THE ASTROPHYSICAL JOURNAL, 416:L71–L74, 1993 October 20

USING THE SCHRÖDINGER EQUATION TO SIMULATE COLLISIONLESS MATTER

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Received 1993 May 26; accepted 1993 August 3

ABSTRACT

A new numerical technique for following the evolution of collisionless matter under the influence of gravity is proposed. Matter is modeled as a Schrödinger field obeying the coupled Schrödinger and Poisson equations. The de Broglie wavelength, $\lambda_{\rm deB}$, associated with this field enters as a free parameter and is tuned according to the specifications of the simulation one is doing. In the limit $\lambda_{\rm deB} \to 0$ (a limit which would require infinite computing power) the equations reduce to the coupled Vlasov and Poisson equations as they should. Our method can handle multiple streams in phase space and is competitive in terms of computation time with particle-mesh N-body simulations. Results from a simple one-dimensional collapse of a self-gravitating object as well as a two-dimensional simulation of a cold dark matter universe are used to illustrate the viability of the technique.

Subject headings: dark matter — galaxies: kinematics and dynamics — methods: numerical

1. INTRODUCTION

The successful theory of large-scale structure will involve knowledge of both the initial conditions at the time structure formation begins and the set of physical laws that evolves this initial data forward in time. In practice, the numerical techniques used to follow the evolution of a model universe can be just as important as the physics that goes into the model. Indeed, for many theories the physics is extremely simple. Consider, for example, the cold dark matter and hot dark matter scenarios. In either case, one assumes an Einstein-de Sitter universe with the bulk of the mass density (90%–99%) in a collisionless dark component. One also specifies the initial spectrum of density fluctuations: essentially the positions and velocities of the particles. The problem is in finding a scheme for evolving the initial conditions forward in time. Clearly it would be ridiculous to follow individual particles: if dark matter is some elementary particle of mass m, then there will be $\sim 10^{68}$ (m GeV^{-1}) particles in a single galaxy. Even if the dark matter "particles" are brown dwarfs, they will still be far too numerous to follow individually.

The problem simplifies if one models dark matter as a continuous fluid in phase space where the graininess of the particle distribution is smoothed out. This description is valid so long as the structures of interest are larger than the interparticle spacing and the timescales of interest are short compared with the two body relaxation time. Fortunately, both of these conditions are satisfied for nearly all forms of dark matter considered to date.

A collisionless fluid obeys the Vlasov equation or collisionless Boltzmann equation:

$$\frac{\partial f}{\partial t} = \sum_{i=1}^{3} \left(\frac{\partial V}{\partial x^i} \frac{\partial f}{\partial v_i} - v_i \frac{\partial f}{\partial x_i} \right) \tag{1}$$

(Binney & Tremaine 1987). $f(\boldsymbol{x}, \boldsymbol{v}) d^3x d^3v$ is the number of particles in the six-dimensional phase-space volume element $d^3x d^3v$ centered on the point $(\boldsymbol{x}, \boldsymbol{v})$, and $V = V(\boldsymbol{x})$ is the gravitational potential. Three approaches exist for solving this equation: "phase-space methods" which evolve the (smooth) distribution function directly in phase space (White 1981; Fujiwara 1981); N-body (or particle) simulations in which N fictitious superparticles are used to provide a statistical description of the distribution function (Hockney & Eastwood 1988); and fluid methods in which the first few moments of the collisionless Boltzmann equation (typically mass conservation and Euler equations) are solved using standard techniques for numerical hydrodynamics (Peebles 1987).

Each of these techniques has advantages and disadvantages. In N-body techniques, which are by far the most popular in astrophysics and cosmology, N "superparticles" are chosen with random positions and velocities taken from the initial distribution function, thereby providing a statistical coverage of the distribution function. The particles are then evolved according to Newton's Law, and their final positions and velocities are used to approximate the final distribution function.

