Chaotic mixing of granular material in slowly rotating containers as a discrete mapping

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Chaotic mixing of granular material in a two-dimensional slowly rotating noncircular container in the absence of granular diffusivity is studied analytically and numerically as a discrete mapping. The noncircularity of a drum produces a time periodic disturbance and chaotization of the flow field. The location of the fixed points of the mapping and the separatrices of the hyperbolic points are determined in a closed analytical form.
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Mixing of granular material in a partially filled rotating container is encountered in many technological operations in metallurgy, pharmaceutical and chemical industries, food processing, etc. It was a subject of numerous studies during the last few years (see, e.g., Refs. 1–10 and references therein). Mixing of particulate solids through random scattering of granules in the avalanches was extensively investigated recently.[1,2–4] In this study we showed that even when particles are not scattered at all when they fall down at the free surface, the flow of granular material can be chaotic. The cause of the chaos is as follows. When granular material flows in a circular drum without diffusion the flow is steady. However a noncircular container produces some time periodic disturbances of the flowfield that can highly improve the mixing.[9,11,13] We consider advection of a tracer in a noncircular drum filled with particles with the same physical properties. After some assumptions the motion of the tracer can be described by a two dimensional discrete mapping. This model, although it is highly simplified, allows us to study the dynamics of mixing.

I. INTRODUCTION

There are several types of flow which result in a random dispersion of particles in a rotating drum and mixing of granular material, namely, convection, diffusion and shear.[12] Note, that while the particle diffusion is uncontrollable, the macroscopic advection can be effectively changed by a proper choice of the mixer's geometry.[1,9] Flowing granular mixtures of nonidentical particles often segregate due to percolation of smaller or heavier particles through a shearing layer. Thus, random diffusion and interparticle percolation constitute a net segregation flux.[6] Results of computational and experimental study of mixing and segregation of granular materials in rotating cylindrical drum were reported in Refs. 5, 6, and 9. The process is governed by two factors: net segregation flux and stretching of the granular material due to the different periods of rotation of particles located along different radii. The authors plotted the intensity of segregation vs number of rotation of the drum. Mixing proceeds in two well distinguishable stages: rapid initial mixing and long time evolution. Notably, the mixing curves obtained from the experiments and from the computations with different values of the net segregation flux coincide at the first stage with the mixing curve that corresponds to the *zero segregation flux*. In the recent work of Khakhar *et al.*[13] the authors considered mixing of granular materials in half filled drums which are symmetric with respect to the rotation by *180°*. Computational and scaling analyses showed that mixing in a noncircular mixer was faster then in the circular mixer, and the difference in the mixing time was found to increase with the mixer size. The latter suggests that the study of the particles advection by the macroscopic flow can provide a useful information about the first more rapid and also more controllable stage of the mixing process.

II. DISCRETE MAPPING

Flow field of granular material in a drum comprises two different regions, namely, a stationary rotated bulk and a thin cascading layer. Particles slowly rotate with the stationary bulk and then rapidly fall down in the cascading layer, continuously or intermittently, depending on the flow regime. When a period of rotation is much larger then an avalanching time, the analysis can be considerably simplified. In the present study we use the model described in Ref. 8, namely, a two-dimensional convex mixer $r=r(\phi)$ (see Fig. 1) partially filled with a granular material with a constant bulk density. The container slowly rotates around a horizontal axis with a constant angular velocity $\dot{\theta}=1$. The free surface of the granular material is flat and it is inclined at a constant angle of repose. The height of the free surface is $z=h(\theta)$ can be easily calculated from the equation of mass conservation. The center of the free surface is located at $x_C=dh(\theta)/d\theta$. Each particle rotates with the bulk of the material and when it reaches the free surface at a point x', it immediately falls

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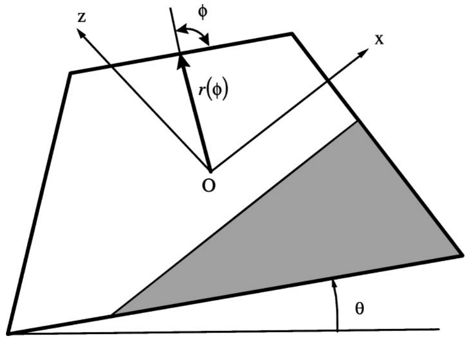

FIG. 1. Rotating container partially filled with a granular material. X axis is parallel to the free surface of the material, i.e., the angle of repose of the granular material is eliminated from the analysis.

down and sediments at the bulk at the new position $x=x_C-(x'-x_C)=2x_C-x'$ which is symmetrical with respect to the center of the free surface.

