

Experimental validation of phase space conduits of transition between potential wells

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Abstract. A phase space boundary between transition and non-transition, similar to those observed in chemical reaction dynamics, is shown experimentally in a macroscopic system. We validate the phase space flux across rank one saddles connecting adjacent potential wells and confirm the underlying phase space conduits that mediate the transition. Experimental regions of transition are found to agree with theory to within 1%, suggesting the robustness of phase space conduits of transition in a broad array of two or more degree of freedom experimental systems, despite the presence of small dissipation.

Introduction: prediction of transition events in transient dynamics

Prediction of transition events and the determination of governing criteria has significance in many physical, chemical, and engineering systems where rank-1 saddles are present. To name but a few, ionization of a hydrogen atom under electromagnetic field in atomic physics, transport of defects in solid state and semiconductor physics, isomerization of clusters, reaction rates in chemical physics, buckling modes in structural mechanics [1], ship motion and capsize [2], and escape and recapture of comets, asteroids, and spacecraft in celestial mechanics [3]. The theoretical criteria of transition and its agreement with laboratory experiment have previously been shown for 1 degree of freedom (DOF) systems. Detailed experimental validation of the geometrical framework for predicting transition in higher dimensional phase space (≥ 4 , i.e., for 2 or more DOF systems) is still lacking. The geometric framework of phase space conduits in such systems, termed tube dynamics [3] has not before been demonstrated in a laboratory experiment. Here we present a direct experimental validation of the accuracy of the phase space conduits, as well as the transition fraction obtained as a function of energy, in a 4 dimensional phase space using a laboratory experiment of a macroscopic system, with implications for other mechanical systems.

Our setup consists of a mass rolling on a multi-well surface [4], Fig. 1(a), that is representative of potential energy underlying systems that exhibit transition/escape behavior. The equations of motion are obtained from the Lagrangian; $\mathcal{L}(x, y, \dot{x}, \dot{y}) = T(x, y, \dot{x}, \dot{y}) - V(x, y)$. The kinetic energy (translational plus rotational for a ball rolling without slipping) is, $T(x, y, \dot{x}, \dot{y}) = \frac{1}{2} \left(\frac{7}{5}\right) (\dot{x}^2 + \dot{y}^2 + (H_x \dot{x} + H_y \dot{y})^2)$ and the potential energy is $V(x, y) = gH(x, y)$, where $H(x, y)$ is the height function for the multi-well surface and g is the acceleration due to gravity. Small damping is present, but over short time-scales, the motion approximately conserves energy, and the conservative dynamics are the dominant contributor to transition between wells. Let $\mathcal{M}(E)$ be the *energy manifold* given by setting the energy integral ($\mathcal{E}(x, y, v_x, v_y) = T(x, y, \dot{x}, \dot{y}) + V(x, y)$) equal to a constant, i.e., $\mathcal{M}(E) = \{(x, y, v_x, v_y) \in \mathbb{R}^4 \mid \mathcal{E}(x, y, v_x, v_y) = E\}$ where $E \in \mathbb{R}$ is a constant. The projection of the energy manifold onto configuration space, the (x, y) plane, is the region of energetically possible motion for a ball of energy E , $M(E) = \{(x, y) \mid V(x, y) \leq E\}$. The zero velocity curves are the boundary of $M(E)$ and are the locus of points in the (x, y) plane where the kinetic energy vanishes. The ball's state is only able to move on the side of this curve where the kinetic energy is positive, shown in white in Fig. 1(c) (the left panel). The critical energy of escape, E_e , is the same as the energy of the saddle points in each bottleneck (which are all equal), and divides the global behavior into two cases, according to the sign of excess energy, $\Delta E = E - E_e$:

Case 1, $\Delta E < 0$: the ball is safe against escape since potential wells are not energetically connected.

Case 2, $\Delta E > 0$: ‘bottlenecks’ between all the potential wells open up around the saddle points, permitting the ball to move between any two adjacent wells (e.g., Fig. 1(c) shows this case).

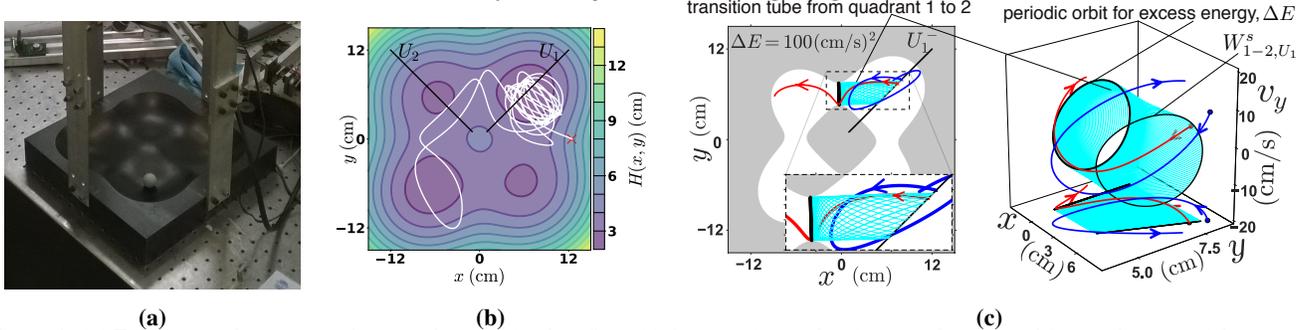


Figure 1: (a) Experimental apparatus showing the machined surface (b) An experimental trajectory, shown in white, on the potential energy surface where the contours denote isoheights. Release from rest is marked by a red cross. (c) For a fixed energy E above a critical value E_e (i.e., $\Delta E > 0$), the permissible region (in white) has potential wells connected by bottlenecks around saddle-type equilibria. All motion from quadrant 1 to quadrant 2 must occur through the interior of a stable manifold tube associated to a periodic orbit in the bottleneck between them (video: <https://youtu.be/gMqrFX2JkLU>). Example transition (red) and non-transition (blue) trajectories are shown.