Phase-space methods work directly with the distribution function $f(\boldsymbol{x}, \boldsymbol{v})$. In addition, by describing dark matter as a continuous field (which for all intents and purposes it is!) they avoid two-body relaxation effects which can limit N-body simulations. Phase-space methods have seen very limited success, in part because of the large number of dimensions in phase space and in part because distribution functions in general develop fine-grained structures which are difficult to follow numerically. (See Rasio, Shapiro, & Teukolsky 1989 for a discussion of phase-space methods and their limitations.)

Peebles (1987) has used a pressureless fluid model to study the growth of nonlinear density perturbations in an expanding universe. The mass conservation and Euler equations for the density and velocity fields are evolved numerically and compared with analytic and numerical N-body results. As with

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phase-space methods, matter is treated as a continuous field. The model can describe cold collisionless matter where the velocity dispersion of the particles is negligible and where there are only single streams in phase space. However, since the velocity field is single-valued, the model is unable to handle "hot" systems where there is a nonnegligible velocity dispersion. In addition, the method fails as soon as orbit crossing (multistreaming) occurs.

Our goal here is to find a model for collisionless matter that (1) describes matter as a field rather than particles, (2) is a function only of the three spatial coordinates and time, (3) can follow multiple streams in phase space as well as hot collisionless matter, and (4) is competitive with N-body techniques in terms of computation time.

Our approach is to describe collisionless matter as a Schrödinger field $\psi(\boldsymbol{x}, t)$ obeying the coupled Schrödinger and Poisson equations:

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + mV(\boldsymbol{r})\psi \quad \nabla^2 V = 4\pi G \psi\psi^* , \qquad (2)$$

where ψ has units of $(\text{density})^{1/2}$ and should be thought of as a classical field rather than the wavefunction for a single particle as in quantum mechanics. (We set $c = 1$ but keep factors of $\hbar$.)

The validity of this approach, which will be established in detail below, follows from the equivalence between the classical mechanics of point particles and wave mechanics in the geometric optics limit, with the squared modulus of ψ corresponding to the density of matter. An interesting difference between this and the more standard approaches is that here $\psi(\boldsymbol{x}, t)$ encodes both position and momentum information in a single position-space function. Phase-space information can be extracted from $\psi(\boldsymbol{x}, t)$ by constructing a "Schrödinger" distribution function, $\mathscr{F}(\boldsymbol{x}, \boldsymbol{p}, t)$. To compute $\mathscr{F}(\boldsymbol{x}, \boldsymbol{p}, t)$ we multiply ψ by a window function of width η centered on $\boldsymbol{x}$, take the Fourier transform, and then square the result. Below we show that the Schrödinger distribution function obeys an equation approximately equal to the Vlasov equation provided that $\lambda_{\rm deB} \ll \eta \ll L$, where L is the typical spatial scale of interest, $\lambda_{\rm deB} \equiv \hbar/mv$ is the "de Broglie wavelength," and the typical "velocity" of the field is $v \sim |\nabla\psi/(\partial\psi/\partial t)|$. Finally, we require $\lambda_{\rm deB} \gtrsim d$, where d is the grid spacing for the simulation.

A limit on the accuracy with which one can follow the evolution of collisionless matter is given by the resolution in phase space, $(\Delta x\, \Delta v)^3$. Consider a virialized system of size L with velocity dispersion σ. In a Schrödinger code, the spatial resolution is $\Delta x \sim \eta$, while the resolution in velocity space is $\Delta v \sim \sigma d/\eta$. The resolution in phase space is then $(\Delta x\, \Delta v)^3 \sim \sigma^3 L^3/N_G$, where $N_G = (L/d)^3$ is the number of grid points in the simulation.

For a phase-space code the resolution in position space is $\Delta x \sim L/N_p$, where N_p is the number of grid points for a given direction in position space. Likewise, $\Delta v \sim \sigma/N_v$, where N_v is the number of grid points for a given direction in velocity space. $N_G = N_p^3 N_v^3$, and we see that phase-space methods will have roughly the same accuracy for a fixed number of total grid points. Similarly, in an N-body simulation, the expected resolution in phase space is $(\Delta x\, \Delta v)^3 \sim \sigma^2 L^3/N$, where N is the number of particles used in the simulation. In particle-mesh (PM) codes, the lattice used to calculate forces has N gridpoints, and again $(\Delta x\, \Delta v)^3 \sim \sigma^3 L^3/N$. Thus, in each case, the resolution for a given number of particles or grid points is the same.

