INVARIANT TORI FOR A CLASS OF SINGLY THERMOSTATED HAMILTONIANS

LEO T. BUTLER

ABSTRACT. Let $H$ be a $C^r$ proper hamiltonian on $T^*\Sigma$ where $\Sigma = \mathbb{R}$ or $\mathbb{T}$ and $r > 4$. This paper proves sufficient conditions for the existence of a positive measure set of invariant KAM tori in an associated singly thermostated vector field on $T^*\Sigma \times \mathbb{R}$. We apply this result to 4 important single thermostats in the literature. This extends results of Legoll, Luskin & Moeckel [7, 8].

1. INTRODUCTION

In equilibrium statistical mechanics, a mechanical Hamiltonian $H$ is viewed as the internal energy of an infinitesimal system that is immersed in, and in equilibrium with, a heat bath $B$ at the temperature $T$. A dynamical model of the exchange of energy was introduced by Nosé [10], based on earlier work of Andersen [2]. This consists of adding an extra degree of freedom $s$ and rescaling momentum by $s$:

$$ F = H(q, ps^{-1}) + N(s, p_s), $$

where $N(s, p_s) = \frac{1}{2M} p_s^2 + nkT \ln s$, \hspace{1cm} (1)

$n$ is the number of degrees of freedom of $H$, $M$ is the “mass” of the thermostat and $k$ is Boltzmann’s constant. Solutions to Hamilton’s equations for $F$ model the evolution of the state of the infinitesimal system along with the exchange of energy with the heat bath.

Hoover reduced Nosé’s thermostat by eliminating the state variable $s$ and rescaling time $t$ \hspace{1cm}[4]:

$$ q = q, \quad \rho = ps^{-1}, \quad \frac{d}{d\tau} = \frac{d}{dt}, \quad \xi = \frac{ds}{d\tau}. $$

The Nosé-Hoover thermostat of the 1 degree of freedom Hamiltonian $H$ is the following vector field:

$$ \dot{q} = H_\rho, \quad \dot{\rho} = -H_q - \epsilon \xi \rho, \quad \dot{\xi} = \epsilon (\rho \cdot H_\rho - T), $$

where $\epsilon^2 = 1/M$.

Hoover observed in his original paper that this thermostat was ineffective in producing the statistics of the Gibbs-Boltzmann distribution from single orbits of the thermostated harmonic oscillator \hspace{1cm}[4]. Numerous extensions of the Nosé-Hoover thermostat have appeared. This note focuses on those which model the exchange

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of energy with the heat bath using a single, additional thermostat variable ($\xi$ in \ref{sec:thermostat}), the so-called single thermostats.

The main result of this paper is

**Theorem 1.1.** Let $\Sigma = \mathbb{R}$ or $\mathbb{T}^1$ and $H : T^*\Sigma \rightarrow \mathbb{R}$ be a real-analytic, mechanical hamiltonian that is Morse. If $T$ is a

1. Nosé-Hoover thermostat (\ref{sec:nose-hoover});
2. Tapias, Bravetti & Sanders logistic thermostat (\ref{sec:tapias-bravetti-sanders});
3. Watanabe-Kobayashi thermostat (\ref{sec:watanabe-kobayashi}); or
4. Hoover-Sprott-Hoover thermostat (\ref{sec:hoover-sprott-hoover}),

then for each inverse temperature $\beta > 0$, there is an $\epsilon(\beta) > 0$ such that for all $\epsilon \in [0, \epsilon(\beta))$, the thermostated vector field $X_H + \epsilon T$ has a positive measure set of invariant tori.

Legoll, Luskin and Moeckel \cite{7, 8} prove the existence of KAM tori for the Nosé-Hoover thermostated harmonic oscillator; they indicate that the general case reduces to proving the non-isochronicity of an associated averaged hamiltonian. The present note derives the averaged hamiltonian and uses this to prove case (1) of the above theorem (see \ref{sec:nose-hoover} and remark \ref{rem:isochronicity}). Watanabe and Kobayashi \cite{17} introduce a 2-parameter family of thermostats. They show, with the thermostated harmonic oscillator, that the associated averaged hamiltonian has a first integral. The present note extends this by deriving the hamiltonian and symplectic structure of the averaged thermostat in the general setting in order to prove case (3) above. The thermostats of Tapias, Bravetti & Sanders and Hoover, Sprott & Hoover have been investigated by computationally-oriented researchers with the aim of finding ergodic single thermostats \cite{15, 5, 6}.

A related obstruction is observed in the classical adiabatic piston problem. In one variant of this problem, a box of fixed size is filled with a gas that is separated by a massive piston. The piston is free to move parallel to an axis of the box without friction. Neishtadt & Sinai and Wright \cite{9, 18} show that the Anosov-Kasuga averaging theorem, combined with ergodicity of the gas dynamics, imply that in the infinite mass limit the piston oscillates deterministically and for large but finite mass $M$ the piston’s motion is approximately oscillatory for an $O(\sqrt{M})$ time period. Shah, et. al. \cite{14} explain that in slow-fast systems the Gibbs volume entropy of the fast subsystem is conserved, so ergodicity of the fast subsystem frustrates ergodicity of the whole. Indeed, for the Nosé-Hoover thermostat, it is proven that in the decoupled limit of $\epsilon = 0$, the thermostat’s state oscillates in a potential well $U$ where $U$ is an analogue of the free energy of the fast subsystem (see eq. \ref{eq:thermostat-energy}).

The outline of this paper is: \ref{sec:thermostat} introduces a definition of a single thermostat for a hamiltonian system; \ref{sec:notation} establishes notation and terminology to discuss 1 degree-of-freedom hamiltonian systems; \ref{sec:poincare} derives a Poincaré return map, invariant symplectic form, & hamiltonian for the averaged thermostated vector field; \ref{sec:proof} proves Theorem \ref{thm:main} using the results of the previous section.

### 2. Single Thermostats

Let $\Sigma$ be a smooth manifold, $T^*\Sigma$ its cotangent bundle and $\{,\}$ the canonical Poisson bracket. Let $\pi : P \rightarrow T^*\Sigma$ be a trivial line (or circle) bundle over $T^*\Sigma$. One should think of $P$ as an extended phase space which models the state of a mechanical system with points $(q, p) \in T^*\Sigma$ and the thermostat’s local state with
Given a smooth Hamiltonian $H : T^* \Sigma \to \mathbb{R}$, let $X_H = \{H \circ \pi, \cdot\}$ be the Hamiltonian vector field lifted to $P$. Say that a probability measure

$$d\mu_\beta = Z_\beta(1)^{-1} \exp(-\beta G_\beta(q,p,\xi)) \, dq \, dp \, d\xi$$

projects to the probability measure

$$dm_\beta = Z(\beta)^{-1} \exp(-\beta H(q,p)) \, dq \, dp$$

if $dm_\beta = \int_\Sigma d\mu_\beta$, i.e. if $dm_\beta$ is a marginal of $d\mu_\beta$. It is a natural convention in the literature on thermostats to postulate that the invariant measure $d\mu_\beta$ of the thermostated vector field projects to the Gibbs-Boltzmann probability measure $dm_\beta$ of the mechanical system. Somewhat surprisingly, the main result of this paper does not require such an assumption.

**Definition 2.1.** A smooth vector field $T$ on $P$ is a thermostat for $H$ if there is a smooth probability measure $d\mu_\beta$ on $P$ such that the following holds

1. $d\mu_\beta$ is invariant for $Y_\epsilon = X_H + \epsilon T$ for all $\epsilon$;
2. $G_\beta$ is proper for all $\beta > 0$;
3. there exists an interval of regular values of $H$, $[c_-, c_+]$, and constants $d_\pm$ such that
   a. the average value of $(d\xi, T)$ is of opposite sign on $H^{-1}(c_-) \cap \xi^{-1}([d_-, d_+])$ and $H^{-1}(c_+) \cap \xi^{-1}([d_-, d_+]);$
   b. the average value of $(dH, T)$ is of opposite sign on $\xi^{-1}(d_-) \cap H^{-1}([c_-, c_+])$ and $\xi^{-1}(d_+) \cap H^{-1}([c_-, c_+]).$

The requirement that the (log of the) density of the invariant measure $d\mu_\beta$ be proper may appear unnatural at first sight. However, it implies that the Hamiltonian $H$ is proper—which is natural—and it is a property shared by all examples in the literature known to the author (see section below).

