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Dynamics of SHS in periodic media

Michael Frankel^{a,*}, Victor Roytburd^b^a*Department of Mathematical Sciences, Indiana University Purdue University, Indianapolis,
IN 46202-3216, USA*^b*Department of Mathematical Sciences, Rensselaer Polytechnic Institute, Troy, NY 1218-3590, USA*

Abstract

Solutions of a 1-D free-interface problem modeling a solid combustion front (SHS) propagating in a combustible mixture with periodically varying concentration of the reactant, either smooth or discontinuous, exhibit the classical phenomenon of mode locking. Numerical simulation shows a variety of locked periodic, quasi-periodic, and chaotic solutions. A bifurcation diagram obtained via the correlation dimension of the orbits suggests the existence of a dense set of Arnold's tongues.

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1. Introduction

In a recent letter, [1] we reported observations of frequency locking for the Stefan problem with kinetics in response to a spatially periodic nonhomogeneity of the medium. The current paper presents a brief discussion of a further investigation of this phenomenon.

The free-interface problem under consideration arises naturally as a mathematical model of condensed-state combustion (also known as self-propagating high-temperature synthesis or SHS [10]), solidification [6], crystallization in thin films [9], etc. The numerical experiments described in [4] demonstrated that the unperturbed problem generates a variety of complex thermokinetic oscillations including Hopf bifurcation, period doubling cascades, Shilnikov–Hopf bifurcation, etc.

* Corresponding author.

E-mail address: mfrankel@math.iupui.edu (M. Frankel).

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The new feature that was added in [1] was a periodic perturbation of the initial concentration of the so-called deficient component which controls the reaction rate in the case of the combustion synthesis. We observed a variety of quasi-periodic and complex periodic regimes with periods that are various multiples of the perturbation period. This is a clear manifestation of the classical phenomenon of frequency locking. Moreover, as we demonstrate below, *these features occur persistently even for a discontinuous concentration* modeling layered materials in combustion synthesis (global well-posedness of the problem with discontinuous coefficients is briefly discussed in Section 2).

The physical phenomena modeled by periodically driven dynamical systems appear in many fields (see e.g. [11]) such as lasers, superconductors (Josephson's junctions), mechanical engineering, etc. These systems are known to exhibit rich patterns of behavior that oftentimes includes mode locking, with the mode-locked bands usually having the structure of the so-called Arnold's tongues in the amplitude–frequency parameter space.

It is necessary to mention that the analysis of externally periodically (in time) forced systems is usually carried out for an appropriate ansatz which consequently leads to a low-dimensional ODE. In our case, however, we make no attempt of such reduction, neither are we aware of any ansatz for a solution leading to it, while *the internal “forcing” is periodic in space*, and the system is formally autonomous.

Below, we present several examples of numerical solutions and a rather detailed map of resonance bands in the amplitude–frequency parameter space showing typical Arnold's tongues. The map was obtained by computing the correlation dimension of the orbit in the phase space of the solutions of the problem. We remind the reader that every point in the parameter space is a result of numerical simulation of a nontrivial free-interface problem for a partial differential equation. It turns out that even a rough approximation of the correlation dimension is sufficient to distinguish between the periodic and aperiodic problems. To the best of our knowledge, this method has not been previously employed for bifurcation diagrams of such type.

2. Free-interface problem

The combustion of condensed matter represents a wave of exothermic chemical reaction that transforms a solid combustible mixture directly into a solid product. The 1-D model consists of differential equations for the temperature u of the mixture and the relative concentration of the so-called deficient reactant Z (see e.g. Shkadinsky et al. [8]):

$$u_t = \kappa u_{xx} + qW(Z, u), \quad Z_t = -W(Z, u),$$

where κ is the thermal diffusivity, W is the chemical reaction rate, and q is the heat release.

Due to a strong temperature dependence of the reaction rate, there is a well-defined narrow region (flame front) where the bulk of chemical reaction and the heat release occur. Thus, the distributed chemical reaction can be modeled by the δ -function, $W = Z(s(t))g(u)\delta(x - s(t))$, located at the interface $x = s(t)$ between the fresh $Z = Z(s(t))$ and burned $Z = 0$ material (see [12]). In the context of solidification [6] or crystallization of thin films [9], the free-interface model is conceptually even simpler: the latent heat of the phase transition at the interface is diffused into the surrounding matter.