Another important consideration is the timestep required for accurate integration of the equations of motion. In the Schrödinger method, the timestep will be $\Delta t \sim \psi/\dot{\psi} \sim m\hbar/p^2 \sim \lambda_{\rm deB}/v$, which is just the time for a particle of velocity v to cross a spatial resolution element, so again we would expect the necessary timestep to be similar for PM and Schrödinger methods. Though PM and Schrödinger methods provide roughly the same resolution in phase space for a fixed amount of computer power, the two methods are based on entirely different assumptions and are therefore subject to different systematic errors.

2. MOTIVATION AND JUSTIFICATION

There are a number of ways to motivate the Schrödinger model, the most concrete of which will be discussed below. A more heuristic approach though comes from first considering a coherent scalar field, such as axion, as a potential dark matter candidate. Axions provide a curious example of dark matter. They are extremely light (the favored axion has a mass of $m_a \sim 10^{-5}$ eV) yet nonrelativistic, essentially because they are born in a zero-momentum Bose condensate. Nevertheless, axions should behave like any other dark matter candidate. However, the favored axions moving in the gravitational field of a galaxy or cluster would have a de Broglie wavelength of ~ 10 m, making it unreasonable to follow them if we are interested in galaxies and clusters. Instead, we can follow a fictitious superlight particle whose de Broglie wavelength is smaller than the scales of interest but not so small that it becomes prohibitively expensive in terms of computer time. To put things in perspective, with N-body simulations, we use too few superheavy particles, whereas here we are using too many superlight particles.

A classical scalar field obeys the coupled Klein-Gordon (K-G) and Einstein equations:

$$\nabla_\mu \nabla^\mu \phi + \left(\frac{m}{\hbar}\right)^2 \phi = 0 \quad G_{\mu\nu} = 8\pi G T_{\mu\nu} , \qquad (3)$$

where

$$T_{\mu\nu} = \partial_\mu \phi \partial_\nu \phi - \frac{1}{4} g_{\mu\nu}\left[\partial_\kappa \phi \partial^\kappa \phi - \left(\frac{m}{\hbar}\right)^2 \phi^2\right] . \qquad (4)$$

For nonrelativistic fields ($|\Delta\psi/\dot{\psi}| \ll 1$) we can write

$$\phi = \frac{\hbar}{\sqrt{2m}} (\psi e^{-imt/\hbar} + \psi^* e^{imt/\hbar}) , \qquad (5)$$

where ψ is a slowly varying function of time in the sense that $|m\psi| \gg |\hbar \partial\psi/\partial t|$. (This is an excellent approximation for dark matter axions.) For weak gravitational fields, only the Newtonian potential enters into the metric. The Schrödinger and Poisson equations follow by direct substitution where we neglect $\ddot{\psi}$ terms.

The K-G equation was originally introduced to describe a single relativistic quantum-mechanical spin-zero particle. To describe a large number of ϕ particles we should really "second-quantize" the K-G equation, which then becomes an equation for the evolution of field operators with appropriate commutation rules. However, in the limit of very large occupation numbers, the classical description of equations (3)–(5) is adequate. Likewise, the Schrödinger approach can be interpreted as a classical wave equation.

The Schrödinger approach is by no means limited to the case of spin-zero bosons. To see the validity of the model in a more general context, consider a phase-space representation of ψ. In this work we use the coherent state or Husimi representation (Husimi 1940). Let

$$\Psi(p, x, t) = \left(\frac{1}{2\pi\hbar}\right)^{1/2}\left(\frac{1}{\pi\eta^2}\right)^{1/4} \times \int e^{-(x-x')^2/2\eta^2 - ip(x'-x/2)/\hbar}\psi(x', t)dx' , \quad (6)$$

where η has units of length and roughly gives the resolution in position space. (For now, we consider one coordinate or two phase-space dimensions. The generalization to higher dimensions is straightforward.) The quantity

