INVARIANT TORI FOR MULTI-DIMENSIONAL INTEGRABLE
HAMILTONIANS COUPLED TO A SINGLE THERMOSTAT

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ABSTRACT. This paper demonstrates sufficient conditions for the existence of KAM tori in a singly thermostated, integrable Hamiltonian system with n degrees of freedom with a focus on the generalized, variable-mass thermostats of order 2—which include the Nosé thermostat, the logistic thermostat of Tapias, Bravetti and Sanders, and the Winkler thermostat. It extends Theorem 3.2 of Legoll, Luskin & Moeckel, (Non-ergodicity of Nosé-Hoover dynamics, Nonlinearity, 22 (2009), pp. 1673–1694) to prove that a “typical” singly thermostated, integrable, real-analytic Hamiltonian possesses a positive-measure set of invariant tori when the thermostat is weakly coupled. It also demonstrates a class of integrable Hamiltonians, which, for a full-measure set of couplings, satisfies the same conclusion.

1. Introduction

A central model in statistical mechanics is an isolated mechanical system, modeled by a Hamiltonian \( H \), that is in equilibrium with a heat bath at the temperature \( T \). Khinchin stressed ergodic theory as the foundations of statistical mechanics—approximately twenty years after Fermi’s ill-fated effort to prove the quasi-ergodic hypothesis for mechanical systems \([35, 20]\). By the early nineteen-sixties, the Kolmogorov-Arnol’d-Moser theory and the Fermi-Pasta-Ulam numerical results demonstrated that there are fundamental difficulties in the project to reduce statistical mechanics to classical mechanics \([36, 37, 4, 5, 48]\;[21, 23]\).

This note studies thermostated systems used in the computational statistical-mechanics and molecular-dynamics literature. Many of the results in the mathematical literature on the properties of these systems are negative, in a sense: they demonstrate the existence of positive-measure sets of KAM tori and hence the failure of ergodicity.

1.1. Thermostated mechanics. Nosé \([49, 50]\), after Andersen \([3]\), introduced an “extended system” to create a system with an invariant measure that projects onto the Gibbs-Boltzmann measure in physical phase space. This consists of adding an extra degree of freedom \( s \), re-scaling momentum by \( s \), and coupling the extra state \( s \) thus:

\[
H = H(q, ps^{-1}) + N_T(s, p_s), \quad \text{where} \quad N_T(s, p_s) = \frac{1}{2Q}p_s^2 + gkT \ln s, \quad (1)
\]

Date: 2021–07–14 11:21:15.

2020 Mathematics Subject Classification. 70H08; 37J40, 82B05, 70F40.

Key words and phrases. thermostats; Nosé-Hoover thermostat; Hamiltonian mechanics; KAM theory; degenerate KAM theory.
where $g$ is a parameter, $Q$ is the “mass” of the thermostat (a proxy for the thermal coupling) and $k$ is Boltzmann’s constant. In this note, it is assumed that units are chosen so that $gk = 1$. Solutions to Hamilton’s equations for $H$ model the evolution of the state of the infinitesimal system along with the exchange of energy with the heat bath [51, p. 187].

Hoover’s reduction eliminates the state variable $s$ and re-scales time $t$ [27]:

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

The Nosé-Hoover thermostat for an $n$-degree of freedom Hamiltonian $H$ can be put in the form (c.f. [27], eq. 6):

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

(2)

where $\epsilon^2 = 1/Q$ and $z = \epsilon \xi^2$.