Consider an individual particle which is trapped by the bulk of the granular material at a moment θ_i at a point $(x_i, z_i=h(\theta_i))$. The equations of motion of the particle in the bulk read: $dx/d\theta=-z$, $dz/d\theta=x$. Solving these equation with the initial condition $x(\theta_i)=x_i$, $z(\theta_i)=h(\theta_i)$ we find that

$$x=-h(\theta_i)\sin(\theta-\theta_i)+x_i\cos(\theta-\theta_i),$$

$$z=h(\theta_i)\cos(\theta-\theta_i)+x_i\sin(\theta-\theta_i).$$

The latter expressions imply that the particle will reach again the free surface at the moment $\theta_{i+1}>\theta_i$ which is the next root of the equation:

$$h(\theta_{i+1})=h(\theta_i)\cos(\theta_{i+1}-\theta_i)+x_i\sin(\theta_{i+1}-\theta_i).$$

The particle will appear at the free surface at the point $x'=-h(\theta_i)\sin(\theta_{i+1}-\theta_i)+x_i\cos(\theta_{i+1}-\theta_i)$, it will fall down and reenter the bulk of the granular material at the new position $x_{i+1}=2x_C-x'$. Thus, the motion of a grain in a two-dimensional slowly rotating container can be described by a two-dimensional implicit area preserving discrete mapping $M:(\theta_i, x_i)\rightarrow(\theta_{i+1}, x_{i+1})$ which has the following form:

$$\begin{aligned} h(\theta_{i+1})&=h(\theta_i)\cos(\theta_{i+1}-\theta_i)+x_i\sin(\theta_{i+1}-\theta_i)\\ x_{i+1}&=2\frac{dh(\theta_{i+1})}{d\theta}+h(\theta_i)\sin(\theta_{i+1}-\theta_i)-x_i\cos(\theta_{i+1}-\theta_i) \end{aligned} \quad (1)$$

where the height of the free surface $h(\theta)$ is a known periodic function which depends on the shape of the container.

III. TIME PERIODIC FLOW, FIXED POINTS AND SEPARATRICES OF THE MAPPING

Since the inertial forces are neglected, any change of the center of rotation of the container does not affect the flow of granular material. One can easily verify that the equations (1) are invariant with respect to the transformation: $h'(\theta)=h(\theta)+R\sin(\theta)$, $x'=x+R\cos(\theta)$ for an arbitrary constant R. Therefore the height of the free surface $h(\theta)$ is $2\pi/N$-periodic function of the angle θ, where $N\geqslant 1$ is an integer constant, and the first harmonic in $h(\theta)$ always can be canceled by a translation of the origin of the coordinates.

Flow of granular material in a circular drum was considered in Ref. 10. In this case the height of the free surface $h(\theta)=\text{constant}$, and the coordinate x enters the Eqs. (1) as a parameter. The system is integrable, and each particle in less and more than a half filled drum moves along its own closed trajectory with periods $2\arctan(x/h)$ and $2(\pi+\arctan(x/h))$, respectively. Due to the time-periodic disturbances induced by the deviation of the shape of the drum from a circular cylinder, the system becomes non-integrable. The latter causes an enhancement of the mixing rate (for discussion of time-periodic Hamiltonian systems, chaos and mixing see Ref. 11).