$$\mathscr{F}(p, x, t) \equiv |\Psi(p, x, t)|^2 \quad (7)$$

gives the density of the Schrödinger field in phase space. By direct calculation one finds that

$$\frac{\partial \mathscr{F}}{\partial t} = \sum_{i=1}^{3}\left(m\frac{\partial V}{\partial x_i}\frac{\partial \mathscr{F}}{\partial p_i} - \frac{p_i}{m}\frac{\partial \mathscr{F}}{\partial x_i}\right) + \left[O\left(\frac{\eta^2}{L^2}\right) + O\left(\frac{\hbar^2}{\eta^2 P^2}\right)\right]\frac{\partial \mathscr{F}}{\partial t} \quad (8)$$

(Skodje, Rohrs & van Buskirk 1989), where again L is the typical scale for spatial variations in the system and P is the typical momentum. Therefore, $\mathscr{F}$ obeys the collisionless Boltzmann equation so long as the last two terms on the right-hand side are small, that is, $\lambda_{\rm deB} \ll \eta \ll L$, where $\lambda_{\rm deB} \simeq \hbar/P$. Note that the extra terms on the right-hand side vanish in the limit $\hbar \to 0$ so long as the aforementioned conditions are satisfied.

3. DOING SIMULATIONS

We first describe how one constructs a wave function $\psi(x)$ corresponding to a given distribution function $f(x, p)$. (Again we focus on one spatial dimension.) Consider the Ansatz

$$\psi(x_k) = \frac{1}{\sqrt{N}}\sum_{n=0}^{N-1}\sqrt{f(x_k, p_n)}e^{ip_n x_k/\hbar}R_n , \quad (9)$$

where $p_n = 2\pi\hbar n/N\Delta$ and $x_k = k\Delta$ are grid points in a discrete phase-space lattice, N is the number of lattice points in position or momentum space, and R_n is a complex random number with $\langle |R| \rangle = 1$. We wish to show that

$$\mathscr{F}(x, p) \simeq f(x, p) , \quad (10)$$

where $\mathscr{F} = |\Psi(p, x)|^2$ and

$$\Psi(p, x) = \left(\frac{1}{2\pi\hbar}\right)^{1/2}\left(\frac{1}{\pi\eta^2}\right)^{1/4} \times \sum_{k=0}^{N-1} e^{-(x_k-x)^2/2\eta^2 - ip(x_k - x/2)/\hbar}\psi(x_k) . \quad (11)$$

The key assumption is that f is slowly varying in p and x in the sense that $|\partial f/\partial p| \ll \eta f/\hbar$ and $|\partial f/\partial x| \ll f/\eta$. These conditions allow us to take $f(p_n, x_n) = f(p, x)$. Doing the x-transform we find

$$\mathscr{F}(x, p) = \left(\frac{\eta}{\sqrt{\pi}\hbar N}\left|\sum_{n=0}^{N-1} R_n e^{ip_n x/\hbar} e^{-(p_n-p)^2\eta^2/2\hbar^2}\right|^2\right) f(p, x) . \quad (12)$$

The term in parentheses is a real random function of p and x with correlation length η in x and $\hbar/\eta$ in p and with average value 1. Therefore, f and $\mathscr{F}$ are effectively equivalent when averaged on scales greater than η in x and $\hbar/\eta$ in p. Figure 1 (Plate L3) gives the wave function $\psi(x)$ and the corresponding function $\mathscr{F}(x, p)$ for the distribution function $f(x, p) = e^{-x^2/x_0{}^2 - p^2/p_0{}^2}$.