The model with the δ -function source is then rewritten as a system of two heat equations coupled at the interface:

$$u_t = u_{xx}, \quad x \neq s(t), \quad u(x, 0) = u_0(x) \geq 0, \tag{1}$$

$$Z_0(s(t))g[u(s(t), t)] = v(t), \quad u_x^+(s(t), t) - u_x^-(s(t), t) = v(t), \tag{2}$$

where $v(t)$ is the interface velocity, $s(t) = \int_0^t v(\tau) d\tau$ is its position, u is the temperature, and u_x^+ and u_x^- are the right-side and left-side derivatives. At $-\infty$, the surrounding matter is assumed to be at the temperature of the fresh combustible, while the temperature of the burned matter as well as its gradient is bounded: $u(-\infty, t) = 0$, $u(\infty, t) < C$, $|u_x(\infty, t)| < C$.

Under reasonable assumptions on the kinetic function g , one can rigorously prove that problem (1)–(2) possesses global in time, uniformly bounded classical solutions (see [3]).

Theorem 1. *Let $0 < Z_{\min} \leq Z_0(x) \leq Z_{\max}$ be a Lipschitz continuous function. Suppose that the kinetic function g satisfies the following assumptions: $g(u)$ is a continuous, monotone decreasing, negative function with bounded derivative on $(0, \infty)$ and $g(0) = -g_0$ for some $g_0 > 0$; $\lim_{u \rightarrow \infty} g(u)/u = 0$. Then for continuous and bounded initial data there exists one and only one classical solution of the free-interface problem (1)–(2). The solution is uniformly bounded for all $t > 0$.*

Note that $v_0 = g_0 Z_{\min}$ is the minimal possible speed of the interface. The main point of the global existence proof is the a priori estimate.

Theorem 2. *Let $u(x, t), v(t)$ be a classical solution of the free-interface problem (1)–(2) and $\sup_{-\infty < x < \infty} |u_0(x)| = M$; then $|u(x, t)| \leq 2(g_1/v_0 + M)/Z_{\min}$, where g_1 is a constant dependent on the kinetic function g . Since $v = Z_0[s(t)]g[u(s(t), t)]$, for the velocity we have the obvious bound $|v| \leq Z_{\max}g(2(M + g_1/v_0)/Z_{\min})$.*

So far the concentration Z_0 has been assumed to be continuous. For some applications it is natural to use discontinuous or, rather, piecewise continuous Z_0 , which corresponds to layered structures. It is easy to extend the previous results to this case.

Proposition 3. *The results of Theorems 1–2 hold if $Z_0(x)$ is a uniformly piecewise Lipschitz continuous function.*

Proof. It is convenient to introduce the change of variables $\tau = s(t)$, $x = x$. Denote $w(\tau) = v(t(\tau))$; then $\partial/\partial t = w(\tau)\partial/\partial\tau$, and the original temporal variable can be recovered through $t = \int_0^\tau d\eta/w(\eta)$. As a result, the problem takes the form of a forced autonomous problem

$$w(\tau)u_\tau = u_{xx}, \quad x \neq \tau, \quad \tau > 0, \tag{3}$$

$$Z_0(\tau)g[u(\tau, \tau)] = w(\tau), \quad u_x^+(\tau, \tau) - u_x^-(\tau, \tau) = w(\tau).$$

Obviously the existence result (Theorem 1) for a continuous Z_0 yields a corresponding result for the system in (3). Thus, we can solve the problem “piecewise” from $\tau = 0$ to $\tau = \tau_1$, where the first discontinuity of Z_0 occurs. The final values of dependent variables at $\tau = \tau_1$ serve as initial conditions for the problem on the interval (τ_1, τ_2) etc. \square

Unlike typical forcing, the initial concentration in (1)–(2) is a function of the dependent variable of the problem $s(t)$. Thus, strictly speaking, the problem is autonomous. Although in terms of the new variables the perturbation becomes “time dependent” (3), a highly variable coefficient $1/v$ at the “time” derivative of the heat equation makes numerics substantially more challenging. For this reason, we use the original formulation for the numerical solution. Consequently, the driving frequency ω and the frequency of the periodic solution, as seen in the power spectra and temporal dynamics in the figures below, are not the same.