Definition 2.1 encompasses that of Ramshaw [11, Section V]. This latter work, which develops a formalism that encapsulates earlier single thermostats, posits specific forms of $G$ and $T$.

The main result of this paper is to give necessary conditions on the triple $(H, G, T)$ for the existence of a positive-measure set of invariant tori in the weakly-coupled limit of $\epsilon = 0$.

**3. Preliminary Materials**

This section establishes notation and terminology for subsequent sections. Throughout, $\Sigma = \mathbb{R}$ or $\mathbb{T}$ and $T^*\Sigma = \{(q,p) \mid q \in \Sigma, p \in \mathbb{R}\}$ is the cotangent bundle. A smooth function $H : T^*\Sigma \to \mathbb{R}$ (also called a Hamiltonian function) is Morse if, at each critical point its Hessian is non-degenerate; it is a topological Morse function if each critical point has a neighbourhood homeomorphic to a neighbourhood of a critical point of a Morse function $H'$ and $H'$ is conjugate to $H$ by this homeomorphism; $H$ is proper if the pre-image of each compact set is compact; $H$ is mechanical if $H(q,p) = \frac{1}{2}p^2 + V(q)$ and quasi-mechanical if $H(q,p) = F(p) + V(q)$ where $F$ is
even, $F(0) = 0$ and $F'(p)/p > 0$ for all $p \neq 0$; and, when $\Sigma = \mathbb{R}$, asymptotically convex if $H^{-1}((-\infty, c])$ is a convex set for all $c$ sufficiently large.

The Morse property for quasi-mechanical hamiltonians is equivalent to $F''(0) > 0$ and $V''(q_c) \neq 0$ at every critical point $q_c$. Properness implies that $V(q) \to \infty$ as $|q| \to \infty$. Asymptotic convexity is equivalent to positivity of the signed curvature of all sufficiently large energy levels. It implies, for example, that the critical set is finite.

This paper is primarily concerned with asymptotically convex, proper, mechanical, topological Morse hamiltonians $H(q, p) = \frac{1}{2}p^2 + V(q)$. Such functions do not have local maxima, only local minima and saddle critical points. Moreover, properness implies that $V$ is bounded below and it attains that lower bound (which will be assumed to be 0 henceforth). The Morse property plus asymptotic convexity implies that there are only finitely many critical points. If $c$ is a local minimum, then $H^{-1}(c)$ is a union of a finite number $r_c$ of regular circles and $k_c$ minimum points. A neighbourhood $N_c$ of the critical level is a disjoint union of $r_c$ annuli and $k_c$ disks. On the other hand, if $c$ is a saddle critical value, then since $H$ has no local maxima, $H^{-1}(c)$ also has a simple description: there are $r_c \geq 0$ regular circles, and $s_c > 0$ singular path components. When $\Sigma = \mathbb{R}$, the $i$-th singular component of $H^{-1}(c)$ consists of $k_{c,i} + 1 > 1$ circles pinched at $k_{c,i}$ distinct points. A small neighbourhood $N_c$ of $H^{-1}(c)$ is a disjoint union of $r_c$ annuli and $s_c$ disks where the $i$-th disk has $k_{c,i} + 1$ disjoint, smaller disks removed from its interior. The boundary of $N_c$ consists of the boundary of those deleted smaller disks and the “lower half” of the annuli boundaries (which make up $H^{-1}(c-\epsilon)$) and the boundary of the larger disk and “upper half” of the annuli boundaries (which make up $H^{-1}(c+\epsilon)$). When $\Sigma = \mathbb{T}^1$, the above description holds except for the largest saddle critical value: in that case, a neighbourhood $N_c$ of $H^{-1}(c)$ is easiest to describe: it is a cylinder with $k_c$ disjoint disks removed. The boundary of $N_c$ consists of 2 essential circles (= $H^{-1}(c+\epsilon)$) and $k_c$ inessential circles (= $H^{-1}(c-\epsilon)$); $N_c$ retracts onto $H^{-1}(c)$, which is max $\{2, k_c\}$ circles pinched at $k_c$ points. Finally, if $c$ is a critical value of mixed type (i.e. $H^{-1}(c)$ contains both a local minimum and a saddle), then $H^{-1}(c)$ contains $r_c$ regular circles, $k_c$ local minima and $s_c$ saddle components and the above descriptions of a neighbourhood $N_c$ are combined. Because the saddle components are most important for the purposes here, a critical value $c$ will be said to be a saddle value if $s_c > 0$, i.e. if $H^{-1}(c)$ contains a saddle.

The preceding paragraph implies that coarse topological structure of the levelsets of $H$ can be summarized in a directed tree $\Gamma_H$ with the following structure: (see figure 3)

$\Sigma = \mathbb{R}$: $\Gamma_H$ is a finite tree with each branch either terminating at a vertex (a local minimum) or branching into $s_c > 1$ separate branches (a saddle), the root vertex is labeled $\infty$ and the highest vertices are labeled 0; or

$\Sigma = \mathbb{T}^1$: $\Gamma_H$ is obtained from a finite tree similar to that described in the first case by splitting the root branch and vertex in two (and labeling the latter as $\pm \infty$).

Each edge of $\Gamma_H$ is naturally homeomorphic to a closed interval by $H$, and $H$ partially orders the graph, too.

The graph $\Gamma_H$ has a second, equally valuable description. Each point $\gamma \in \Gamma_H$ is a path-connected component of a level set of $H$. When $dH|_{\gamma}$ does not vanish (i.e. when $\gamma$ lies in the interior of an edge), $\gamma$ is a circle and an orbit of the hamiltonian
flow $\varphi^t$ of $H$. Moreover, there is a canonical quotient map $\psi$ and functions $I, \tilde{I}$ such that

$$\bigcup T^1 \times \mathbb{R}$$

commutes. The quotient map $\psi$ is the quotient map obtained from the equivalence relation $\sim$ where $X \sim X'$ iff $H(X) = H(X')$ and $X$ and $X'$ lie in the same path-connected component of $H^{-1}(H(X'))$. The function $\tilde{I}$ is defined by

$$2\pi \tilde{I}(\gamma) = \oint_{\gamma} p \, dq.$$

$\tilde{I}$ is continuous on $\Gamma_H$ less the set of saddle vertices. At a saddle vertex $\sigma$ one has the identity

$$\lim_{\gamma \to \sigma} \tilde{I}(\gamma) = \sum_{\gamma \sim \sigma} \lim_{\gamma \to \sigma} \tilde{I}(\gamma),$$

where the right-hand sum is the sum over all edges incoming to $\sigma$. This also holds for vertices of local minima, with the convention that the sum over an empty set is 0 (i.e. $\tilde{I}$ is continuous at local minimum vertices).

If $B_H = \Gamma_H - V_H$ is the set of points that are not vertices, i.e. $B_H$ is the union of the interiors of the edges of $\Gamma_H$, and $L = \psi^{-1}(B_H)$, then $\psi|L$ is a proper submersion whose fibres are circles. Classical constructions yield the existence of angle-action variables $(\theta, I) : L \to \bigcup T^1 \times \mathbb{R}$ where the disjoint union is taken over the edge set of $\Gamma_H$ \cite{3}. In these variables, $H = H(I)$ and $H_I > 0$ since $\tilde{I}$ is monotone increasing in $H$. If $\sigma$ is a saddle vertex, then as $\gamma \to \sigma$ (from above or below), $H_I(\tilde{I}(\gamma)) \to 0$ since the period goes to $\infty$; if $\sigma$ is a local minimum vertex, then as $\gamma \sim \sigma$, $H_I(\tilde{I}(\gamma)) \to \omega_{\sigma} > 0$ where $\omega_{\sigma}$ is the frequency of the linearized oscillations at $\sigma$. It follows that the function

$$K(I) = I \cdot H_I(I)$$

(5)

is a continuous, non-negative function that vanishes only on the vertex set of $\Gamma_H$ and is smooth on $B_H$.