Consider now the flow of granular material in a triangular containers $(N=3)$ although the obtained results can be applied to an arbitrary convex container with $2\pi/N$ periodic $(N\geqslant 3)$ variation of the free surface. Consider a case when the container is less than half filled, and the height of the free surface is always negative. One can now seek for the fixed points of the mapping M [see Eqs. (1)] in the form:

$$\theta_i=\frac{2\pi}{N}i+\theta_*,\quad x_i=x_*.$$

After some algebra equations (1) yield the following expressions:

$$\frac{dh(\theta_*)}{d\theta}=0,\quad x_*=\tan\left(\frac{\pi}{N}\right)h(\theta_*).$$

Thus, the fixed points correspond to the extrema of function $h(\theta)$. The behavior of the system near the fixed points is given by the linearized discrete mapping. Introduce the new variables: $\theta_i=\theta_*+\Theta_i$, $x_i=x_*+X_i$. Then after some algebra we obtain

$$h(\theta_*)\tan\left(\frac{\pi}{N}\right)(\Theta_{i+1}-\Theta_i)=X_i\sin\left(\frac{2\pi}{N}\right),$$

$$X_{i+1}-2\frac{d^2h}{d\theta^2}\Theta_{i+1}-h(\theta_*)(\Theta_{i+1}-\Theta_i)=-X_i\cos\left(\frac{2\pi}{N}\right).$$

The eigenvalues of the above linear algebraic system of equations are given by the following expressions:

$$\lambda_{1,2}=1+\chi\pm\sqrt{(1+\chi)^2-1}, \quad (2)$$

where

$$\chi=\frac{1+\cos(2\pi/N)}{h(\theta_*)}\cdot\frac{d^2h(\theta_*)}{d\theta^2}.$$

Thus, the fixed points corresponding to the maxima of $h(\theta)$ are saddle points while those corresponding to the minima of the height of the free surface are centers.

We shall call a periodic point of the mapping (1) that is mapped q times during the time interval $\Theta=p(2\pi/N)$ and returns to its initial position a fixed point of the order p/q. The fixed points considered above are of the order 1/1. A direct calculation of the fixed points of the higher orders is quite involved. Instead let us consider the time periodic flow induced by a small noncircularity of a drum $r=r_0+\varepsilon^2 r(\phi)$. Thus, the height of the free surface is $h(\theta)=h_0+\varepsilon^2 h'(\theta)$, where $h_0<0$ and ε is a small parameter.

Introduce the following change of variables:

$$\theta_i = i\,\theta_0 + \theta_i',$$

$$x_i = h_i \tan\left(\frac{\theta_0 + \theta_{i+1}' - \theta_i'}{2}\right) + x_i',$$

where $\theta_0 = (p/q)(2\pi/N)$. Then, Eqs. (1) read

$$h(\theta_0 + \theta_{i+1}') - h(\theta_i') = x_i' \sin(\theta_0 + \theta_{i+1}' - \theta_i'),$$

$$h(\theta_i')\tan\left(\frac{\theta_0 + \theta_{i+1}' - \theta_i'}{2}\right) - h(\theta_{i-1}' - \theta_0) \times \tan\left(\frac{\theta_0 + \theta_i' - \theta_{i-1}'}{2}\right) = 2\,\frac{dh(\theta_i')}{d\theta} - x_i' - x_{i-1}' \cos(\theta_0 + \theta_i' - \theta_{i-1}'). \tag{3}$$

Based on the numerical experiments with the mapping (1) we can assert that when ε is small and when the particle initially was located near the resonance of the mapping (1) of the order p/q, the differences between the consequent values of the angle θ' are also small, and the discrete variable i can be replaced by a continuous parameter ξ as follows:

$$\theta_{i+1}' - \theta_i' = \varepsilon\frac{\theta_{i+1}' - \theta_i'}{\varepsilon} = \varepsilon\frac{d\theta'}{d\xi} + \frac{\varepsilon^2}{2}\frac{d^2\theta'}{d\xi^2} + \cdots,$$

where the scaling $\theta_{i+1}' - \theta_i' \sim \varepsilon$ is chosen in order to balance different terms in Eqs. (3). Thus, $x' \approx \varepsilon^2(h'(\theta_0 + \theta_{i+1}') - h'(\theta_i'))/\sin(\theta_{0i})$.