The situation is somewhat different with cold dark matter. There, the velocity dispersion is negligible, and the distribution function is a three-dimensional surface in six-dimensional phase space. Suppose orbit crossing has not yet occurred. The distribution function can then be described by the density and momentum fields $\rho(\boldsymbol{x})$ and $\boldsymbol{p}(\boldsymbol{x})$ and the Ansatz for the wave function is

$$\psi(\boldsymbol{x}) = \sqrt{\rho(\boldsymbol{x})}\, e^{i\theta(\boldsymbol{x})/\hbar} , \quad (13)$$

where $\nabla\theta(\boldsymbol{x}) = \boldsymbol{p}(\boldsymbol{x})$. The Ansatz works so long as $\rho(\boldsymbol{x})$ and $\theta(\boldsymbol{x})$ are slowly varying functions. We can take $\rho(x') = \rho(x)$ and $\theta(x') = \theta(x) + (\boldsymbol{x}' - \boldsymbol{x})\nabla_x \theta$. Substituting into equations (6) and (7) we find

$$\mathscr{F}(\boldsymbol{x}, \boldsymbol{p}) = \frac{\eta}{\sqrt{\pi}\hbar}\, p(\boldsymbol{x})\, e^{-(\boldsymbol{p} - \hbar\nabla_x\theta)^2\eta^2/\hbar^2} . \quad (14)$$

In the limit $\hbar/\eta \to 0$, $\mathscr{F} = \rho(\boldsymbol{x})\delta(\boldsymbol{p} - \hbar\nabla\theta)$ as it should. For finite $\hbar/\eta$, $\mathscr{F}$ is proportional to a Gaussian in (p) of thickness $\hbar/\eta$.

It is convenient to write our equations in terms of the dimensionless quantities $\boldsymbol{y} = x/L$, $\tau = t/T$, and $\chi = (4\pi/\rho)^{1/2}\psi$, where L and ρ are the typical size and density of the system of interest and $T = 1/(G\rho)^{1/2}$ is roughly the timescale for collapse. The Schrödinger and Poisson equations then become

$$2i\mathscr{L}\frac{\partial \chi}{\partial \tau} = \nabla_y^2 \chi + 2\mathscr{L}^2 U(\boldsymbol{y})\chi \quad \nabla_y^2 U = \chi\chi^* , \quad (15)$$

where $\mathscr{L} \equiv mL^2/\hbar T$. $\mathscr{L}$ is roughly the ratio of the size of the system to the de Broglie wavelength and is typically $\sim N$, and y, τ, and χ are of order unity.

The Schrödinger equation is solved numerically using Cayley's Method (Goldberg, Schey, & Schwartz 1967), an implicit finite-differencing scheme. The potential field is obtained from the density field using the fast Fourier transform, just as in PM codes.

In Figure 2 (Plates L4 and L5) we give the results for a self-gravitating one-dimensional system solved by both the Schrödinger method and a simple N-body code. The initial conditions are those of a "cold" system with $\boldsymbol{v}(\boldsymbol{x}) = 0$ and $\rho(\boldsymbol{x}) = \rho \exp(-x^2/L^2)$. The length of the simulation is such that particles near the center of the distribution make two complete orbits, well within the regime where multistreaming is occurring.

4. COSMOLOGICAL SIMULATIONS

Consider now an Einstein-de Sitter universe dominated by a nonrelativistic ψ field. Since we are dealing with weak gravity and nonrelativistic fields, only the Newtonian potential (in a Robertson-Walker background) enters the field equations. We find

$$i\hbar\frac{\partial \psi}{\partial t} = -\frac{h^2}{2ma^2}\nabla^2\psi + mV(\boldsymbol{r})\psi$$

$$\nabla^2 V = \frac{4\pi G}{a}(\psi\psi^* - \langle\psi\psi^*\rangle) , \quad (16)$$

where $a(t) = (t/t_0)^{2/3}$ is the Robertson-Walker scale factor, t_0 is the current age of the universe, and we have set $a(t_0) = 1$. ψ has