Let it be noted that $\Gamma_H$ is defined for all $C^2$ proper hamiltonians, but it is not as nice in the general case. If $H$ is proper, topologically Morse, has a compact critical set and no local maxima, then $\Gamma_H$ has the structure and properties described above. An interesting question is when does there exist a symplectic diffeomorphism $\varphi$ such that $H$ and $H'$ are conjugate by $\varphi$, $H' = H \circ \varphi$, and more precisely, is every hamiltonian with the 4 properties listed in the previous sentence conjugate to a (quasi)-mechanical hamiltonian?

### 4. Weakly Coupled Single Thermostats

In the sequel, $H : T^* \Sigma \to \mathbb{R}$ is a proper, smooth function; $T$ is a thermostat for $H$ in the sense of definition 2.1 and $d\mu_\beta$ is an invariant probability measure in the same sense.
In the variables \((\theta, I, \xi)\) on \(\pi^{-1}(L) \subset P\), one has
\[
X_H = H_I \partial_\theta, \quad T = a \partial_\theta + b \partial_I + c \partial_\xi
\]
where \(a, b, c\) are smooth functions of \((\theta, I, \xi)\). The invariance of \(d\mu_\beta\) implies that
\[
\langle dG, X_H \rangle \equiv 0, \quad \text{so} \quad G = G(I, \xi) \quad \text{and} \quad (7)
\]
\[
\beta \langle dG, T \rangle - \text{div}(T) \equiv 0, \quad \text{so} \quad a_\theta = \beta b G_I - b_I + \beta c G_\xi - c_\xi. \quad (8)
\]
Let \(\bar{x}\) denote the mean value of \(x\) over \(\theta\): \(\bar{x}(I, \xi) = \frac{1}{2\pi} \int x(\theta, I, \xi) d\theta\). If \(x = \bar{x}\), then the over-bar will be omitted. Equations 7–8 imply that
\[
0 \equiv \beta \bar{b} G_I - \bar{b}_I + \beta \bar{c} G_\xi - \bar{c}_\xi. \quad (9)
\]
Let \(P_{c,d} = H^{-1}([c_-, c_+]) \cap \xi^{-1}([d_-, d_+])\) be the compact set from part (2) of definition 2.1. The Hamiltonian \(H\) is critical-point free on the invariant set \(P_{c,d}\), so \(H_I \neq 0\) on this set. Therefore, one can rescale the vector field \(Y_\epsilon\) to \(\hat{Y}_\epsilon = \frac{\epsilon}{H_I} H_I (b \partial_I + c \partial_\xi) + O(\epsilon^2) \quad (10)\)
\[
= \epsilon \hat{R}_0 + O(\epsilon^2),
\]
where \(\tau \equiv \theta \mod 2\pi\) is the time along solutions; then \(F_\epsilon = \varphi_\epsilon^{2\pi}\).
Lemma 4.1. The 2-form  
\[ \omega_\beta = Z(\beta)^{-1} H_I \exp(-\beta G(I, \xi)) \, dI \wedge d\xi. \]  
is preserved by \( \varphi_t \).

Remark 4.1. If we abuse notation by writing \( G(H, \xi) \) for \( G(I(H), \xi) \), then \( \omega_\beta = Z(\beta)^{-1} \exp(-\beta G(H, \xi)) \, dH \wedge d\xi \), too.

Proof. Let \( R_e = (H_I + c_0) \times \tilde{R}_e \); this is the vector field \( Y_e \) projected onto the Poincaré section \( S \) as a time-dependent vector field. The invariance of \( d\mu_\beta \) for \( Y_e \) implies that \( \omega_\beta = \exp(-\beta G(I, \xi)) \, dI \wedge d\xi \) is invariant for \( R_e \). This implies that the Lie derivative of \( \omega_\beta \) with respect to \( R_e \) is
\[ \mathcal{L}_{R_e} \omega_\beta = -\frac{bH_I}{H_I^2} \omega_\beta = -\langle d\ln(H_I), \tilde{R}_e \rangle \omega_\beta. \]
If one writes \( \omega_\beta = e^u \omega_\beta \), then this implies that \( \omega_\beta \) is invariant if \( u = \ln(H_I) \).

Lemma 4.2. The 1-form \( z = z_{e, \beta} = \iota_{\tilde{R}_e} \omega_\beta \) is exact.

Proof. From lemma 4.1, \( z \) is closed. Since the Poincaré section \( S \) is contractible, it is exact. \( \blacksquare \)

Let \( z_{e, \beta} = dG_{e, \beta} \) where (eq. 10) implies that \( G_{e, \beta} = \epsilon G_{0, \beta} + O(\epsilon^2) \) and \( dG_{0, \beta} = \iota_{\tilde{R}_e} \omega_\beta \).

Lemma 4.3. There exists a smooth 1-parameter family of symplectic averaging transformations \( \alpha_e : S \rightarrow S \) that transforms \( \tilde{R}_e \) and \( G_{e, \beta} \) to their first-order averages:
\[ \tilde{R}_e = \epsilon \tilde{R}_0 + O(\epsilon^2), \quad G_{e, \beta} = \epsilon G_{0, \beta} + O(\epsilon^2), \]
\[ \tilde{R}_0 = \frac{1}{H_I} (\tilde{b} \partial_I + \tilde{c} \partial_\xi), \quad G_{0, \beta}(I, \xi) = \int_c^\xi Z(\beta)^{-1} \exp(-\beta G(I, x)) \tilde{b}(I, x) \, dx \mod I \]
where \( c = -\infty \) if \( \xi \) is real-valued, and \( c = 0 \) otherwise.

Proof. The existence of the averaging transformation \( \alpha_e \) follows from, for example, [13, Chapter 2]. It is is straightforward that this averaging theory produces a family of symplectomorphisms when the unaveraged vector field is (time-dependent) Hamiltonian.

The formula for \( G_{0, \beta} \) follows from (eq. 9). \( \blacksquare \)

Lemma 4.4. \( G_{0, \beta} \) has a critical point \( (I_0, \xi_0) \) in the interior of \( (H \times \xi)^{-1}(W) \), \( W = [c_-, c_+] \times [d_-, d_+] \).

Proof. Let \( \tilde{b}(H, \xi) = \tilde{b}(I(H), \xi) \) and similarly for \( \tilde{c} \). The averaged value of \( \langle dH, T \rangle \) (resp. \( \langle d\xi, T \rangle \)) is \( H_I \tilde{b} + O(\epsilon) \) (resp. \( \tilde{c} + O(\epsilon) \)). We will assume, without loss of generality, that
\begin{enumerate}
  \item \( s \tilde{b}(u, d_s) > 0 \) for all \( s \in \{+, -\}, u \in [c_-, c_+] \); and
  \item \( s \tilde{c}(c_s, v) > 0 \) for all \( s \in \{+, -\}, v \in [d_-, d_+] \).
\end{enumerate}

Define the map \( r = r(H, \xi) \), by
\[ r(H, \xi) = (\tilde{c}(H, \xi), \tilde{b}(H, \xi)), \quad r : W \rightarrow \mathbb{R}^2. \]
By definition 2.1 and the fact that \( H_I \) does not change sign, for all \( \epsilon \) sufficiently small, \( r(\partial W) \subset \mathbb{R}^2 - \{0\} \). Since \( W \) is affinely homeomorphic to the square \([-1, 1] \times [-1, 1] \), the present lemma now follows from the topological lemma 4.6. \( \blacksquare \)
Lemma 4.5. Assume that the critical points of $\tilde{G}_{0,\beta}$ are isolated and that for some $B,C \in \{-1,1\}$,

1. $sB\dot{b}(u,d_s) > 0$ for all $s \in \{+,-\}$, $u \in [c_-,c_+]$; and
2. $sC\dot{c}(c_s,v) > 0$ for all $s \in \{+,-\}$, $v \in [d_-,d_+]$.

Then the sum of the indices of the critical points of $\tilde{R}_0$ in $(H \times \xi)^{-1}(W)$ is $-BC$. In particular, if the critical points are non-degenerate and $BC = -1$, then there is an elliptic critical point.