Expanding Eqs. (3) with respect to the small parameter ε in the leading order term we obtain

$$h_0\frac{\theta_{i+1}' - 2\theta_i' + \theta_{i-1}'}{\varepsilon^2} = 4\cos^2\left(\frac{\theta_0}{2}\right)\frac{\partial h'(\theta_i')}{\partial\theta'} - \cot\left(\frac{\theta_0}{2}\right) \times (h'(\theta_i' + \theta_0) - h'(\theta_i' - \theta_0)). \tag{4}$$

The right-hand side of the above equation can be represented in a potential form as follows:

$$\frac{\partial U_{p/q}^i}{\partial\theta'} = \frac{\partial}{\partial\theta'}\left[4\cos^2\left(\frac{\theta_0}{2}\right)h'(\theta_i') - \cot\left(\frac{\theta_0}{2}\right)\int_{\theta_i'-\theta_0}^{\theta_i'+\theta_0} h'(\varsigma)\,d\varsigma\right].$$

After summation of Eq. (4) from i to $i+q-1$ we obtain that the leading order term in the mapping (3) near the resonance of the order p/q corresponds to a one dimensional motion in a potential $\overline{U_{p/q}^i} = \Sigma_{j=0}^{q-1} U_{p/q}^{i+j}$:

$$-h_0\frac{d^2\theta'}{d\xi^2} = -\frac{\partial\overline{U}_{p/q}(\theta')}{\partial\theta'}. \tag{5}$$

The maxima of the potential $\overline{U}_{p/q}$ correspond to hyperbolic points of the mapping (1) of the order p/q while the minima indicate location of the centers of the same order. Equation (5) has separatrices that extend from the saddle to the saddle as $\xi \to \pm\infty$, and they can be determined from the energy conservation integral $\overline{U} - (h_0/2)(d\theta'/d\xi)^2 = \max(\overline{U})$. Thus, the separatrices of the order p/q of the discrete mapping (1) can be approximated by the separatrices of the Eq. (5) as follows:

$$x_{(p/q),i} \approx h(\theta_i)\tan\left(\frac{\pi p}{Nq} \pm \varepsilon\left(\frac{2(\overline{U}_{p/q}(\theta_i) - \max(\overline{U}_{p/q}))}{h_0}\right)^{1/2}\right) \tag{6}$$

IV. CHAOTICAL MIXING: NUMERICAL RESULTS AND DISCUSSION.

Consider for simplicity the fixed points of order 1/1 of a $2\pi/N$ periodic ($N \geqslant 3$) flow. The potential of Eq. (5) reduces to $\overline{U} = 4\cos^2(\theta_0/2)h'(\theta_i')$. The question is whether the mapping (1) has separatrices of order 1/1 given by Eq. (6) extending from the saddle to saddle or stable and unstable manifolds of the saddle points split. Keeping the next order terms in the expansion of (3) we obtain:

$$\frac{\varepsilon^2 h_0}{24}\frac{d^4\theta'}{d\xi^4} + h_0\cos^2\left(\frac{\pi}{N}\right)\frac{d^2\theta'}{d\xi^2} - 4\cos^4\left(\frac{\pi}{N}\right)\frac{\partial h'(\theta')}{\partial\theta'} = \varepsilon^3 NL, \tag{7}$$

where NL are nonlinear terms which vanish in a neighborhood of the saddle. Thus, the above equation and mapping (3) can be viewed as singular perturbations of the integrable system (5). Solution of the Eq. (7) linearized near the saddle point is $\theta' = \Sigma_{j=1}^4 C_j \exp(\kappa_j\xi)$ where κ_j are characteristic values

$$\kappa_{1,2} \approx \pm\sqrt{24}\cos\left(\frac{\pi}{N}\right)\sqrt{\frac{1}{h_0(0)}\frac{\partial^2 h'(0)}{\partial\theta^2}},$$

$$\kappa_{3,4} \approx \pm i\varepsilon^{-1}\sqrt{24}\cos\left(\frac{\pi}{N}\right).$$

Thus, in order to obtain a solution passing through the saddle point as $\xi \to \infty$ we must apply three boundary conditions, that is $C_1 = C_3 = C_4 = 0$, and similarly, when $\xi \to -\infty$ the boundary conditions are $C_2 = C_3 = C_4 = 0$. Thus we obtained an overdetermined set of six boundary conditions for the fourth order differential Eq. (7). Therefore, generally, one can not expect that the singularly perturbed Eq. (7) and, consequently, mapping (1), have an invariant manifold which connects two saddle points. The more physically plausible picture is that stable and unstable manifolds of a saddle point split and intersect.

