26]. Details concerning the type of boundary conditions employed were not discussed in these works but, in contrast with Eq. (27) above, the Zeldovich approximation, as normally derived, does not depend on the system center of mass. Gabrielli *et al.* studied the behavior of an infinite system of sheets perturbed from lattice positions [19]. They also employed the screening function introduced by Kiessling to obtain an analytical expression for the field so, in spirit, their work is closely related to ours. However, there is a surprising difference in the expression they obtained for the gravitational field for the case of periodic boundary conditions, which is also given by Eq. (26). Since it lacks the explicit dependence on x_c, it is not translation invariant on the torus and there is a discontinuity in the field when a particle passes through a coordinate boundary at $x= \pm L$. Consequently, it does not represent true motion on a torus. While it is tempting to contemplate that the reintroduction of particles that leave from $x=L$ at $x=-L$ and vice versa is adequate to guarantee periodic boundary conditions, this is not the case. An additional difficulty is that the field they present is self-referential, i.e., since $E_{1p}(x=x_1) \neq 0$ [see Eq. (26)], the field generated by a single particle will induce an acceleration of itself.

In conclusion, we have derived analytic solutions for the potential and field in a one-dimensional system of masses or charges with periodic boundary conditions, i.e., the Ewald sums for one dimension. We have seen that each particle in such a system carries with it its own neutralizing background, without which the potential energy cannot be defined. For a system of particles, we have shown that the system polarization or the center of mass must be explicitly included in the force law. We have also provided a set of tools for exploring the system evolution and have shown that it is possible to construct an efficient algorithm for accomplishing this. In the cosmological setting we have shown that

the difference between the choice of completely symmetric and just periodic boundary conditions plays an insignificant role in the evolution until the number of clusters becomes small, at which time the influence of any boundary condition will become important. In subsequent work we will explore other settings where boundaries play a more prominent role.

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