Proof. From lemma 4.4, there is at least one critical point in the pre-image of $W$. The sum of the indices of the critical points is $-BC \times \deg(r|\partial W) = -BC$. □

Lemma 4.6. Let $W = [-1,1] \times [-1,1] \subset \mathbb{R}^2$ and $f : W \to \mathbb{R}^2$ be a continuous map such that

$$f(u,v) = (x(u,v),y(u,v)) \quad \text{and} \quad sy(u,s) > 0, \ sx(s,v) > 0$$

where $s \in \{1,-1\}$, $u,v \in [-1,1]$. (13)

Then, $0 \in f(W)$.

Proof. This is clear; see figure 4. □

Theorem 4.1. Assume either

1. that conditions (1–2) of lemma 4.5 hold with $BC = -1$ and the period of the vector field $\tilde{R}_0$ is not constant in a neighbourhood of the elliptic critical point $(I_0,\xi_0)$; or
2. the averaged Hamiltonian $\tilde{G}_{0,\beta}$ is proper and $\tilde{R}_0$ has a non-constant period,

then for all $\epsilon$ sufficiently small the Poincaré return map $F_{\epsilon} : S \to S$ has a positive measure set of invariant circles.

Corollary 4.1. Assume the hypotheses of Theorem 4.1. For all $\epsilon$ sufficiently small, the thermostated vector field $Y_{\epsilon}$ (2.1) possesses a positive measure set of invariant tori.

Proof of Theorem 4.1 and Corollary 4.1. Let $(I_0,\xi_0)$ be either (1) an elliptic critical point; or (2) a regular point. In either case, there exists angle-action variables $(\rho,J)$ for $\tilde{G}_{0,\beta}$ which are defined in a neighbourhood of $(I_0,\xi_0)$. In these coordinates, $\tilde{G}_{0,\beta} = \tilde{G}_{0,\beta}(J)$. We will let $'$ denote $\partial/\partial J$. Since the period of $R_0$ is $P = 2\pi/\tilde{G}_{0,\beta}'$ is a smooth function, non-constancy of $P$ implies that $\tilde{G}_{0,\beta}''$ is non-zero in some neighbourhood of $(I_0,\xi_0)$. Then KAM theory is applicable [16, Chapter 2]. □
Remark 4.2. The proof of Theorem 4.1 is similar to the proofs in [7, 8]. The distinctive aspect here is that the coarse, topological, properties of the thermostat vector field $T$ (it tries to heat the mechanical system $H$ when $H$ is small, and tries to cool when $H$ is large) combined with the existence of a Poincaré section force the existence of KAM tori.

5. Examples

In this section, we will apply theorem 4.1 to a number of single thermostats that appear in the literature.

5.1. Separable Thermostats. This section describes an abstract type of thermostat vector field that satisfies the properties of 2.1.

Definition 5.1 (Separable Thermostat). Let

$$
T = A \partial_q + B \partial_p + C \partial_\xi,
$$

where

$$
A = A_0(q, p) A_1(\xi), \quad B = B_0(q, p) B_1(\xi), \quad C = C_0(q, p) C_1(\xi).
$$

If $d\mu_\beta$ (eq. 3) is invariant for $T$ and if there is an interval of regular values $[c_-, c_+]$ for $H$ such that on $H^{-1}([c_-, c_+])$,

1. $A_0 H_q$ and $B_0 H_p$ are both non-negative and at least one is positive;
2. $C_0$ changes sign; and
3. both $A_1$ and $B_1$ are odd functions of $\xi$;
4. $C_1$ is a positive function.

then $T$ is called a separable thermostat for $H$.

Theorem 5.1. Let $T$ be a separable thermostat for $H$ and assume, in addition, that on $H^{-1}([c_-, c_+])$,

1. $(\text{sign}(A_1) + \text{sign}(B_1)) \text{sign}(\xi) < 0$ and;
2. $\overline{C}$ is increasing.

Then, the conclusions of Theorem 4.1 and Corollary 4.1 apply.

Proof. One verifies that these conditions imply conditions (1–2) of lemma 4.5 hold with $[d_-, d_+] = [-1, 1]$ and the sign terms $B = -1, C = 1$. □

5.2. Nosé-Hoover Thermostat. In this case [4], the thermostat vector field is separable and

$$
G_\beta = H + \frac{1}{2} \xi^2, \quad A_0, A_1 = 0.
$$

$$
B_0 = p, \quad B_1 = -\xi, \quad C_0 = p \cdot H_p - T, \quad C_1 = 1.
$$

(15)

If one lets $K = B_0 H_p = p \cdot H_p$ (twice the averaged kinetic energy), then $\overline{C} = \overline{\xi} = K - T$ and $H_1 \overline{b} = -K \xi$. Note that a straightforward change of variables [8] eq. 18 shows that

$$
K = \overline{p} \cdot \overline{H}_p = \frac{1}{2\pi} \oint p \frac{dq}{dt} d\theta = I \cdot H_1.
$$

(16)

(Compare to [8] eqs 34–5.) From lemma 4.3 it follows that the hamiltonian of the vector field $\overline{R}_0$ is

$$
\overline{G}_{0, \beta} = (\beta Z(\beta))^{-1} I \exp (-\beta G_\beta).
$$

(17)
The integral found in [8][17] can be obtained by noting that $\tilde{R}_0$ is also hamiltonian with respect to the area form $T\omega_3/\tilde{G}_{0,3} = H_I I^{-1} dI \wedge d\xi$. If one changes to Darboux coordinates $(\sigma, \xi)$ where

$$\sigma = \int_{I_0}^{I} H_I dI / I$$

and $(I_0, \xi_0 = 0)$ is the critical point (where $I_0 \cdot H_I(I_0) = T$), then the hamiltonian $\tilde{G}_{0,T}$ of $\tilde{R}_0$ with respect to $d\xi \wedge d\sigma$ is

$$\tilde{G}_{0,T} = \frac{\xi^2}{2} + H(I(\sigma)) - T \ln I(\sigma).$$

**Remark 5.1.** A formula similar to (eq. 19) appears in [8, eqs. 33–35, 41], although the explicit form of $U_I$ is not there because the formula (eq. 16) was not used by the authors. A similar expression appears in [17, p. 040102-3] for the special case of the harmonic oscillator. [8] defines the canonical coordinates $(\xi, \sigma)$ via $I = I_0 e^\sigma$. This is due to an oversight: although the authors mention normalization of the return time to the Poincaré section, in their calculations the normalization is omitted with the consequence that the symplectic form used there omits the $H_I$ term. The reader may trace this back to the use of the vector field $Y_\epsilon$ (and the projected vector field $R_\epsilon$) rather than the normalized vector field $\tilde{Y}_\epsilon$ (and $\tilde{R}_\epsilon$)—see Lemma 4.1 and the surrounding discussion. Consequently, the differential equations satisfied by the averaged vector field are incorrectly stated in [8, eq. 41], because it is implicitly assumed that $H_I \equiv 1$ (or $\omega(\alpha) \equiv 1$ in [8, eq. 37]). This is mentioned only because the proof of the following theorem is significantly less involved if one omits the $H_I$ term in the definition of $\sigma$ (eq. 18).

**Theorem 5.2.** Let $H : T^* \Sigma \to \mathbb{R}$ be a proper real-analytic mechanical hamiltonian which is Morse. Then the period of $\tilde{R}_0$ is not constant in a neighbourhood of the critical point $(I_0, 0)$.

**Proof of Theorem 5.2** Since $H$ is bounded below, it can be assumed without loss that 0 is its (and $V^*$'s) global minimum. Let $H_0 = H(I_0)$ be the value of $H$ at the thermostatic equilibrium action $I_0$.

Assume that the period of $\tilde{R}_0$ is constant in a neighbourhood of the elliptic critical point $(I_0, 0)$. Real analyticity implies that the period is constant on the entire phase space. Since $(\sigma, \xi)$ are Darboux coordinates and $\tilde{G}_{0,T}$ is a mechanical hamiltonian, the potential $U = U_T$ must be isochronous and real analytic. In particular, $U$ must increase to the right of $I_0$ and decrease to the left.