We performed calculations with a small model disturbance of the height of the free surface of the form $h(\theta) = -1 + 0.01\cos(3\theta)$. A small blob of particles was initially placed in a close vicinity of the saddle. The results are presented in Fig. 2. We see that the unstable manifold of the hyperbolic point approaches the saddle but in a close neighborhood of the singular point there appear oscillations with the increasing frequency. Thus, the oscillating unstable solution intersects with a stable solution that tends to the saddle point as $i \to -\infty$. An intersection of separtrices is recognized as one of the most striking signatures of chaos. When the

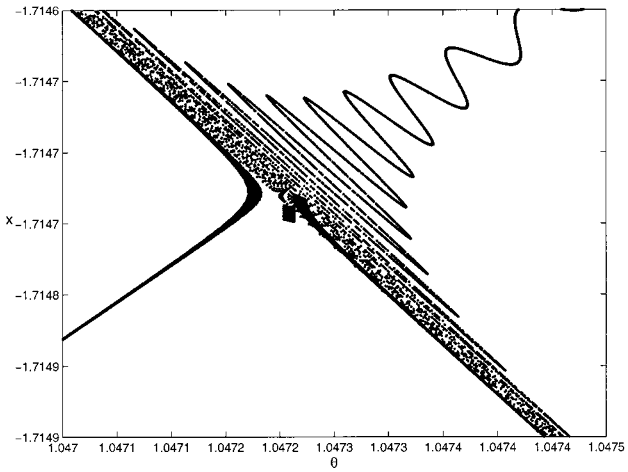

FIG. 2. Evolution of a blob of granular material initially placed in a vicinity of the hyperbolic point. The oscillating tail of the unstable manifold of the saddle approaches the fixed point.

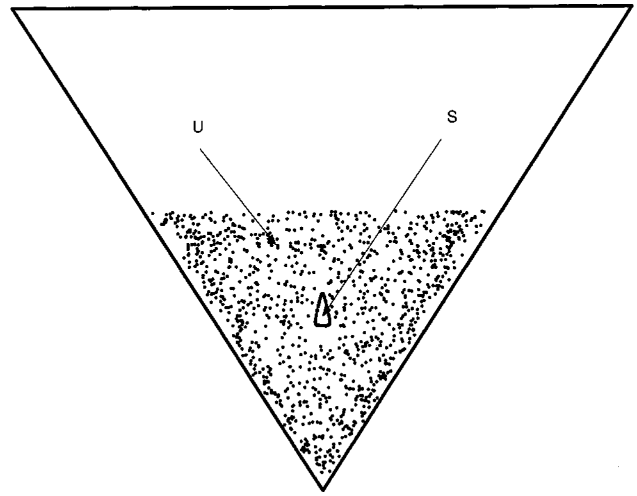

FIG. 4. Poincaré section for a filling level $f=0.33$ with stable and unstable fixed points.

motion along the separtrices of a saddle point becomes more intensive, the chaotic region expands and fills a substantial part of the phase space.

In order to enhance a mixing rate, it is necessary to maintain a high stretching rate near the saddle points. The Eq. (2) shows that large values of the eigennumbers λ_i are attained in a container which provides a sharp maximum of $h(\theta)$. It is intuitively clear that polygons (e.g., triangle) satisfy this requirement. We examined numerically different container shapes of the form $r=r_0+\Sigma r_n\cos(3n\phi)$ and found that a triangular shape provides the best mixing.

In Figs. 3 and 4. we showed the Poincaré sections for different initial positions of a particle. The chaotic region corresponds to the initial locations near the saddle point while the particles initially located in a vicinity of the elliptic point move along the closed quasiperiodic trajectories. When the filling level of the container increases, the fixed points of the mapping become close to each other, and the region with a quasiperiodic behavior shrinks.

When the maximum value of the free surface height reaches zero, the saddle points with a period $2\pi/N$ disappear, and a new type of a regular motion emerges (see Fig. 5).

