Journal of Statistical Physics, Vol. 117, Nos. 1/2, October 2004 (© 2004)

Relaxation to a Perpetually Pulsating Equilibrium

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Received January 7, 2004; accepted April 29, 2004

Paper in honour of Freeman Dyson on the occasion of his 80th birthday. Normal N-body systems relax to equilibrium distributions in which classical kinetic energy components are $1/2kT$, but, when inter-particle forces are an inverse cubic repulsion together with a linear (simple harmonic) attraction, the system pulsates for ever. In spite of this pulsation in scale, $r(t)$, other degrees of freedom relax to an ever-changing Maxwellian distribution. With a new time, τ, defined so that $r^2\mathrm{d}/\mathrm{d}t = \mathrm{d}/\mathrm{d}\tau$ it is shown that the remaining degrees of freedom evolve with an unchanging reduced Hamiltonian. The distribution predicted by equilibrium statistical mechanics applied to the reduced Hamiltonian is an ever-pulsating Maxwellian in which the temperature pulsates like r^{-2}. Numerical simulation with 1000 particles demonstrate a rapid relaxation to this pulsating equilibrium.

KEY WORDS: N-body dynamics; limit cycles; Maxwellian equilibrium.

1. INTRODUCTION

In classical mechanics when N bodies interact with forces derived from a potential

$$V = \sum_n V_n, \tag{1}$$

where V_n is of inverse nth power in $|\mathbf{x}_i - \mathbf{x}_j|$, the Virial theorem reads

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$$\frac{1}{2}\frac{\mathrm{d}^2 I}{\mathrm{d}t^2} = 2T + \sum_n n V_n = 2E + \sum_n (n-2) V_n. \tag{2}$$

Here

$$I = \sum_i m_i |\mathbf{x}_i - \bar{\mathbf{x}}|^2 = Mr^2 = 1/2 \sum_i \sum_j M^{-1} m_i m_j |\mathbf{x}_i - \mathbf{x}_j|^2, \tag{3}$$

and indices i, j run over the particles and $\bar{\mathbf{x}} = \sum m_i \mathbf{x}_i / \sum m_i$. We notice that the term with $n = 2$ disappears from the second sum in Eq. (2). Furthermore if the simple harmonic term is $V_{-2} = 1/2\omega^2 \sum_{i<j} \sum M^{-1} m_i m_j |\mathbf{x}_i - \mathbf{x}_j|^2$ then it can be re-expressed as $\omega^2 I/2$. We now specialise to the problem in which only V_2 and V_{-2} are present, so that any two particles of separation r_{ij} repel each other as r_{ij}^{-3} and attract like r_{ij}. We consider this special problem because Eq. (2) now reads

$$\frac{1}{2}\frac{\mathrm{d}^2 I}{\mathrm{d}t^2} = 2E - 2\omega^2 I, \tag{4}$$

so I vibrates harmonically about the value E/ω^2. If this excitation is present initially it will continue vibrating at the same amplitude for ever, despite the complication of the r_{ij}^{-3} repulsions of the particles. Multiplying Eq. (4) by $\mathrm{d}I/\mathrm{d}t$ and integrating,

$$\frac{1}{4}\left(\frac{\mathrm{d}I}{\mathrm{d}t}\right)^2 = 2EI - \omega^2 I^2 - M^2 \mathcal{L}^2, \tag{5}$$

where the last term is the integration constant. Using $I = Mr^2$ this becomes

$$1/2(\dot{r}^2 + \mathcal{L}^2 r^{-2} + \omega^2 r^2)M = E, \tag{6}$$

which may be compared with the energy of a particle of mass M orbiting with specific angular momentum $\mathcal{L}$ under a central simple harmonic force. Evidently

$$\frac{\mathrm{d}^2 r}{\mathrm{d}t^2} = \mathcal{L}^2 r^{-3} - \omega^2 r. \tag{7}$$