From this, it follows that $U$ is bounded below, with a unique critical point at $\sigma = 0$. Moreover,

$$U_\sigma = I - TI_H = I (1 - T/K(I))$$

$$U_{\sigma\sigma} = I (I_H - TI_{H_H}).$$

**Claim 5.2.1.** $H$ has no critical values in $[H_0, \infty)$.

We use the notation and terminology introduced in section 3. Let $\gamma_0 \in \Gamma_H$ be the connected component of $H^{-1}(H_0)$ where the thermostatic equilibrium is attained. Since $K(I_0) = T$, the point $\gamma_0$ is not a vertex, so let $c_0 \subset \Gamma_H$ be the interior of the edge containing $\gamma_0$. The claim 5.2.1 is equivalent to the claim that $\sup c_0 = \pm \infty$.

Assume otherwise, so $v = \sup c_0$ is a saddle vertex. But $\lim_{\gamma \searrow v} I(\gamma) > 0$ and $K(I(v)) = 0$ from section 3 which implies that $U_{\sigma} \searrow -\infty$ at $\gamma \nearrow v$. Since $U$ is
increasing to the right of \( \sigma = 0 \) (i.e. for \( \gamma \in c_0 \) such that \( \gamma_0 < \gamma < \nu \)), this is a contradiction. Therefore, the sup \( c_0 \) is not a saddle vertex so it can only be \( \pm \infty \).

It is a tautology that the following dichotomy holds.

**Definition 5.2 (Critical Dichotomy).** Let \( c_0 \in \Gamma_H \) be the interior of the edge described above. Either \( \min c_0 \) is

1. a saddle vertex; or
2. a local minimum vertex.

**Claim 5.2.2.** In case (2) of the critical dichotomy the minimum is degenerate.

Since \( \Gamma_H \) is connected and sup \( c_0 = \pm \infty \), one concludes that \( \min c_0 \) must be the unique global minimum vertex of \( \Gamma_H \). Since \( \hat{I}(\gamma) \searrow 0 \) and \( H \searrow 0 \) as \( \gamma \searrow \min c_0 \), therefore \( U \nearrow \infty \). If \( \lim \inf U_\sigma = -\infty \), then (eq. 20) implies that \( \lim \sup I_H = \infty \) (\( \lim \inf H_I = 0 \)) and so the minimum must be degenerate.

Therefore, to complete the proof of claim 5.2.2, it remains to show that \( \lim \inf_{I \to -\infty} U_\sigma = -\infty \). Assume that \( U_\sigma \) is bounded below by \( -1/c \) for some \( c > 0 \). Let \( \sigma_{\pm}(u) \) be the inverses of \( U(\sigma) \): \( U(\sigma_{\pm}(u)) = u \) for all \( u \geq 0 \) and \( \pm \sigma_{\pm}(u) > 0 \) for all \( u > 0 \). Then \( \sigma'_-(u) \) is bounded above by \( -c \), so there is a \( d > 0 \) such that \( \sigma_{\pm}(u) \leq -cu + d \) for all \( u \). Since \( \sigma_{\pm}(u) \geq 0 \), it follows that \( \Delta(u) = \sigma_{\pm}(u) - \sigma_{\mp}(u) \geq cu - d \) for all \( u > 0 \).

But, it is known [12] that if \( U \) is an isochronous potential, then \( \Delta(u) \) is a constant multiple of \( \sqrt{u} \). This contradiction proves that \( \lim \inf U_\sigma = -\infty \), as required.

**Claim 5.2.3.** In case (1) of the critical dichotomy the following holds:

As \( \gamma \searrow \min c_0 \),

1. \( I \searrow I_1 > 0 \);
2. \( I_H \nearrow \infty \);
3. \( U_\sigma \searrow -\infty \). And,
4. \( U \) is bounded.

1 & 2 follow from section 3 since \( \min c_0 \) is a saddle vertex. \( 3 \) follows from (eq. 20) and 2. From 1 and (eq. 19) it follows that \( U \) is bounded from above on the interval \( [\min c_0, \gamma_0] \) and 3 implies that \( U \) does not extend to the left of \( \min c_0 \); on the other hand, \( U \) reaches its minimum value at \( \gamma_0 \) (where \( \sigma = 0 \)). But the image of \( [\gamma_0, \sup c_0] \) equals that of \( (\min c_0, \gamma_0] \). Therefore, \( U \) is bounded, hence 4.

Finally, the finite value \( g = \sup U_T(\sigma) \) is a critical point of \( G_{0,T} \) since the topology of the level sets of \( G_{0,T} \) change at height \( g \). This contradicts the constancy of the period of \( R_0 \).

Therefore, only case (2) of the critical dichotomy can hold, in which case claim 5.2.2 holds, too.

**Remark 5.2 (Isochronous potentials).** The proof of claim 5.2.2 uses the fact that if \( U \) is an isochronous potential, then \( \Delta(u) \) is proportional to \( \sqrt{u} \). A more elementary proof consists in showing that the action function \( J \) satisfies \( 2\pi J(g) \geq cg^{\frac{3}{2}} - 2dg^{\frac{5}{2}} \) while \( J \) is proportional to \( g \).

**Remark 5.3 (Degenerate global minimum).** In case (2) of the critical dichotomy, above, it is shown that the critical point at \( H = 0 \) must be degenerate. Since \( H \) is real analytic, the degeneracy is finite, so a straightforward calculation shows that \( I = cH^r + o(H^r) \) for some constant \( c > 0 \) and integer \( r \geq 2 \) with \( r = \frac{1}{2}(1 + 1/n) \). Therefore, the infimum \( \sigma_1 \) of \( \sigma \) is finite.
Let’s examine a particular example: \( V(q) = (\omega q)^{2n} \) for \( n \geq 2 \). A computation shows that \( I = \gamma H^{r} \) where \( r = \frac{1}{2}(1 + 1/n) \) and \( \gamma \) is a structural constant, \( H_{0} = rT, \sigma = (H^{s} - H_{0}^{s})/(s\gamma) \) where \( s = 1 - r \) (so \( \sigma_{1} = -H_{0}^{s}/(s\gamma) \)), and

\[
U/H_{0} = (1 + \sigma/\sigma_{1})^{1/s} - \ln(1 + \sigma/\sigma_{1})^{1/s}.
\]

The third-order Birkhoff normal form of \( \tilde{G}_{0,T} \) is, up to a \( T \)-dependent constant,

\[
\omega \gamma J - A \gamma^{2} J^{2} + B \gamma^{3} J^{3} + O(J^{4}),
\]

where \( \omega = H_{0}^{1/2-s}, A = \frac{6s^{2} - 6s + 1}{24H_{0}^{2s}}, \)

and \( B = \frac{180s^{4} - 312s^{3} + 168s^{2} - 36s + 5}{1728H_{0}^{3s+1/2}} \)

Since the resultant of the numerators of \( A \) and \( B \) is \(-6912\), the Hamiltonian is not isochronous for any value of \( s \), hence \( n \).

On the other hand, one can try to “design” a hamiltonian \( H \) given \( U \) using (eq. 18) & (eq. 19). In this case, one gets

\[
H(\sigma) = H_{0} - T \ln \left( 1 - \beta I_{0} \int_{0}^{\sigma} \exp(-\beta \tilde{U}(\sigma)) \, d\sigma \right), \quad \text{(21)}
\]

where \( \tilde{U} = U - U_{0} \) is a function defined on \((\sigma_{1}, \infty)\); \( U_{0} = U(0) = H_{0} - T \ln I_{0} \). The function \( \tilde{U} \) satisfies

\[
\int_{\sigma_{1}}^{\infty} \exp(-\beta \tilde{U}(\sigma)) \, d\sigma = \frac{T}{I_{0}} \times \exp(\beta H_{0}), \quad \text{(22)}
\]

\[
\int_{0}^{\infty} \exp(-\beta \tilde{U}(\sigma)) \, d\sigma = \frac{T}{I_{0}}, \quad \text{(23)}
\]

so the integral of \( \exp(-\beta \tilde{U}) \) over \((\sigma_{1}, \infty)\) is \( T \).