It is important to emphasize that the rigorous results of existence and uniform boundedness of solutions provide a firm foundation for the numerical simulations presented in the paper.

3. Unforced dynamics

Prior to turning to the nonhomogeneous case, consider the basic problem with $Z_0(x) \equiv 1$. It is convenient to represent the kinetics in the form

$$g(u) := 1 + \alpha J(u), \quad (4)$$

where the function $J(\xi) = (g(\xi) - 1)/\alpha$ is normalized so that $J(1) = 0$, $J'(1) = -1$. This makes the problems with different kinetics identical in terms of linearization about the basic solution, while $\alpha > 0$ can be treated as the principal instability parameter of the problem. The spatial variable x is selected so that the *interface propagates to the left*.

For the Arrhenius-type kinetics

$$v = g(u) = -\exp\left[\frac{\alpha(u-1)}{\sigma + (1-\sigma)u}\right], \quad (5)$$

which has been employed for the DNS of the paper, α is the scaled activation energy for the exothermic chemical reaction that occurs at the interface, and σ is the ratio of temperatures of the fresh and burned material for the traveling wave solution.

The problem (1)–(2) has a unique traveling wave solution

$$u_b(x, t) = \begin{cases} \exp(x+t), & x \leq -t, \\ 1, & x > -t, \end{cases} \quad s_b = -t,$$

provided J is monotone. A linear stability analysis indicates that the loss of stability occurs via a Hopf bifurcation at $\alpha_{\text{cr}} = \sqrt{5} + 2$, with the corresponding frequency $\omega_{\text{cr}} \simeq 1.03$ and $T_{\text{cr}} = 2\pi/\omega_{\text{cr}} \simeq 6.1$. This frequency can be viewed as a “natural” frequency of the problem that predicates the existence of locked regimes described in the next sections. Depending on the parameters, the system exhibits a classical transition to chaos through Feigenbaum’s cascade, a Shilnikov–Hopf bifurcation, etc. (see [4] for details).

4. Frequency locking for harmonically varying media

In this section, we discuss the phenomenon of frequency locking for the free-boundary problem (1)–(2), with the periodically varying mass concentration

$$Z_0(x) = 1 + a \cos(2\pi\omega x). \quad (6)$$

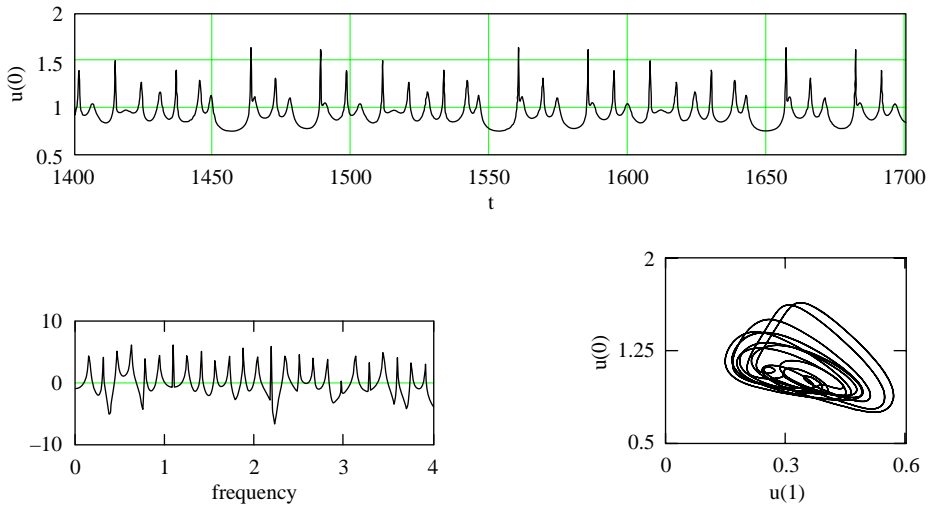


Fig. 1. $a = 0.1$, $\omega = 0.1$: ultraharmonic frequency locking of large multiplicity. Top: interface temperature profile; bottom-left: power spectrum; bottom-right: 2-D projection of the orbit.