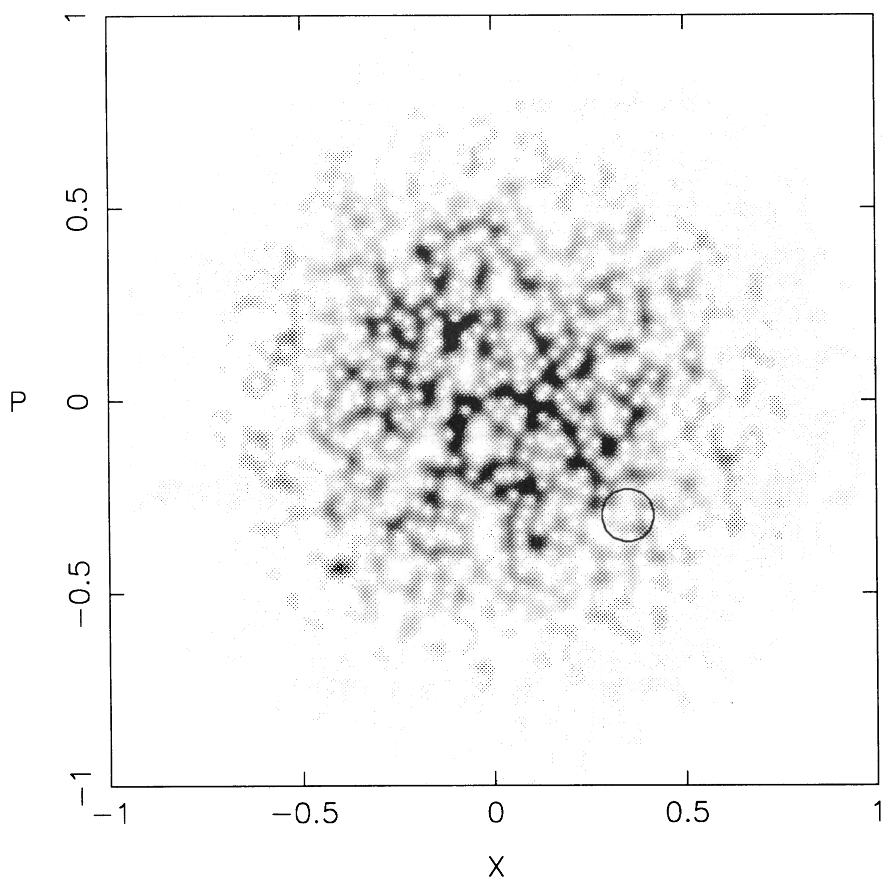

FIG. 1.—$\mathscr{F}(x, p)$ calculated from the Ansatz equation (9) using equations (6) and (7). $N = 2048$ gridpoints were used, and we have taken $\eta = (1/2\pi N)^{1/2} \simeq 0.0088$. If the distribution function were instead mapped with particles as in B-body simulations, then there would be approximately 10 particles in the circle shown on the plot.