One can use equations (eq. 21)–(eq. 23) to reconstruct \( H \) and \( I \) as functions of \( \sigma \). A tractable case is when \( \tilde{U} \) is rational; since the isochronous case is of particular interest one can assume, without significant loss of generality, that

\[
\tilde{U}(\sigma) = (\sigma + 1) - (\sigma + 1)^{-1} \right)^{2}. \quad \text{(24)}
\]

In this case, one computes

\[
\int_{-1}^{\infty} \exp(-\beta \tilde{U}(\sigma)) \, d\sigma = \sqrt{\frac{\pi}{4\beta}}, \quad \text{(25)}
\]

\[
\int_{0}^{\infty} \exp(-\beta \tilde{U}(\sigma)) \, d\sigma = \sqrt{\frac{\pi}{4\beta}} W_{0}, \quad W_{0} = W(0), \quad \text{(26)}
\]

where \( W = W(\sigma) \) is defined in (eq. 28). Combined with (eq. 22) & (eq. 23), one finds that

\[
H_{0} = -T \ln(W_{0}), \quad I_{0} = \frac{2T^{\frac{1}{2}}}{\sqrt{\pi} W_{0}}. \quad \text{(27)}
\]

From this one determines that (with \( \sigma = \tau - 1 \))

\[
H = -T \ln W, \quad I = H_{0} - \frac{2T^{\frac{1}{2}}}{\sqrt{\pi} W} \times \exp(-\beta(\tau - 1/\tau)^{2}), \quad \text{(28)}
\]

where \( 2W = e^{4\beta} \text{erf} \left( \sqrt{\beta}(\tau + 1/\tau) \right) + \text{erf} \left( \sqrt{\beta}(\tau - 1/\tau) \right) \),
and erfc is the complementary error function [1, Chapter 7]. One finds that
\[ \lim_{I \to 0^+} H/I^\alpha = 0 \text{ if } \alpha = 1 \text{ and } \infty \text{ if } \alpha > 1. \] On the other hand, for the oscillator with potential \( V = (\omega q)^{2n} \) the same limit is 0 for \( 1 \leq \alpha < 1/r \) and \( 1/r > 1 \) when \( n > 1 \). So, by the arguments of the first paragraph of this remark, the Hamiltonian \( H \) cannot be mechanical and real analytic. Indeed, I am uncertain if \( H \) extends to a \( C^2 \) Hamiltonian, mechanical or otherwise, in the \((q,p)\) coordinates.

To rule out all possibilities for \( H \), one needs to know the general form of an iso-chronous potential. Bolotin & MacKay [12, p. 220] prove that if \( U \) is a \( C^r \) \((r \geq 2)\) iso-chronous potential on \( \mathbb{R} \) with a critical point at 0, and \( U''(0) = 2 \), then there is a continuous (shear) function \( \delta : [0, \infty) \to \mathbb{R} \) such that \( \delta(u) = o(\sqrt{u}) \) at 0, \( \delta \) is \( C^r \) on \((0, \infty)\), \( |\delta'(u)| < \frac{1}{2} u^{-\frac{1}{2}} \) for \( u > 0 \) and the function \( U = U(\sigma) \) is defined implicitly as the zero locus of the function \( K(\sigma, u) = u - (\sigma - \delta(u))^2 \). Geometrically, the graph of the potential \( U \) is obtained from the parabola \( u = \sigma^2 \) by the shearing transformation \( (\sigma, u) \to (\sigma - \delta(u), u) \). The general case is obtained from this result by rescaling \( u \) and restricting the domain of \( K \). However, even with this additional information, I am unable to prove if the example with \( U \) determined by (eq. 24) is illustrative of the general case or a singular case.

Remark 5.4 (The averaged kinetic energy). As mentioned above, the formula for the averaged kinetic energy (eq. 16) is not used in [8]. Nonetheless, the authors numerically compute this integral, called \( k_0 \) there, for the planar pendulum \( H = \frac{1}{2} p^2 - \cos q \) by integrating Hamilton’s equations. On the other hand, it follows from (eq. 16) and [3] eqs. 11–13] that

\[
K = \frac{2(H + 1)}{1 - kK'(k)/K(k)}, \quad H + 1 = \frac{2}{k^2}, \quad I = \frac{8K(k)}{\pi k},
\]

where \( K(k) \) is an elliptic integral described in [3]. Figure 3 (resp. 4) reproduces figure 10 (resp. 11) of [8] using only these formulas.

Figure 3. \( K \) vs. \( H \) for the planar pendulum \( H = \frac{1}{2} p^2 - \cos q \), c.f. [8 Figure 10]. The vertical red line is the energy level of the saddle fixed point.
Figure 4. \( W \) vs. \( a \) for the planar pendulum \( H = \frac{1}{2}p^2 - \cos q \), c.f. [8, Figure 11]. The vertical red line is the action of the saddle fixed point.

Figure 5. \( \sigma \), \( \ln I \) and their difference for the planar pendulum.

5.3. Logistic Thermostat of Tapias, Bravetti & Sanders. In [15], Tapias, Bravetti & Sanders introduce a “logistic thermostat”, which is very similar to Hoover’s with:

\[
\begin{align*}
G_\beta &= H + F, & A_0, A_1 &= 0, \\
B_0 &= p, & B_1 &= -F', & C_0 &= p \cdot H_p - T, & C_1 &= 1,
\end{align*}
\]

(29)

where \( F = \ln (\cosh (\xi)) \) and \( F' = \tanh (\xi) \). [15] uses the variable \( \zeta \) for the thermostat and parameter \( Q \) (which would be \( \sqrt{Q} \) in Hoover’s thermostat). These are related to \( \xi \) and \( \epsilon \) by \( \xi = \epsilon \zeta / 2 \) and \( \epsilon = 1/Q \). That paper also uses \( 2TF \) in lieu of \( F \), but there is no qualitative difference in the analysis below. The choices here are dictated by the desire to portray clearly this thermostat as a perturbation of Hoover’s (which it is), since with the choices made, \( F = \frac{1}{2} \xi^2 + O(\xi^4) \).
Indeed, let $F_\eta(\xi) = \eta^{-2}F(\eta \xi) = \frac{1}{2}\xi^2 + \eta^2 \bar{F}_\eta(\xi)$. For $\eta = 0$, one has Hoover’s thermostat and for $\eta = 1$, the logistic thermostat. Equations (eq. (29)) hold for the averaged thermostat from equations (eq. (29)) (with $\frac{1}{2} \xi^2$ replaced by $F(\xi)$ in the latter equation). Let $\varphi_{\eta} : (\rho, J) \rightarrow (\xi, \sigma)$ be the angle-action map for $\bar{G}_{0, T; \eta}$ where $T$ is held fixed. The thermostatic equilibrium is at $(\sigma, \xi) = (0, 0)$ independently of $\eta$. If $H$ is real analytic, then $\eta \mapsto \bar{G}_{0, T; \eta}''(J)$ is a real-analytic function that does not vanish at $\eta = 0$ for some $J$. Therefore, it is non-zero for all but a countable set without accumulation points. This “almost” proves that the averaged hamiltonian is never isochronous.

**Theorem 5.3.** Let $H : T^* \Sigma \rightarrow \mathbb{R}$ be a proper real-analytic mechanical hamiltonian that is Morse. If $F$ (eq. (29)) satisfies $F(\xi)/|\xi| \rightarrow c > 0$ as $|\xi| \rightarrow \infty$, then the period of $\bar{H}_0$ is not constant in a neighbourhood of the critical point $(I_0, 0)$.

**Remark 5.5.** It is clear that $F(\xi) = \ln \cosh(\xi)$ satisfies the hypothesis of this theorem. The strategy of the proof is similar to that employed for Theorem 5.2 with a similar result: if $\bar{H}_0$ has a constant period, then $H$ has a single, degenerate minimum point.

**Proof.** Assume the stated hypotheses. Condition 3 of definition 5.1 requires that $F$ is even, so $F'(0) = 0$ and without loss, $F(0) = 0$. If $U_T(I(\sigma))$ is bounded above, $\gamma = \sup \{U_T\}$ is a critical value of $\bar{G}_{0, T}$. If $U_T$ is not constant, then $\bar{G}_{0, T}$ has two distinct critical values, which contradicts isochronicity. Therefore, $U_T$ is unbounded from above and has only one critical value (an absolute minimum, which may be assumed to be 0) at the point $\sigma = 0$.

Claim 5.2.1 holds here, with the same proof as above.

To prove that claim 5.2.2 holds here, it suffices to prove that $\lim \inf U_\sigma = -\infty$. To do this, one uses a method similar to that mentioned in remark 5.2.