For DNS below, we employed a finite-difference scheme in the coordinate system attached to the interface $\eta = x - s(t)$ (see [4] for details). In mathematical terms, the free-boundary problem in (1)–(2) governs the temporal evolution in the infinitely dimensional “phase” space of functions $u(\eta, t)$ and scalars v .

The results are represented by the time histories of the interface temperature $u(\eta, t)|_{\eta=0}$. We also describe dynamics through projections of the infinitely dimensional phase space onto the plane $[u(-1, t), u(0, t)]$, i.e., the temperature profile at each t is represented by two values, at $\eta = -1$ and $\eta = 0$. The corresponding figures below contain three graphs: an interface temperature profile (top), its power spectrum (bottom-left), and a two-dimensional projection of the orbit (bottom-right).

Fig. 1 depicts a complex periodic orbit that is a result of frequency locking of large multiplicity in the ultraharmonic region (note that the forcing has a *spatial* not temporal period). As parameters of forcing vary, one encounters a whole range of complex periodic, quasi-periodic, and chaotic orbits. For example, Fig. 2 shows a typical quasi-periodic orbit in the subharmonic domain. We remark that quasi-periodic solutions with more than two basic periods have also been observed.

5. Bifurcation structure via correlation dimension

To demonstrate possible dynamic scenarios in the parameter space, as the main technical device we employ the asymptotic (for t large) correlation dimension of the orbits (see [2] for a discussion of correlation dimension in the context of unperturbed free-interface problems). To the best of our knowledge, *this is the first application of correlation dimension for the investigation of bifurcation structure, in particular for PDEs.*

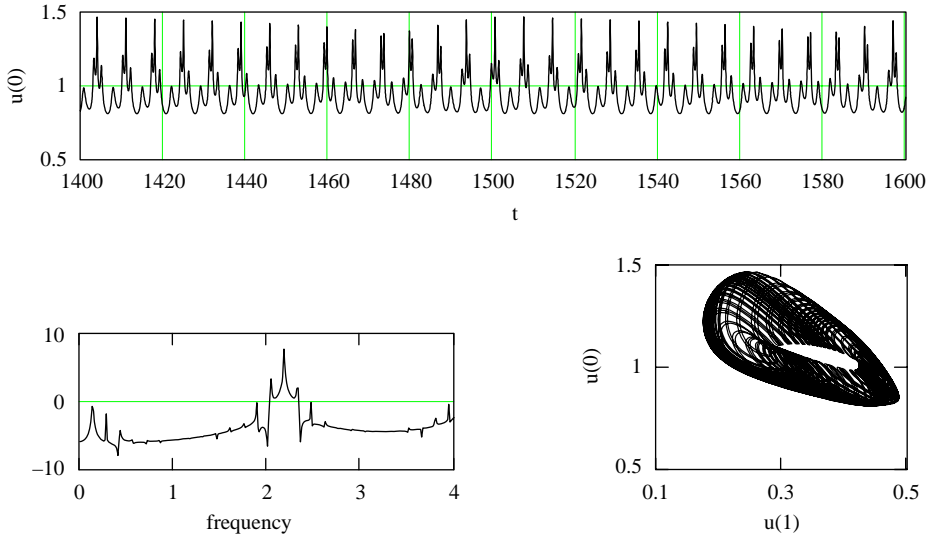


Fig. 2. A quasi-periodic orbit in the subharmonic region, $a = 0.3$, $\omega = 0.65$.

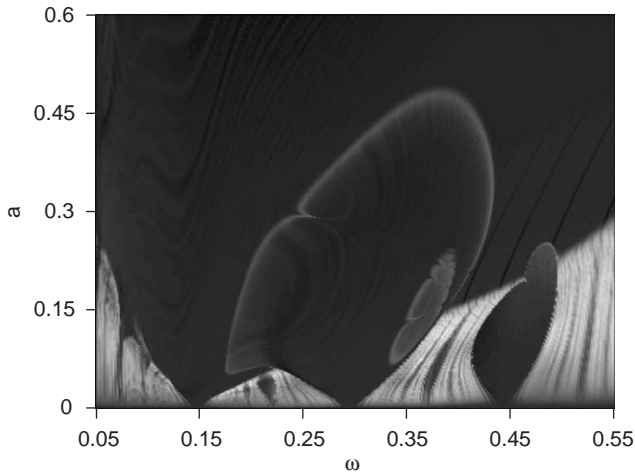


Fig. 3. Bifurcation diagram in the ωa plane.