Tube dynamics and the transition fraction

Within a given potential well, there are phase space conduits leading to escape/transition to a different potential well which are cylindrical manifolds or *tubes*, as shown in Fig. 1(c). Based on these tubes, we can calculate the fraction of energetically permissible trajectories which will transition from/into a given well by calculating the transition rate of trajectories crossing the rank-1 saddle in the bottleneck connecting the wells. For computing this rate—surface integral of trajectories crossing a bounded surface per unit time—we use the geometry of the tube manifold cross-section on the Poincaré section U_1 . For low excess energy, we employ the theory of flux over a rank-1 saddle [?], which corresponds to the action integral around the periodic orbit of period T_{po} at energy ΔE . The transition fraction is given in 2 DOF to leading order in ΔE by $p_{trans} = \frac{T_{po}}{A_0} \Delta E$ where A_0 is the symplectic area of the energy surface as it intersects the Poincaré section at energy $\Delta E = 0$. For small positive excess energy, the predicted growth rate for our system is $T_{po}/A_0 \approx 0.87 \times 10^{-3}$ (s/cm)².

Experimental results

Dynamics on the Poincaré section are best written in polar coordinates; $U_1^- = \{(r, p_r) \mid \theta = \frac{\pi}{2}, \text{sign}(p_\theta) = -1\}$. We take Poincaré sections of 120 experimental trajectories to reveal the tube cross-sections. We determine the instantaneous ΔE for every point on the Poincaré section U_1^- , and consider narrow ranges of ΔE to approximate a single energy manifold. In Fig. 2(a) we see an example of the Poincaré section U_1^- for all intersections in the energy range $40 < \Delta E < 140$ (cm/s)². The intersection points which are about to transition from quadrant 1 to 2, determined by following the experimental trajectories forward in time, and are marked with red circles.

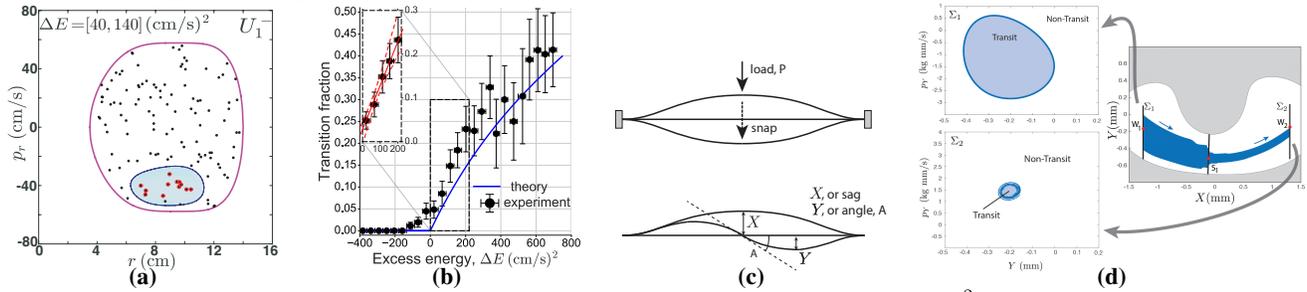


Figure 2: (a) On the Poincaré section U_1^- we show a narrow range of energy ($\Delta E \in (40, 140)$ (cm/s)²) and label intersecting trajectories as no transition (black) and imminent transition (red) to quadrant 2, based on their experimentally measured behavior. The theoretical tube cross-section leading to transition at excess energy $\Delta E = 140$ (cm/s)² intersects U_1^- along the blue curve. Its interior is shown in cyan and includes the experimental transition trajectories. The outer closed curve (magenta) is the boundary of the energy surface $\mathcal{M}(\Delta E)$ on U_1^- . See video: <https://youtu.be/YZKYx0N9Zug> (b) Transition fraction of trajectories as a function of excess energy. The theoretical result is shown (blue curve) and experimental values are shown as filled circles (black) with error bars. For small excess energy above critical, the transition fraction shows linear growth (see inset) with slope $1.0 \pm 0.23 \times 10^{-3}$ (s/cm)², in agreement with the analytical result. (c) The two dominant degrees of freedom of the shallow arch, symmetric and asymmetric modes, represented by coordinates X and Y , resp. (d) In the shallow arch model, the transition tube from the left well to the right well with damping present is shown.

Connection with structural mechanics: the buckled beam model example

The laterally-loaded, mildly buckled, beam (or moderately shallow arch) is an archetypal nonlinear structural system in mechanics [1] (Fig. 2(c)). The trivial equilibrium and its snapped-through counterpart are potential energy minima. For a range of geometries, a 2 DOF model (symmetric and asymmetric modes, Fig. 2(c)) captures the main behavior, and shows the energetically expedient dynamic transitions as trajectories are influenced by the lowest energy unstable equilibria in passing through (or not) to the snapped-through configuration, as in Fig. 2(d).

Conclusions

The transitioning points at each energy interval are found to be within the theoretical tube boundary (blue curve); as in, e.g., Fig. 2(a). Furthermore, the fraction of transitioning trajectories increases linearly with ΔE , Fig. 2(b), as expected from arguments related to the phase space flux over a rank-1 saddle [4], and agreement between observed and theoretical values is within experimental error. This experimental validation of tube dynamics establishes a framework which can be exploited for control, e.g., avoiding or triggering transition between metastable states in systems of 2 or more degrees-of-freedom [4, 1, 2]. The authors acknowledge NSF grants 1537349 & 1537425.

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