To save writing unimportant details hereafter we take all the masses equal, so that $m_i = m = M/N$. The equation of motion for $\mathbf{x}_i$ now reads

$$m\,\frac{\mathrm{d}^2\mathbf{x}_i}{\mathrm{d}t^2} = -\,m\omega^2(\mathbf{x}_i - \bar{\mathbf{x}}) - \frac{\partial V_2}{\partial \mathbf{x}_i}, \tag{8}$$

where the simple harmonic forces were combined using Eq. (3). We now employ rescaled variables defined by

$$\mathbf{X}_i = \mathbf{x}_i - \frac{\bar{\mathbf{x}}}{r}. \tag{9}$$

Then

$$\begin{aligned}\frac{\mathrm{d}^2\mathbf{x}_i}{\mathrm{d}t^2} &= \frac{\mathrm{d}^2 r}{\mathrm{d}t^2}\mathbf{X}_i + 2\frac{\mathrm{d}r}{\mathrm{d}t}\frac{\mathrm{d}\mathbf{X}_i}{\mathrm{d}t} + r\frac{\mathrm{d}^2\mathbf{X}_i}{\mathrm{d}t^2}\\ &= (\mathcal{L}^2 r^{-3} - \omega^2 r)\mathbf{X}_i + r^{-3} r^2 \frac{\mathrm{d}}{\mathrm{d}t}\left(r^2\frac{\mathrm{d}\mathbf{X}_i}{\mathrm{d}t}\right).\end{aligned} \tag{10}$$

Introducing a new 'time' τ by $\mathrm{d}/\mathrm{d}\tau = r^2\mathrm{d}/\mathrm{d}t$, we notice that $\mathcal{L}\tau$ is the azimuth of the particle in the imaginary orbit introduced under Eq. (6). The equations of motion become

$$m\mathrm{d}^2\mathbf{X}_i/\mathrm{d}\tau^2 = -\,m\mathcal{L}^2\mathbf{X}_i - \partial\mathcal{V}_2/\partial\mathbf{X}_i, \tag{11}$$

where $\mathcal{V}_2 = r^2 V_2$. Since V_2 is homogeneous of degree -2 in the $\mathbf{x}_i$, one merely replaces the $\mathbf{x}_i$ by $\mathbf{X}_i$ to make $\mathcal{V}_2$ from V_2. The result does not depend on r explicitly. Equation (11) is thus an autonomous equation for the evolution of the reduced variables $\mathbf{X}_i$, but as functions of τ rather than t.

From their definition (9) the $\mathbf{X}_i$ are constrained so that both

$$\sum \mathbf{X}_i = 0, \qquad \sum \mathbf{X}_i^2 = N. \tag{12}$$

Now the E in Eq. (1) is the energy relative to the centre of mass since the I is measured in that frame, see Eq. (3). Our energy equation is therefore

$$\begin{aligned}E &= \frac{1}{2}\sum m\left[\frac{\mathrm{d}(\mathbf{x}_i - \bar{\mathbf{x}})}{\mathrm{d}t}\right]^2 + V_{-2} + V_2\\ &= \frac{1}{2}M(\dot{r}^2 + \omega^2 r^2) + r^{-2}\left[\frac{1}{2}\sum m\left(\frac{\mathrm{d}\mathbf{X}_i}{\mathrm{d}\tau}\right)^2 + \mathcal{V}_2\right].\end{aligned} \tag{13}$$

Eliminating $\dot{r}$ via Eq. (6) and multiplying by r^2 we obtain

$$\frac{1}{2}M\mathcal{L}^2 = \frac{1}{2}\sum m\left(\frac{\mathrm{d}\mathbf{X}_i}{\mathrm{d}\tau}\right)^2 + \mathcal{V}_2. \tag{14}$$

So the "energy" of the reduced variables in τ-time is $M\mathcal{L}^2/2$. Had we directly integrated equation (11) to find this energy, it would not have been obvious that the integration constant was zero.