We are primarily interested in the qualitative understanding of dynamics, in particular in the rough distinction between periodic and aperiodic regimes. Our experience shows that the bifurcation structure computed via correlation dimension is largely insensitive to the sample (finite-dimensional projection of the phase space) size ≥ 2 . It is only because of this circumstance that we are able to obtain a detailed bifurcation map at a reasonable computational cost.

Fig. 3 depicts a bifurcation map obtained for the kinetics (5) with $\sigma = 0.15$, $\alpha = 5.2$. The perturbation amplitude and frequency range in the intervals $[0, 0.6]$ and $[0.05, 0.55]$,

respectively, with 400 mesh points in each variable. Note that every point is a result of DNS of a free-interface problem, and the computational cost of a detailed map becomes prohibitive. To make the problem with 16×10^4 DNS tractable from the computational viewpoint, we have to choose a rather crude space mesh size. Consequently, the critical values for the bifurcation parameter α undergo shift from the theoretical values: for example, the value $\alpha=5.2$ corresponds to a simple periodic relaxational oscillation for the unperturbed problem. The darker areas, corresponding to lower correlation dimension, represent periodic orbits, while the lighter areas represent aperiodic orbits. One can clearly recognize the classical Arnolds tongue structure. We observe increasingly narrower secondary tongue corresponding to periodic orbits of higher multiplicity. Remarkably, correlation dimension is able to capture even rather fine transitions between the qualitatively different periodic regimes. Although theoretically the correlation dimension of any periodic regime is equal to 1, in the vicinity of the bifurcation convergence to the attractor is very slow. This is reflected in the higher values of the *numerical* approximation for the dimension. For example, the large lightly shaded oval contour separates between simple periodic (above the oval) and double-periodic (inside) orbits.

There are a number of complex features observed in the dynamical response of the forced van der Pol equation [7] and other similar dynamical systems that one would attempt to verify for our system: for instance, whether the Arnold's tongues represent a dense set with its complement forming a Cantor set in the (a, ω) plane, whether the Feigenbaum sequences occur within the tongues, etc. Since the dynamics of the unforced problem changes dramatically as the bifurcation parameter α increases, it would also be interesting to investigate how the frequency-locking response changes with increasing α .

6. Frequency locking for layered media

Traditionally, the theory of condensed-phase combustion is based on the assumption of homogeneous combustible mixture. However, motivated by emerging engineering applications there was an increased interest in the combustion of heterogeneous media; see [5] and references therein. In [5] the authors propose a mathematical model of flame propagation in a layered heterogeneous system with the medium consisting of layers of combustible material separated by layers of inert heat conducting matter.

Unlike the distributed kinetics model studied in [5], the free-interface formulation (1)–(2) prohibits the velocity to vanish and therefore does not allow for zero reactant concentration (presence of the inert material). We model a layered medium by a piecewise-constant periodic function with the inert material approximated by intervals of lower (but nonzero) concentration:

$$Z_0(x) = 1 + a \begin{cases} 1, & n < \omega x < n + 1/2, \\ -1, & n + 1/2 < \omega x < n + 1. \end{cases}$$

This particular form of the perturbation has been selected for comparison with the harmonic perturbation (6). Some other related questions, such as dependence on the relative size of active and inert layers and homogenization issues, will be addressed elsewhere [3].