Hoover observed that this thermostat is ineffective in producing the statistics of the Gibbs-Boltzmann distribution from single orbits of the thermostated harmonic oscillator [27]. There are numerous extensions of the Nosé-Hoover thermostat that model the exchange of energy with the heat bath using a single, additional thermostat variable ($\xi$ in [2]), the so-called single thermostats. A sample includes [64, 63, 53, 58, 60, 61, 62]. Winkler, in [64], introduces a $p/s^2$ coupling which produces better results than Nosé’s, but precludes the Hooverian reduction (eq. 2) since it is equivalent to a variable-mass variant the Nosé thermostat—see [7, Lemma 3.1]. In [63], Watanabe & Kobayashi thermostat a harmonic oscillator with a thermostat that controls a single moment of momenta and show its first-order averaged system is integrable. Rech, in [53], considers the same variant of the Nosé-Hoover thermostated harmonic oscillator—introduced in [57] by Sprott, Hoover & Hoover—in which the temperature varies with position. Tapias, Bravetti & Sanders, in [58], replace the linear friction of the Nosé-Hoover thermostat with a tanh-friction that saturates at large magnitudes of the thermostat state $\xi$. Wang & Yang, in [60, 61], investigate the Nosé-Hoover thermostated harmonic oscillator and find regions of phase space where apparently chaotic dynamics exist and regions where invariant tori appear. In [62], the same authors visit the variant of the Nosé-Hoover thermostated harmonic oscillator that thermostats total energy, and demonstrate (numerically) the existence of a horseshoe. The present author shows, in a 2-degree of freedom hamiltonian that is integrable and enjoys a saddle-centre critical point, that the Nosé-Hoover thermostat splits the homoclinic connections and creates horseshoes for a suitable parameter regime [7].

The Nosé and Nosé-Hoover thermostats are used to thermostat mixed quantum-classical systems, too. Grilli & Tosatti, in [24] (see also [25]) use a variant of Nosé’s thermostat to couple a combined quantum and classical system with a heat bath. In [44] eqs. 1–3, Mauri, Car & Tosatti couple a mixed quantum-classical system to a Nosé-Hoover thermostat; this work is extended by Alonso, et. al. [2]. Sergi and Sergi & Petruccione, in [55, 56], examine an alternative mixed quantum-classical

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1 Nosé notes that $g = n + 1$ or $g = n$ can be used: the former choice ensures that the microcanonical ensemble of $H$ projects to that of $H$; the latter choice is appropriate when one views the momentum $p' = p/s$ to be “real” and one wishes to obtain ergodic averages in “real” variables (see [59] eq. 2.16), [49] eq. 2.5, p. 513).

2 Hoover puts $g = n$ to ensure that the extended system has an invariant density that projects to the Gibbs-Boltzmann density for $H$. 

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system, based on Wigner’s formalization, coupled to a Nosé-Hoover thermostat (and chains). Thermostats are applied to quantum systems by Mentrup & Schnack [46, 47].

1.2. KAM Tori. Most notable for the purposes of the present note, there are several studies of the Nosé-Hoover thermostat from the point-of-view of near-integrable systems [40, 41, 43]. Legoll, Luskin & Moeckel, in [40], show that the Nosé-Hoover thermostated harmonic oscillator enjoys KAM tori near the $\epsilon = 0$ decoupled limit; they extend this result in [41] to show that an integrable system that is coupled to a Nosé-Hoover thermostat has a first-order averaged system that is also integrable near $\epsilon = 0$ [41, Theorem 3.2]:

**Theorem 1.1** (Legoll, Luskin & Moeckel). _The averaged equations for the Nosé-Hoover dynamics (eq. 2) for a completely integrable Hamiltonian system with $n$ degrees of freedom have $n$ independent first integrals._

The authors speculate that, even if the full system is ergodic, finite-time orbit averages should converge very slowly to the spatial average. They show numerically, using a rotationally-invariant, planar mechanical hamiltonian with potential energy $V(r) = r^2 + r^4$, that the first integrals of the averaged thermostated system appear to display no convergence to a spatial average.