We are now in a position to state our problem in statistical mechanics. Given that the $\mathbf{X}_i$ must satisfy the constraints Eq. (12), what is their statistical equilibrium and how does any such equilibrium translate back into the eternally pulsating variables $\mathbf{x}_i$ and $\dot{\mathbf{x}}_i$? We find the equilibrium in Section 2. In Section 3 we demonstrate by numerical experiment with 1000 particles that a system started well away from that pulsating equilibrium relaxes to the predicted ever-pulsating equilibrium. Finally in Section 4 we remark on the solutions of the corresponding problem in quantum mechanics.

The problem is exceptional in that the normal dissipation of the basic breathing mode is exactly absent. Nevertheless the other modes of the system do dissipate. Although the long range simple harmonic force seems very artificial the net effect is exactly that found by Newton for the gravitational force within a homogeneous body. Such bodies have inspired many delightful studies by the great mathematicians including one by Freeman Dyson.[1] The special case of our problem in which $\mathcal{V}_2$ is zero is the N-body problem exactly solved by Newton in the Principia.[2] The pulsating equilibrium idea arose in our earlier generalisations of his work to other extraordinary N-body problems that are exactly soluble in both classical and quantum mechanics.[3,4] The special case when the harmonic force is absent and the particles are on a line is the exactly soluble Calogero model.[5]

2. STATISTICAL MECHANICS OF THE REDUCED SYSTEM

The constraint $\sum \mathbf{X}_i^2 = N$ tells us that the $3N$ coordinates lie on a hypersphere of radius $\sqrt{N}$ in $3N$ dimensions. Each of the three constraints $\sum \mathbf{X}_i = 0$ gives a hyperplane through the hypersphere's centre so the first of them reduces the $3N$-sphere to a $(3N-1)$-sphere; imposing the others as well reduces that to a $(3N-3)$-sphere. If $\mathcal{V}_2$ were zero the representative point would move freely on such a hypersphere and with $\mathcal{V}_2$ present the motion is still a Hamiltonian one in the angles. The reduced system

Eq. (11) still has a conserved total angular momentum. Writing $\mathbf{X}_i'$ for $\mathrm{d}\mathbf{X}_i/\mathrm{d}\tau$ the conservation law is

$$\sum \mathbf{X}_i \times m\mathbf{X}_i' = \sum (\mathbf{x}_i/r) \times mr^2 \frac{\mathrm{d}}{\mathrm{d}t}(\mathbf{x}_i/r) = \sum \mathbf{x}_i \times m\dot{\mathbf{x}}_i = \mathbf{J}. \tag{15}$$

Incorporating this constraint too, the reduced system has $3N-7$ degrees of freedom. For details of the angles on the hypersphere and their corresponding momenta see the appendix to ref. 4. Using Lagrange multipliers $m\beta^*/2, \boldsymbol{\gamma}, \delta$ to impose the constraints of constant 'energy' $M\mathcal{L}^2/2$, $\mathbf{J}$, and $\sum \mathbf{X}_i^2$ on the equilibrium distribution function, it factorises into a distribution function of momenta $m\mathbf{X}'$ given by,

$$f \propto \exp[-\beta^* m\mathbf{X}'^2/2 - \boldsymbol{\gamma}.(\mathbf{X} \times m\mathbf{X}')], \tag{16}$$

and a distribution function of spatial coordinates.