For $g > 0$, let $\sigma_\pm(g)$ be the local inverse to $U_T$: $g = U_T(I(\sigma(\pm)(g)))$ and $\pm \sigma_\pm(g) > 0$. Let $\Delta = \sigma_+ - \sigma_-$. From the previous paragraph it follows that both $\sigma_+$ and $-\sigma_-$ are increasing, so $\Delta$ is, too.

Let $g \gg 1$. By hypothesis, $F(\xi) = c \xi (1 + k(\xi))$ where $k(\xi) \rightarrow 0$ as $|\xi| \rightarrow \infty$; without loss of generality, it is assumed $c = 1$. The level set $\{\bar{G}_{0, T} = g\}$ satisfies $\xi = g - U_T(I(\sigma)) + o(g)$ for $\xi \gg 1$. Let $J(\rho, J)$ be the angle-action variables for $\bar{G}_{0, T}$. It follows, by comparing inscribed and circumscribed rectangles, that for any $0 < \alpha < 1$,

$$2(1 - \alpha)g\Delta(\alpha g) \leq 2\pi J + o(g) \leq 2g\Delta(g).$$  

Therefore, since $\bar{G}_{0, T} = \omega J$ is linear in $J$,

$$\frac{\pi}{\omega} \geq \lim_{g \rightarrow \infty} \Delta(g) \geq \frac{\pi}{\omega(1 - \alpha)},$$

hence $\Delta(g) \nearrow \pi/\omega$ as $g \rightarrow \infty$. This implies that $\sigma_-(g)$ has an infimum $\sigma_1$ and $\sigma_+(g)$ has a supremum $\sigma_2 = \sigma_1 + \pi/\omega$.

To summarize: $U = U_T(I(\sigma))$ has a bounded domain $(\sigma_1, \sigma_2)$ and diverges to $\infty$ as $\sigma$ approaches either endpoint. Therefore $U_\sigma$ diverges to $-\infty$ at $\sigma_1$ (resp. $\infty$ at $\sigma_2$). This proves claim 5.2.3 holds here, too.

To prove that claim 5.2.3 holds here, one notes that the proof above does not make use of the mechanical nature of $\bar{G}_{0, T}$, only its quasi-mechanical nature. Since 4 of that claim is that $U$ is bounded, one obtains a contradiction.
Therefore, only case (2) of the critical dichotomy can hold, in which case claim 5.2.2 holds, too.

Remark 5.6 (Degenerate global minimum). Similar to remark 5.3, one can examine the case where the potential energy has a degenerate critical point at \( q = 0 \), e.g. \( V = (\omega q)^{2n} \). Similar calculations, using the 4-th order Birkhoff normal form of \( \bar{G}_0, \bar{T} \), show that the isochronicity condition is never satisfied.

5.4. Watanabe & Kobayashi. In [17], Watanabe & Kobayashi generalize Hoover’s thermostat by setting

\[
\begin{align*}
G_\beta &= H + \frac{1}{2} \xi^2, & A_0, A_1 &= 0, \\
B_0 &= p^k, & B_1 &= -\xi, & C_0 &= p^{k-1} (p \cdot H_p - k T), & C_1 &= \zeta_l(\xi)
\end{align*}
\]

where, when \( l = 2n + 1 \), \( \zeta_l \) is the \( n \)-th Maclaurin polynomial of \((2/\beta)^n n! \exp(x)\) evaluated at \( x = \beta \xi^2 / 2 \) [17, eq.s 8–14]. For \((k, l) = (1, 1)\), one has Hoover’s thermostat.

In order to have conditions (1–4) hold in definition 5.1 and (1–2) in Theorem 5.1, one needs both \( k \) and \( l \) to be odd: \( k = 2m + 1 \), \( l = 2n + 1 \). This is assumed in [17]. It is also assumed there that \( H = (q^2 + p^2) / 2 \), but this is not necessary.

The only challenge is condition 2: to locate an interval of regular values \([c_-, c_+]\) such that \( C_0 \) alternates sign. To do this, let us define

\[
f(I) = k p^{k-1}, \quad \bar{K}(I) = \frac{p^{k} \cdot H_p}{f(I)}, \quad C_0 = f(I) \left( \bar{K}(I) - T \right)
\]

where \( f(= f_k) \) and \( \bar{K}(= \bar{K}_k) \) are smooth, positive functions of \( I \). \( \bar{K} \) can be viewed as a weighted average temperature along an orbit similar to that defined in (eq. 16) – indeed, when \( k = 1 \), one recovers the definition of (eq. 16).

If \( H \) is mechanical, \( p = H_p \), so \( \bar{K}_k = (k + 2)^{-1} \times f_{k+2} / f_k \). In addition, the change of variables in (eq. 16) implies that for \( k \geq 3 \), \( 2\pi f_k(I) = k(k-2)H_1(I) \times \int f_{k+3} dp \wedge dq \). These two facts imply that \( \bar{K}_1 \) tends to 0 as \( I \) approaches a critical action, while \( \bar{K}_k \) tends to a non-zero limit for \( k \geq 3 \) when the critical action is positive. Figure 6 plots the graphs of \( \bar{K}_k \) for selected values of \( k \) and demonstrates these facts for a selected example. In addition, when \( H = \frac{1}{2} (p^2 + q^2) \) is a simple harmonic oscillator, \( \bar{K}_k = \frac{2}{k^2+1} I \). This fact is seen in figure 6 too.

If one assumes, when \( \Sigma = \mathbb{R} \), that \( H \) is asymptotically convex, then straightforward comparisons with superscribed and inscribed disks show that \( \bar{K} \) asymptotically grows at least linearly in \( I \). In addition, the critical point set of \( H \) is compact. Therefore, for all \( T > 0 \) sufficiently large, there exist intervals of regular values satisfying condition 2. Since the conditions of Theorem 5.1 are also clearly satisfied, the conclusion follows.

One can prove more. The hamiltonian \( \bar{G}_{0, \beta} \) of the averaged vector field \( \bar{R}_0 \) and the latter’s hamiltonian \( \bar{G}_{0, T} \) with respect to the symplectic form \( -T \omega_\beta / \bar{G}_{0, \beta} \) from
Lemma [4.3] are computed to be
\[ \mathcal{G}_{0,\beta} = (\beta Z(\beta) H_1(I))^{-1} f(I) \tilde{K}(I) \zeta(I) \times \exp(-\beta G_\beta(I, \xi)) \quad (34) \]
\[ \mathcal{R}_0 = \frac{f(I) \tilde{K}(I)}{H_1(I)^2} \times (-\xi \xi \partial_I + \zeta(I) H_1(I) \left[ \tilde{K}(I) - T \frac{\partial_I}{\tilde{K}(I)} \right] \partial_I) \quad (35) \]
\[ \mathcal{C}_{0,T} = Z_l(\xi) + H(I) - T \ln Q_k(I), \quad (36) \]

where \( Z_l(\xi) = \frac{1}{2} \xi^2 - T \ln(\zeta(\xi)/\zeta(0)) \) and \( \ln Q_k = \int_{H_0}^H \frac{dH}{\tilde{K}} \). One checks that \( Z_1(\xi) = \frac{1}{2} \xi^2 \) and \( Q_1(I) = I \), so (eq. 36) reproduces the Hamiltonian in (eq. 19).

Let it be noted that \((I, \xi)\) are not Darboux coordinates for the rescaled symplectic form. One defines Darboux coordinates via
\[ \sigma = \int_{I_0}^{I} \frac{(H_I)^2}{f(I) \tilde{K}(I)} dI, \quad \chi = \int_{0}^{\xi} \frac{d\xi}{\zeta(I)} \quad (37) \]
which for \( k = 1, l = 1 \) specializes to the Darboux coordinates introduced above for the Hoover thermostat.

**Lemma 5.1.** Let \( H : T^*\Sigma \rightarrow \mathbb{R} \) be a proper, smooth Hamiltonian that is convex in momentum. If \( \Sigma = \mathbb{R} \), assume additionally that \( H \) is asymptotically convex. Then for all sufficiently large temperatures \( T \), there exists a unique thermostatic equilibrium \((I, \xi) = (I_0, 0)\) for the averaged vector field (eq. 33). If, in addition, \( l > 1 \), then condition 2 of Theorem 4.1 is satisfied.