1.2.1. Rotationally-invariant potentials. The first result of the current note is the following:

**Theorem 1.2.** Let $M$ be a surface of revolution with local coordinates $(r, \theta)$ on the rotationally-invariant open set $U \subset M$, $(r, \theta) \rightarrow \mathbb{R}^+ \times \mathbb{R}/2\pi \mathbb{Z}$. Let $V : M \rightarrow \mathbb{R}$ be a real-analytic function which is rotationally invariant, so $V(q) = v(r)$. Assume that

H1. $v$ is strictly increasing on an interval $J$;
H2. $rv''(r) + v'(r) > 0$ for all $r \in J$;
H3. $T = r_o^2v'(r_o)$ for some $r_o \in J$;
H4. The mechanical hamiltonian $H : T^*M \rightarrow \mathbb{R}$ is defined by

$$H(r, p_r, \theta, p_\theta) = \frac{1}{2} \left((c(r)p_r)^2 + (p_\theta/r)^2\right) + v(r),$$

where the kinetic energy is induced by the second-fundamental form of $M$ (i.e. the natural metric induced by the inclusion $M \subset \mathbb{R}^3$).

Then, the Nosé-thermostated hamiltonian $H$ (eq. [1]) for each such $T$ enjoys a full-measure set of masses $\Omega \subset \mathbb{R}^+$ such that if $Q \in \Omega$, then $H$ enjoys a set of positive measure of invariant KAM tori.

This theorem is striking because, in contrast to previous work in the area, there is no constraint that the thermostat mass be “sufficiently small”. When this theorem is applied to the case examined in [41] or a Lennard-Jones potential or the spherical pendulum potential, one obtains:

**Corollary 1.1.** If

1. $M = \mathbb{R}^2$, $v(r) = r^2 + r^4$ and $J = \mathbb{R}^+$; or
2. $M = \mathbb{R}^2$, $v(r) = r^{-12} - r^{-6}$ and $J = (0, 3/4)$; or
3. $M = \mathbb{S}^2$, $r = \sin(\varphi)$, $v = -\cos(\varphi)$ for $0 < \varphi < \pi$ and $J = \mathbb{R}^+$,
then, for all $T \in J$, there is a full-measure set of masses $\Omega \subset \mathbb{R}^+$ such that if $Q \in \Omega$, then $H$ enjoys a positive-measure set of invariant KAM tori.

In fact, Theorem 1.2 and its corollary are proven for a more general class of single thermostat, called generalized, variable-mass thermostats of order 2 (see definition 3.2), which include the thermostats of Winkler and Tapias, Bravetti & Sanders [64, 58].

I believe that for a “generic” rotationally-invariant potential $\epsilon$, and temperature $T$, the set of masses $\Omega$ is $\mathbb{R}^+$ less a finite set. However, the calculations used to prove Theorem 1.2 do not appear to lend themselves to a proof of this.

1.2.2. Thermostating integrable hamiltonians. The current paper sharpens Theorem 1.1 of Legoll, Luskin & Moeckel and shows that their speculation is true for 1.2.2. Thermostating integrable hamiltonians. To explain, some terminology rem 1.1 of Legoll, Luskin & Moeckel and shows that their speculation is true for

Theorem 1.3. Let $H : T^*M \to \mathbb{R}$ be a real-analytic hamiltonian that is completely integrable with real-analytic integrals. Assume that $T > 0$ is a regular value of the orbit mean temperature function $\kappa$ and let

$\mathcal{T} = \{(\theta, I, s, p_s) \mid \kappa(I/s) = T, p_s = 0\}$.

Then, there exists a real-analytic symplectomorphism $\varphi : (\theta, I, s, p_s) = \varphi(\theta, \hat{I}, v, V)$, whose image contains a neighbourhood of $\mathcal{T}$, and a real-analytic function $\tilde{G}$ such that the Nosé-thermostated hamiltonian $H$ is transformed to

$H \circ \varphi = \tilde{G}(\hat{I}) + \frac{1}{2} \epsilon \alpha(\hat{I}) (v^2 + V^2) + \epsilon^2 P_\epsilon \circ \varphi$  \hspace{1cm} (3)

where $\epsilon^2 = 1/Q$, $P_\epsilon$ is real analytic in $\epsilon$ for $\epsilon > 0$, continuous in $\epsilon$ at $\epsilon = 0$ and real analytic in the other variables.