In order to elucidate the origin of this regularity let us consider the half-filled drum. It can be easily obtained from symmetry considerations that in this case $h(\theta)=-h(\theta+\pi/N)$ and $dh(\theta)/d\theta=-dh(\theta+\pi/N)/d\theta$ (when N is even, the height of the free surface is zero, while odd values of N correspond to a nontrivial solution). Now we seek for the fixed points of the mapping $M^2=M\cdot M$ in the form: $\theta_{i+2}-\theta_{i+1}=\theta_{i+1}-\theta_i=\pi$. Substituting this formula into (1) one obtains (here we do not distinguish between θ and $\theta+2\pi$):

$$h(\theta+\pi)=h(\theta)\cos(\pi)+x_1\sin(\pi),$$

$$x_2=2\frac{dh(\theta+\pi)}{d\theta}+h(\theta)\sin(\pi)-x_1\cos(\pi), \tag{8}$$

$$h(\theta)=h(\theta+\pi)\cos(\pi)+x_2\sin(\pi),$$

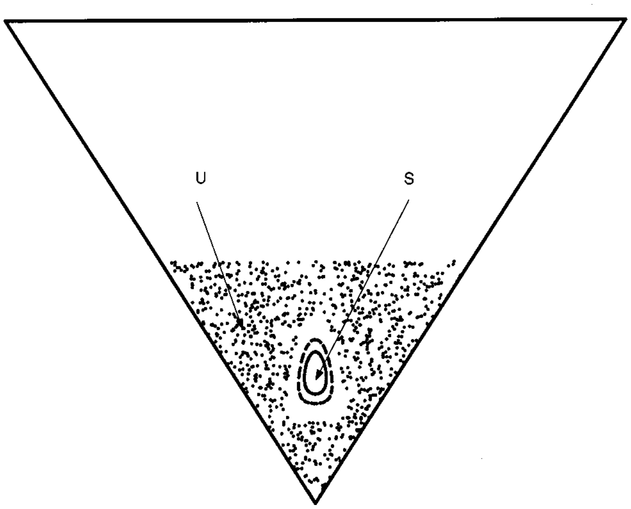

FIG. 3. Poincaré section for a filling level $f=0.25$ with stable and unstable fixed points.

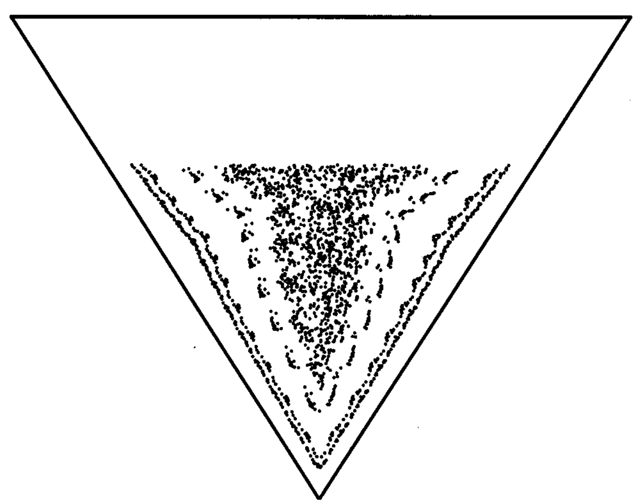

FIG. 5. Poincaré section for a filling level $f=0.45$.

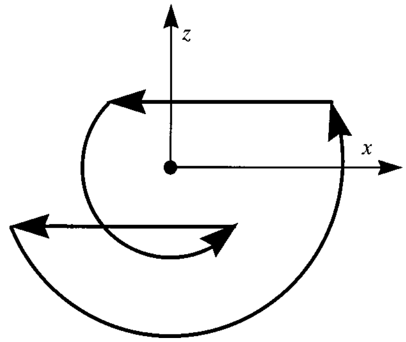

FIG. 6. Particle trajectory in a half filled drum.