Writing $\boldsymbol{\gamma} = -\beta^*\boldsymbol{\Omega}$ and omitting a further function of position

$$f \propto \exp[-\beta^* m(\mathbf{X}' - \Omega \times \mathbf{X})^2/2]. \tag{17}$$

Returning to our original variables $\mathbf{x} = r\mathbf{X}$ and writing $\dot{\mathbf{x}} = \mathbf{v}$, we have $\mathbf{X}' = r[\mathbf{v} - (\dot{r}/r)\mathbf{x}]$ where $r(t)$ is the ever pulsating scale. In terms of our old variables f takes the form

$$f \propto \exp[-\beta^* mr^2(\mathbf{v} - \mathbf{u})^2/2], \tag{18}$$

where $\mathbf{u} = (\dot{r}/r)\mathbf{x} - \Omega r^{-2} \times \mathbf{x}$. We see that $\mathbf{v}$ is distributed Maxwellianly relative to the mean $\mathbf{u}(\mathbf{x}, t)$. This mean moves with a time-dependent 'Hubble' flow (i.e., one with velocity proportional to distance at each time) superposed on a time-dependent rotation $\boldsymbol{\Omega} r^{-2}$. Furthermore the temperature of the distribution is time-dependent with $\beta^* r^2$ taking the place of the normal β so that the temperature is proportional to r^{-2}. We intentionally omitted the spatial distribution from the above as it contains all the complications of the problem. With both attractive and repulsive forces present we expect phase transitions of solids to liquids and gases even in classical physics without quantum phenomena. At low temperatures we expect a solid lattice but it can not be perfectly regular as the spacing must increase outward as the pressure decreases. None of this prevents the whole body undergoing large amplitude rescaling pulsations with the associated time-dependent rotation predicted above. At high enough temperatures $\mathcal{V}_2$ is always small compared with the kinetic energy and it can be neglected except as the means by which the system relaxes to its pulsating equilibrium whose density is then given by

$$\rho = \rho_0 \exp -[\delta Z^2 + q(X^2 + Y^2)], \tag{19}$$

where $\mathbf{X} = (X, Y, Z)$. The coefficient q is best expressed in terms of a reduced omega $\omega^2 = m\beta^*\Omega^2$ and takes the form $4q = 3 - \omega^2 + \sqrt{(3-\omega^2)^2 + 2\omega^2}$. The Lagrange multiplier δ is $\delta = q + \omega^2/2$. Notice that $\delta \to q \to 3/2$ as $\Omega \to 0$. From Eq. (19) we may calculate the moment of inertia and thence the total angular momentum is $\mathbf{J} = \mathbf{\Omega} M/q$. The other Lagrange multiplier is determined from $m\beta^*\mathcal{L}^2 = 3 + \omega^2/q$.

3. SIMULATING THE APPROACH TO THE PULSATING EQUILIBRIUM

Numerical simulations were carried out on a system of 1000 particles of equal mass with pair interactions depending on their separation r_{ij},

$$V(r_{ij}) = \frac{1}{2m^2}\left[r_{ij}^2 + r_{ij}^{-2}\right], \tag{20}$$

using the method of molecular dynamics.[6] The unit of mass was defined so that the total mass $M = 1000\,\mathrm{m}$ was equal to one, and the equations of motion were integrated using the Verlet velocity algorithm with a time step of 0.001. With this choice of parameters the period of the oscillation of r^2 is π time units. The starting configuration was constructed from a cubic array of particles with an initial interparticle spacing of 0.1 and the origin of the coordinates was defined as the cube centre. Velocities were chosen randomly from a Gaussian distribution, and adjusted so that the velocity of the centre of mass was equal to zero and the total energy E was equal to some specified value. The coordinate system was rotated so that the angular momentum was along the z direction. In order to study the approach to equilibrium, the initial velocity and spatial distributions were perturbed by scaling the z velocities and z positions by a factor of two. Such a scaling leaves the angular momentum unchanged.

The perpetual pulsating is illustrated in Fig. 1. The top curve in this figure shows r^2 as a function of time measured in periods of π time units for periods 50–60 since the beginning of the simulation. The harmonic pulsation of r^2 is clear and both amplitude and phase are the same as at the beginning of the simulation. The lower two curves show the total potential energy and the contribution from V_2, the inverse square term. It can be seen that the latter term is only important during the phase of the pulsation when the system is compressed so that r^2 is small.