**Proof.** Inspection of (eq. 35) shows that the averaged vector field \( \mathcal{R}_0 \) vanishes iff \( \xi = 0 \) and \( \tilde{K}(I) = T \).

If \( \Sigma = \mathbb{T} \), then convexity in the momentum implies that the critical-point set of \( H \) is compact; otherwise, asymptotic convexity implies the same. Let \( c \) be the maximal critical value of \( H \) if \( \Sigma = \mathbb{T} \) or the minimal \( c_0 \) for which the sub-level set \( S(h) = H^{-1}(\infty, h) \) is convex for all \( h > c_0 \) if \( \Sigma = \mathbb{R} \). In both cases, it follows that both \( I \) and \( \tilde{K} \) are monotone increasing and smooth in \( H \) for all energies \( H > c \). Then (eq. 38) has a unique solution \((I_0, 0)\) if \( T \) is larger than the maximum of \( \tilde{K}/S(c) \).

Assume that the situation of the previous sentence holds. Let \( H_0 = H(I_0) \) be the energy at the thermostatic equilibrium. One computes the hessian to be
\[ \text{hess} \mathcal{C}_{0,T} = \zeta(I)^{-1} \xi^{l-1} (l - \beta \xi^{l+1}) (d\xi)^2 + T \tilde{K}^{-2} \tilde{K}' (dH)^2. \quad (39) \]

This is positive definite at the thermostatic equilibrium if \( l = 1 \) and otherwise it is degenerate. The lowest order term in the coefficient on \((d\xi)^2\) is of degree \( l - 1 \) in \( \xi \) since \( \zeta(0) = (2T)^n n! \). This implies that for \( l > 1 \), \( \mathcal{C}_{0,T} = ((2T)^n n!)^{-1} (l + 1)^{-1} \xi^{l+1} + \frac{1}{2} T^{-1} \tilde{K}'(H_0) (H - H_0)^2 + O(\xi^{l+3}, (H - H_0)^3) \). Since \( l \) is odd, \( \mathcal{C}_{0,T} \) is proper in a neighbourhood of its critical point. This proves that condition 2 holds if \( l > 1 \).

One is now in a position to prove the analogue to Theorems 5.2 & 5.3

**Theorem 5.4.** Let \( H : T^*\Sigma \rightarrow \mathbb{R} \) be a proper real-analytic mechanical Hamiltonian that is Morse. Then the period of \( \mathcal{R}_0 \) is not constant in a neighbourhood of the critical point \((I_0, 0)\).
Proof. All cases except \( l = 1 \) and \( k \geq 3 \) follow from lemma 5.1 or 5.2, so assume that \( l = 1 \) and \( k \geq 3 \).

As in the proof of Theorem 5.2 let \( \gamma_0 \in \Gamma_H \) be the connected component of the level set of \( H \) where the thermostatic equilibrium \((I_0, 0)\) is attained and let \( c_0 \subset \Gamma_H \) be the edge containing \( \gamma_0 \). One computes, in the Darboux coordinates \((\sigma, \xi)\)\(^{37}\) that

\[
U_\sigma = I_H f \left( \tilde{K} - T \right).
\]

From the discussion in the paragraph following (eq. 33), it is known that if \( s \in \Gamma_H \) is a saddle vertex, then \( I_H f \) and \( \tilde{K} \) are bounded away from 0 in a neighbourhood of \( s \). This implies that if \( s = \sup c_0 \) is a saddle vertex, then \( U \) is bounded on the edge \( c_0 \). This contradicts isochronicity. Hence claim 5.2.1 holds.

If \( s = \min c_0 \) is a saddle vertex, then the reasoning of the previous paragraph shows \( U \) is bounded on \( c_0 \), again contradicting isochronicity.

To prove claim 5.2.2 holds here, assume that the local minimum vertex \( \min c_0 \) is non-degenerate so \( I_H \to \omega^{-2} > 0 \) as \( \gamma \searrow \min c_0 \). On the other hand, both \( f \) and \( \tilde{K} \) approach 0 as \( \gamma \searrow \min c_0 \). This implies that \( U_\sigma \nearrow 0 \) and so \( U_\sigma \) is bounded on \((\min c_0, \gamma_0] \subset c_0 \). By the same argument as in the second paragraph following claim 5.2.2 one obtains a contradiction, thereby proving that claim here. This completes the proof. \( \square \)

Figure 6. \( \tilde{K}_k \), rescaled by \( \frac{k+1}{2} \), for the planar pendulum \( H = \frac{1}{2} p^2 - \cos \theta \) with \( k = 1, 3, 5, 7 \). The inset (upper left) highlights the behaviour near the critical energy level \( H = 1 \).
5.5. **Hoover & Sprott and Hoover, Sprott & Hoover.** In [6], Hoover, Sprott and Hoover obtain numerical results that indicate for some parameter values there are large sets with positive Lyapunov exponents for the thermostat with

\[
G_\beta = H + \frac{1}{4} \xi^4, \quad A_0 = q, \quad A_1 = -\xi^3, \quad B_0 = p^3, \quad B_1 = -\mu\xi^3, \quad C_1 = 1, \quad C_0 = [qH_\xi - T] + \mu p^2 [pH_p - 3T].
\]

For comparison with [6] eq. [HS], p. 237, their \(\xi^4\) term is not multiplied by \(\beta\) and their \(T\) (resp. \(\alpha/T\)) is \(T\) (resp. \(\epsilon, \epsilon\mu\)) here. It is trivial to see that conditions 1, 3 and 4 of definition 5.1 are satisfied. To prove that condition 2 holds, note that on averaging \(C_0\), one obtains

\[
\overline{C}_0 = [K(I) - T] + \mu f(I) \left[ \tilde{K}(I) - T \right],
\]

where \(K\) is the averaged temperature from (eq. 16), \(\tilde{K} = \tilde{K}_3\) is the weighted average temperature from (eq. 33) with \(k = 3\) and \(f = f_3\) is defined likewise.

The Hamiltonian \(\overline{G}_{0,\beta}\) of the averaged vector field \(\overline{T}_0\) and the latter’s Hamiltonian \(\overline{G}_{0,T}\) with respect to the symplectic form \(-T\omega_\beta/\overline{G}_{0,\beta}\) from Lemma 4.3 are computed
to be
\[ \mathcal{G}_{0,\beta} = \left( \beta Z(\beta)H_1(I) \right)^{-1} \left( K(I) + \mu f(I) \hat{K} \right) \exp(-\beta G_\beta(I,\xi)) \]
\[ \mathcal{R}_0 = \frac{1}{H_1} \times \left( -\xi^3(\xi^3)_{-1} \left[ K(I) + \mu f(I) \hat{K}(I) \right] \partial_I + \mathcal{G}_{0} \partial_\xi \right) \]
\[ \mathcal{G}_{0,T} = \xi^4/4 + H(I) - T \ln Q_\mu(I) \]
where \( \ln Q_\mu = \int_{H_0}^{H} dH \left[ \frac{1+\mu f}{K+\mu f} \right] \). One checks that for \( \mu = 0 \) (eq. 45) reproduces the Hamiltonian in (eq. 19), while for \( \mu = \infty \), the potential coincides with that in (eq. 36).

This lemma is clear:

**Lemma 5.2.** Let \( H : T^*\Sigma \to \mathbb{R} \) be a proper, smooth Hamiltonian that is convex in momentum. If \( \Sigma = \mathbb{R} \), assume additionally that \( H \) is asymptotically convex. Then for all sufficiently large temperatures \( T \), there exists a unique thermostatic equilibrium \((I,\xi) = (I_0,0)\) for the averaged vector field (eq. 44). Moreover condition 2 of Theorem 4.1 is satisfied.

The following is an immediate consequence of the preceding lemma.

**Theorem 5.5.** Let \( H : T^*\Sigma \to \mathbb{R} \) be a proper mechanical hamiltonian. Then the period of \( \hat{R}_0 \) is not constant in a neighbourhood of the critical point \((I_0,0)\).

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Department of Mathematics, University of Manitoba, Winnipeg, MB, Canada, R2J 2N2

E-mail address: leo.butler@umanitoba.ca