$$x_1=2\frac{dh(\theta)}{d\theta}+h(\theta+\pi)\sin(\pi)-x_2\cos(\pi).$$

The x-independent solution of the equations (8) reads:

$$h(\theta)=-h(\theta+\pi),\quad \frac{dh(\theta)}{d\theta}=-\frac{dh(\theta+\pi)}{d\theta},$$

$$x_2=2\frac{dh(\theta+\pi)}{d\theta}+x_1.$$

The schematic view of the above solution is presented at Fig. 6. A particle rotates alternatively along two concentric trajectories (half-circles) jumping from one to another when it reaches the free surface. This solution is possible only when the radius of rotation is sufficiently large while in the central part of the container a more complex periodic flow occurs. When the container is nearly half filled, the fixed points of M^2 evolve into a quasi 2π-periodic closed trajectories (see Fig. 7). The reason for this behavior of the model is the assumptions about the zero thickness of the cascading layer and an instantaneous avalanching of the particles which imply the unrealistic result that period of rotation is independent on radial coordinate of a particle. In the real systems a chaotic behavior persists even in a half filled drum.[13]

When the height of the free surface is always positive, we can seek for the fixed points of the mapping M in the form:

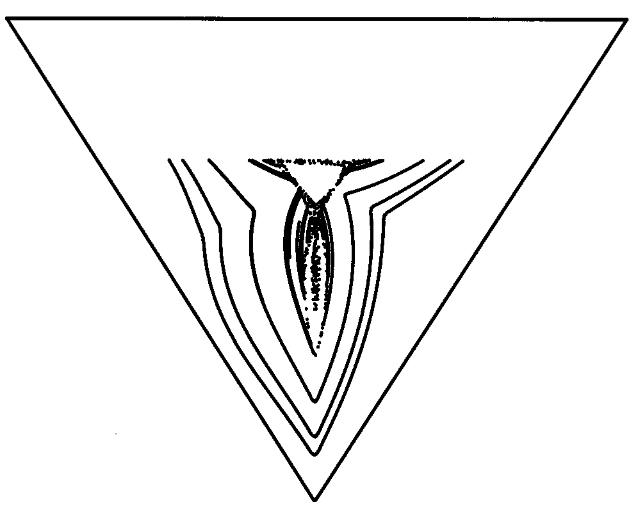

FIG. 7. Poincaré section for a filling level $f=0.5003$.

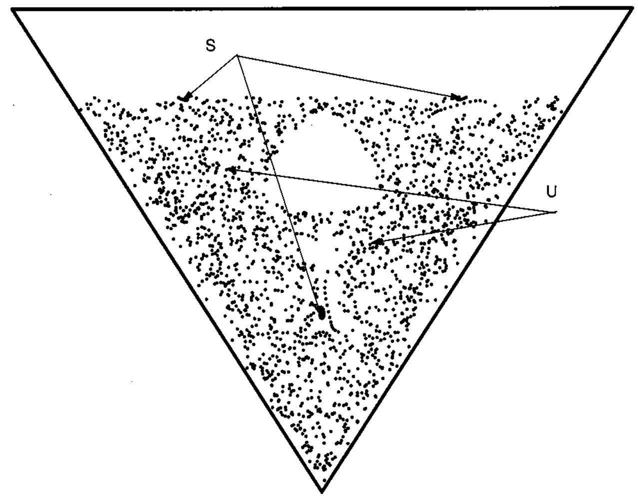

FIG. 8. Poincaré section for a filling level $f=0.66$ with stable and unstable fixed points.

$$\theta_i=\frac{4\pi}{N}i+\theta_*,\quad x_i=x_*.$$

Repeating the previous analysis one can obtain that the fixed points satisfy the following equations:

$$\frac{dh(\theta_*)}{d\theta}=0,\quad x_*=\tan\left(\frac{2\pi}{N}\right)h(\theta_*).$$

The eigenvalues of the linearized mapping are given by formula (2) where the parameter χ is

$$\chi=\frac{1+\cos(4\pi/N)}{h(\theta_*)}\cdot\frac{d^2h(\theta_*)}{d\theta^2}.$$

Contrary to the case of a less then a half filled container, the minima of $h(\theta)$ correspond to the saddle points while the maxima correspond to the centers. The Poincaré section is presented in Fig. 8. The chaotic region corresponds to a particle initially located in a vicinity of a saddle point. The