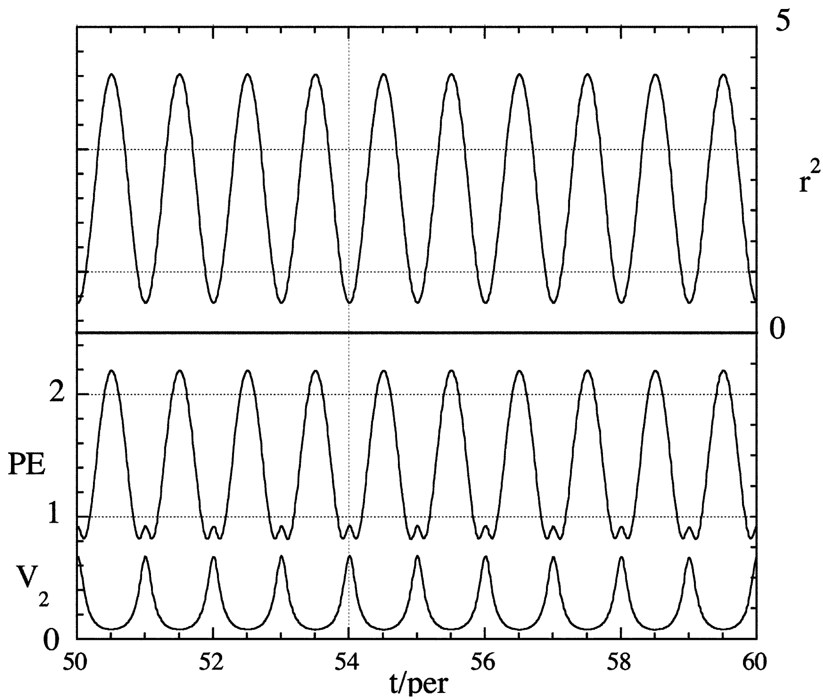

Fig. 1. Variation of r^2 (top), total potential energy (middle) and V_2 (bottom) during 10 pul sations following the first 50 pulsations.

The relaxation toward equilibrium of both the shape of the cluster and the distribution of the peculiar velocities $(\mathbf{v}-\mathbf{u})=\mathbf{v_p}$ towards equilibrium are shown in Figs. 2 and 3. Figure 2 shows the shape of the cluster as measured by the ratio $\left(\sum z_i^2/\sum x_i^2\right)^{1/2}$, which tends to one at equilibrium, since the only angular momentum in the simulation is the small one statistically generated in the initial conditions. Although the system is initially far from equilibrium, the shape relaxes over about five periods to an approximately spherical distribution with equal second moments in x and z, although both quantities are pulsating. Fluctuations in the ratio remain for many periods. Figure 3 shows the changes in $r^2\sum v_{pz}^2$ and $r^2\sum v_{px}^2$ as functions of time. According to Eq. (18) these quantities should be constant and equal at equilibrium. Relaxation of the difference occurs over about five pulsation periods.

The Maxwellian distribution of peculiar velocities $(\mathbf{v_p})$ predicted in Eq. (18) is illustrated in Fig. 4. The top part of the figure shows the velocity distributions at eight different phases of the pulsation. At the phase when the cluster is compact the velocity distribution is broader than when