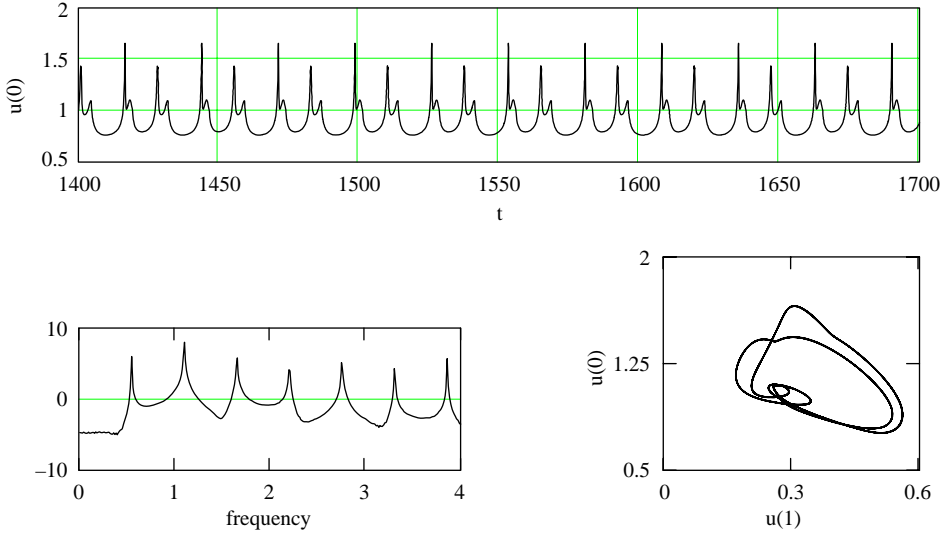


Fig. 4. $a = 0.1$, $\omega = 0.1$: ultraharmonic frequency locking for discontinuous concentration.

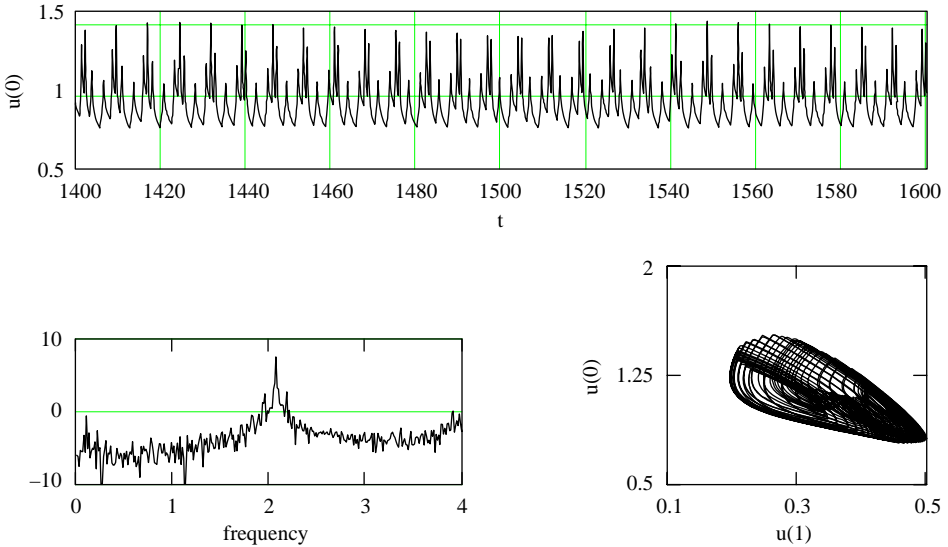


Fig. 5. A subharmonic quasi-periodic orbit for discontinuous concentration $a = 0.3$, $\omega = 0.65$.

Remarkably, even for the discontinuous forcing the problem exhibits the mode-locking phenomenon.

To compare with the harmonic perturbation above, we select the same amplitudes and periods of forcing. Fig. 4 depicts a periodic orbit in the ultraharmonic region (albeit simpler

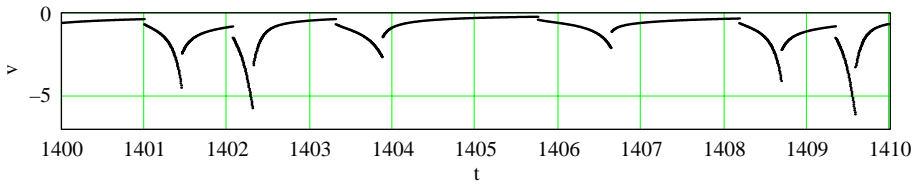


Fig. 6. Velocity profile for $a = 0.3$, $\omega = 0.65$.

than in Fig. 1). Due to the prohibitive computational cost, we have not been able to produce a bifurcation diagram similar to Fig. 3. However, for moderate amplitudes we observed more significant differences in the ultraharmonic region. Fig. 5 shows a quasi-periodic orbit in the subharmonic domain, which appears very similar to its harmonic counterpart (Fig. 2). Yet looking at the velocity profile (Fig. 6) one clearly observes sizable jumps.

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