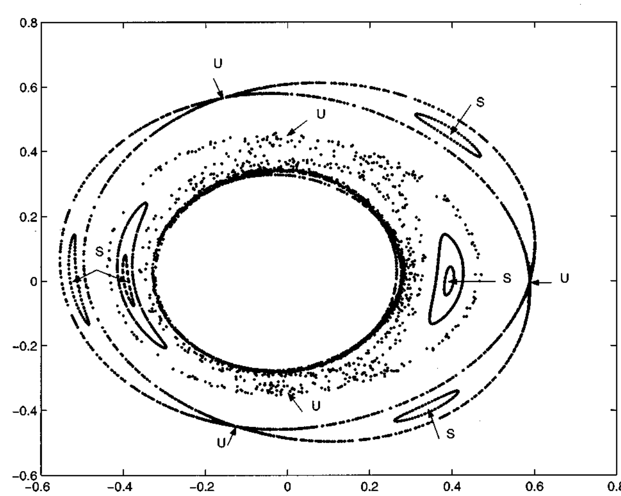

FIG. 9. The phase portrait of particle motion in a noncircular container $r=1+0.12\cos(2\phi)$. The stable and unstable fixed points of the order 1/2 are surrounded by the fixed points of the order 2/3. The elliptical fixed points are surrounded by the closed quasi-periodic trajectories.

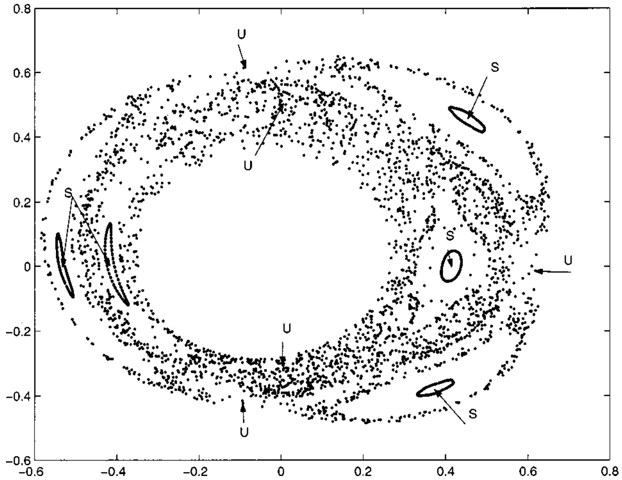

FIG. 10. The particle motion in a noncircular phase portrait of container $r=1+0.19\cos(2\phi)$. The resonance of the order 1/2 and 2/3 overlapped.

small closed trajectories indicate the location of the elliptic fixed points of the mapping (1). The central part of the container is filled by the core of the material which does not get involved in the flow.

While in a triangular container fixed points of the order 1/1 and their separatrices play the major role in mixing, this is not the case in the other containers. For example, in a π-periodic mixer the fixed points of the order 1/1 are possible only in the trivial case when the filling level is 0.5 . Thus, the singular trajectories of the higher orders are of ultimate importance. Consider a π periodic flow in the container $r=1+a\cos(2\phi)$. It is convenient to present the results of the computations in a coordinate system that rotates with the period of $h(\theta)$, i.e., in the polar coordinates $(2\theta,\rho=\sqrt{x^2+h^2})$ (see Figs. 9 and 10). The phase portrait of the system is mainly influenced by the resonances of the lower orders, namely, 1/2 and 2/3. Although for $a=0.12$ the regions near the separatrices are chaotic, the mixing is relatively weak because the resonances are disconnected. According to Eq. (6) one can expect that when the amplitude of $h(\theta)$ increases the difference between $x_{(1/2),i}$ and $x_{(2/3),i}$ tends to zero, and the separatrices of the different resonances overlap. For $a=0.19$ we obtain an enhanced transport between the two resonance and strongly pronounced expansion of the chaotic region.

V. CONCLUSIONS

We analyzed chaotic mixing of granular material in a slowly rotating container as a discrete mapping M. The motion of a particle near a periodic point can be approximated as a one-dimensional motion in a periodic potential. When the radius of a container is a $2\pi/N$ periodic function, the mapping has N saddle points of the order 1/1. The appearance of chaotic motion of granular material can be associated with the intersection of the separatrices of these saddle points.

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