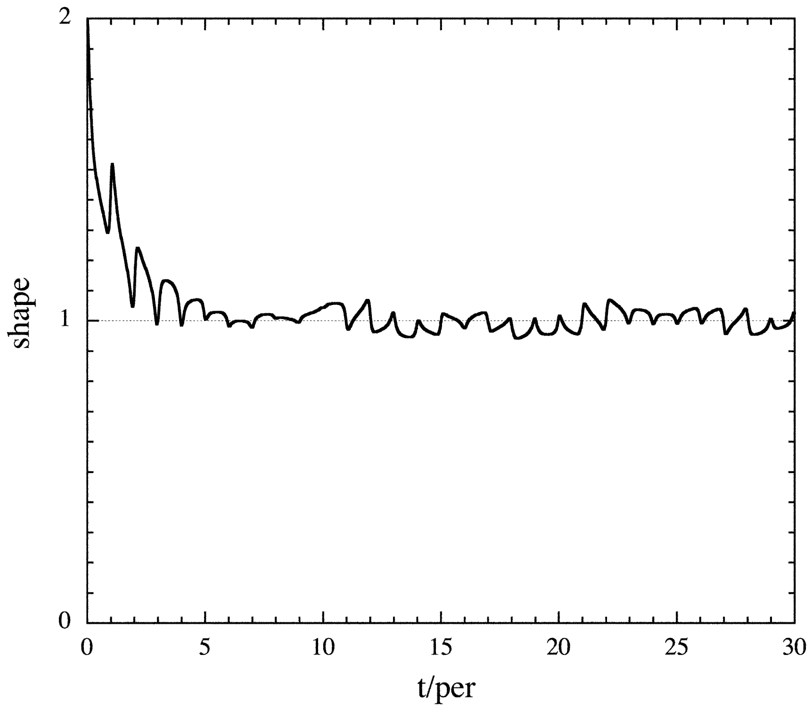

Fig. 2. Variation of the cluster shape $\left(\sum z_i^2 / \sum x_i^2\right)^{1/2}$ at the beginning of the run. Note that the initial anisotropy relaxes in about five pulsations.

the cluster is extended, but in every case the distribution is Maxwellian. The middle part of the figure verifies that the width of the distribution is inversely proportional to r as predicted by Eq. (18), as it shows that, when the velocities are rescaled by r, the distributions coincide. To decrease numerical fluctuations all these graphs average together the distributions of the x, y and z components of velocity relative to the predicted mean and also average the distributions taken at the same phases of 15 pulsations at the end of the run. The logarithmic plot of the distribution function against $(v_{px})^2$ is shown to be linear in the final graph, confirming the Maxwellian form of the distribution.

4. CONCLUSIONS

The predicted pulsating equilibrium is approached and forms a limit cycle. A surprising aspect of this is that so-called 'violent relaxation',[8] the decay of the pulsations of the long-range mean field through its action

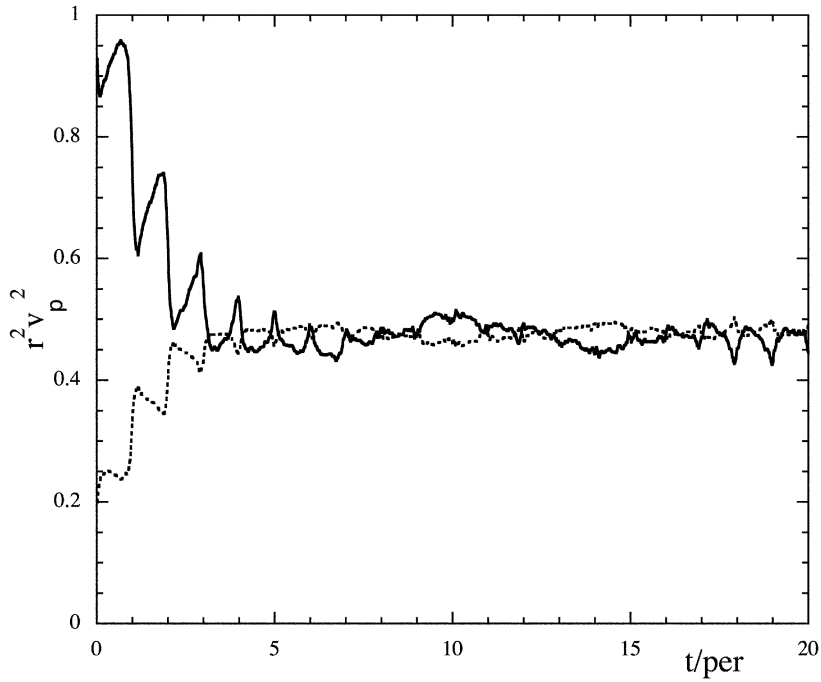

Fig. 3. Variation near the beginning of the run of the mean square peculiar velocities in the z (solid) and x (dashed) directions scaled with r. Note that these relax to equal values in about five pulsations.