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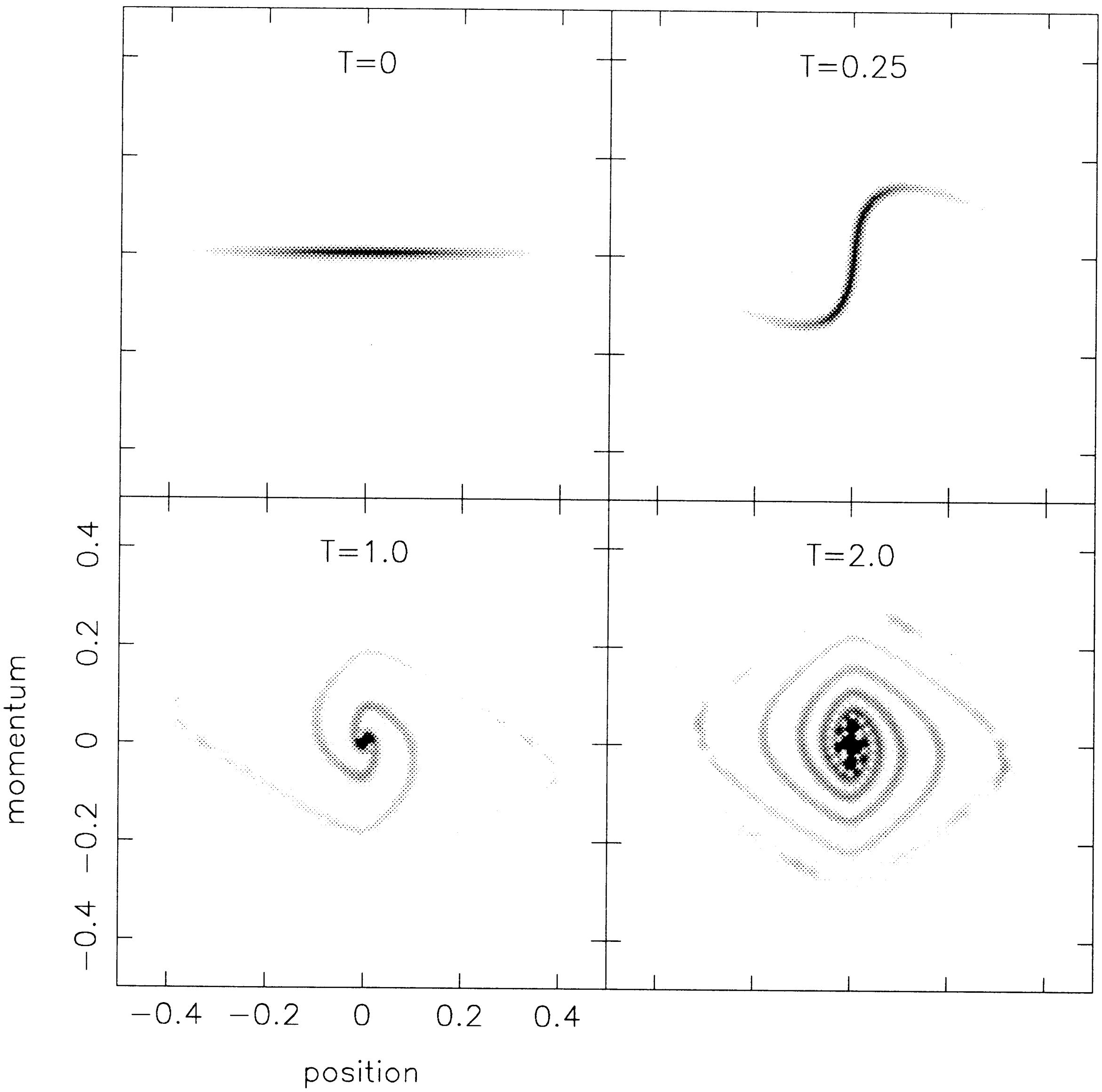

FIG. 2*a*

FIG. 2.—One-dimensional collapse using Schrödinger (*a*) and *N*-body (*b*) methods with 2048 gridpoints and 2048 particles, respectively. Each plot gives the distribution function (eq. [6] for the Schrödinger code). Time *T* is measured in units of the orbit time for particles close to the center of the distribution.

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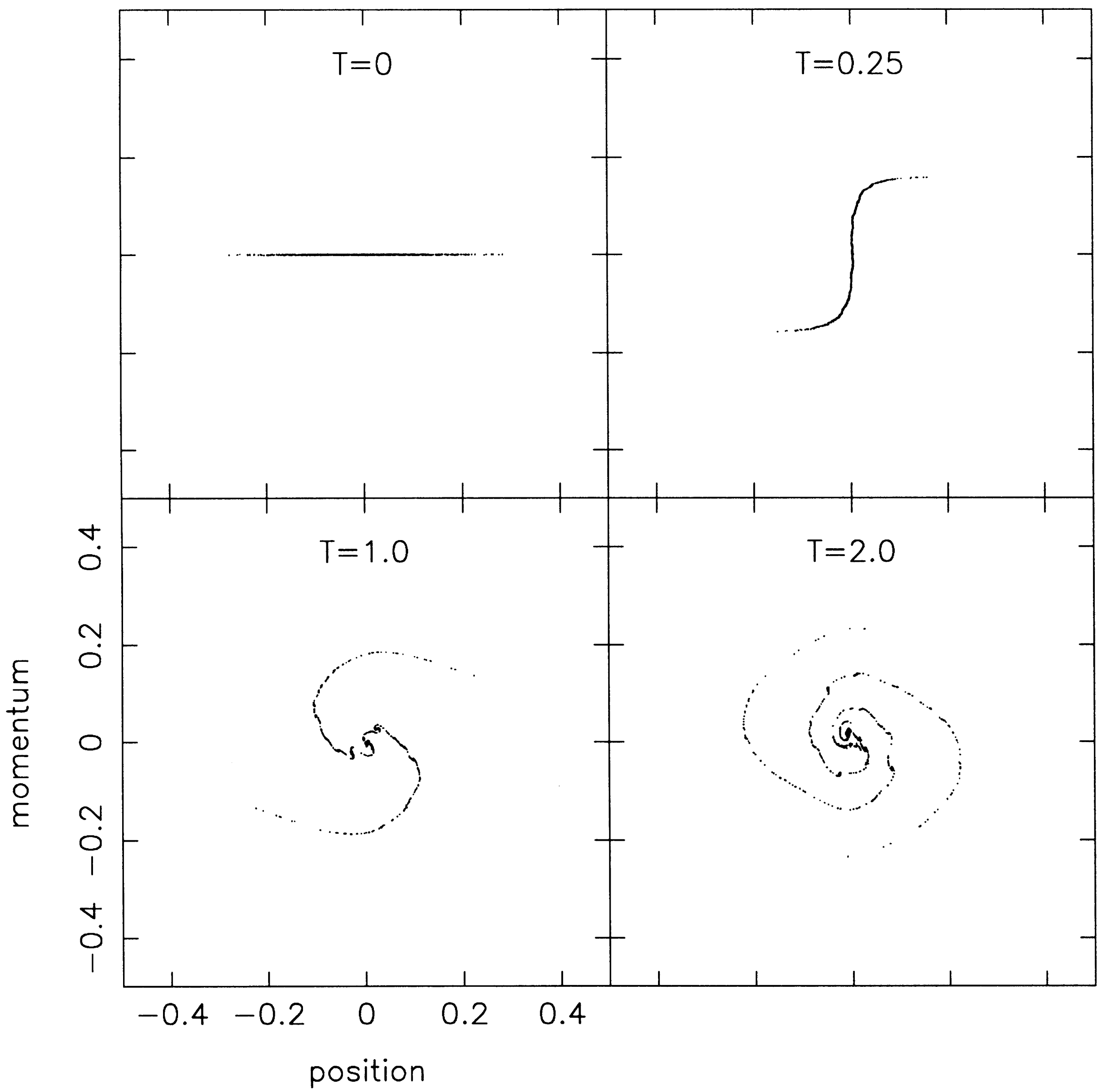

FIG. 2*b*

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been scaled by a factor $a^{-3/2}$ so that $\langle\psi\psi^*\rangle = \rho a^3 = \rho_{\rm crit}$ is the critical density. Writing equation (16) in terms of the dimensionless quantities $y = x/L$, $\chi = (6\pi G t_0^2)^{1/2}\psi$, and $U = 3t_0^2 aV/2L^2$, we find

$$i\,\frac{4\tilde{\mathscr{L}}}{3}\,\frac{\partial\chi}{\partial \ln a}\,\nabla^2 U = \chi\chi^* - 1\ , \tag{17}$$

where $\tilde{\mathscr{L}} = ma^{1/2}L^2/\hbar t_0$ and L is the comoving size of the box used for the simulation. In Figure 3 (Plate L6) we show results for a two-dimensional cold dark matter universe. Simulations using identical initial data ($a = 0.04$, $\delta\rho/\rho \simeq 0.1$) were done using the Schrödinger code discussed here and with a PM code (Kates et al. 1991). Figures 3*a* and 3*b* are for $a = 0.48$. In the Schrödinger simulation, we plot $|\psi|^2$ where in fact, if we are interest in ρ, we should be plotting $\int \mathscr{F}(x, p)dp$. We show $|\psi|^2$ to illustrate multistreaming (ripple effect along sheets). Computation time was comparable, with the Schrödinger method being slightly faster.

It is a pleasure to thank E. Bertschinger, J. R. Bond, M. Choptuik, A. Klypin, L. Kofman, W. Press, A. Stebbins, and S. Tremaine for lively and helpful discussions. Special thanks go to A. Klypin for use of his N-body code. We also thank the referee, J. Binney, for a number of useful suggestions.

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