on particle motions, does not occur for the fundamental mode. Nevertheless the other modes of the system do dissipate. So Violent Relaxation is not totally absent. Limit cycles are well-known in dynamics but it is more unusual to come across a pulsating Maxwellian distribution that continues with no change of entropy. However a related case is found in the Planck distribution of photons which remains rescaled but unchanged in shape or entropy as the universe expands. That is not true of the distribution function of massive particles which need collisions to maintain equilibrium as they cease to be relativistic. There are other many-particle systems known to show continuing changes. For example, Friesecke and Pego[7] show that the Pasta–Fermi–Ulam chain of anharmonic oscillators do not relax to an equilibrium at low energies.

In ref. 4 we discussed the quantum mechanics of a closely related problem including the relevant Fermi–Dirac and Einstein–Bose distributions. The Hamiltonian separates in the form $H = \bar{H}(\bar{\mathbf{x}}) + \tilde{H}(r) + r^{-2}\hat{H}(\mathbf{X})$. The use of momenta allowed us to get the solutions without

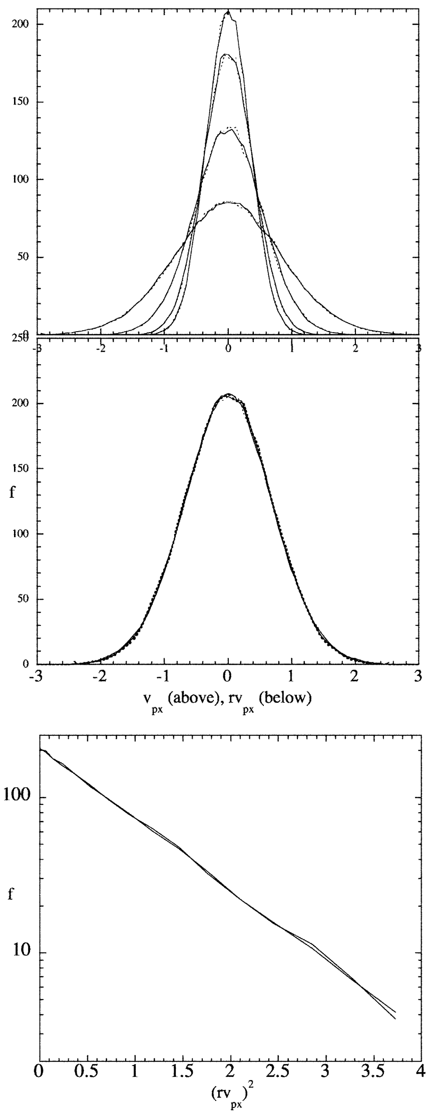

Fig. 4. The equilibrium distribution of peculiar velocities. The upper graph shows the distribution of the peculiar velocities for eight phases of the pulsation cycle. The broad distributions correspond to phases when the cluster is compressed and the narrowest portions to expanded phases. In the middle graph the velocities have been rescaled with r demonstrating that the eight distributions coincide. The bottom portion demonstrates the Maxwellian nature of the distribution by showing the logarithm of the distribution function is linear in $r^2 v_{px}^2$.

the introduction of τ-time but the pulsations of the equilibrium have to be sought out in the correlations whereas they stand out more clearly in the classical case discussed above.

ACKNOWLEDGMENTS

We are grateful to the Institute of Advanced Study for providing the environment at Princeton where this work was done. D.L-B. thanks the Monell Foundation for supporting his visit. R.M.L-B. thanks the Chemical Engineering department of Princeton University.

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