If the re-scaled frequency map $\Omega = (\partial \tilde{G}, \alpha)$ is R-non-degenerate, then, there exists a $Q_0 = Q_0(T, G) > 0$ such that for each $Q \in (Q_0, \infty)$ there is a neighbourhood of $\mathcal{T}$, such that the hamiltonian $H$ has a positive-measure set of invariant tori in that neighbourhood.

Lemma 4.1 has more information about the function $\tilde{G}$ and the neighbourhood of the thermostatic equilibrium set $\mathcal{T}$. Because the first step in creating the symplectomorphism $\varphi$ is indirect, an explicit construction of $\tilde{G}$ seems impossible (except
in some special cases, see remarks 4.7 and 4.8 below). In lieu of this construction, one is able to prove:

**Corollary 1.2.** Assume the hypotheses of Theorem 1.3. Then, the re-scaled frequency map $\Omega$ of $H$ can be made R-non-degenerate by means of a $C^2$-small perturbation of $H$ in the space of real-analytically integrable hamiltonians.

See Corollary 4.1 for the precise, somewhat technical, statement of this corollary.

**Remark 1.1.** Like Theorem 1.2, Theorem 1.3 and its corollary hold for generalized, variable-mass thermostats of order 2. In addition, the theorems hold in the smooth ($C^\infty$) category due to the work of Herman-Féjoz [19]. A puzzling aspect of Theorem 1.3 is that the Nosé-thermostated harmonic oscillator produces a normal form $H \circ \varphi$ whose re-scaled frequency map is not R-non-degenerate (see remark 4.8). So, the theorem here is not proven by reworking an existing proof, but contributes some novel ideas. In addition, it is likely that a better expansion of the thermostat variables $(v, V)$ will also give a proof that the Nosé-thermostated 1-d harmonic oscillator has a frequency map that is R-non-degenerate.

**1.3. Outline.** This note is organized as follows: §2 reviews salient facts about integrable hamiltonian systems and the effect of momentum re-scalings on such systems; §3 defines a general class of single thermostats for which the stated theorems can be proven; §4 contains the material to prove Theorem 1.3 and shows how the theorem implies an improvement on Nosé’s heuristic approximation of the frequency of the thermostat’s oscillations; §5 proves Theorem 1.2 and shows numerical calculations that confirm the theorem’s predictions; §6 contains the necessary material from properly degenerate KAM theory.

## 2. Integrable Hamiltonians

Let $M$ be an $m$-dimensional, real-analytic manifold. The type of Hamiltonian that is considered in this paper is a real-analytic function $H : T^* M \rightarrow \mathbb{R}$ defined on the cotangent bundle $T^* M = \{(q, p) \mid q \in M, p \in T^*_q M\}$ of the real-analytic manifold $M$. Say that $F : T^* M \rightarrow \mathbb{R}$ enjoys fibre-wise super-linear growth if, for each, $(q, p) \neq (q, 0)$, $F(q, \sigma p)/\sigma \rightarrow \infty$ as $\sigma \rightarrow \infty$. The point-wise (or instantaneous) temperature at $(q, p)$ is defined to be $\langle p, H_p \rangle$. If the instantaneous temperature function is bounded above by a constant $C$, then a simple comparison shows that $|H(q, \sigma p)/\sigma|$ is bounded above by $|H(q, p)|/\sigma + C \ln(\sigma)/\sigma$, so $H$ cannot enjoy super-linear growth. Henceforth, it is assumed that $H$ enjoys super-linear growth, whence the instantaneous temperature function is unbounded above on $T^*_q M$ for each $q \in M$.

The cotangent bundle $T^* M$ carries the tautological Liouville 1-form $\lambda$, canonical symplectic form $\Omega = d\lambda$ and its dual, the Poisson bracket $\{\cdot, \cdot\}$. If $q = (q_1, \ldots, q_m)$ are local coordinates on $M$, then any 1-form in $T^*_q M$ is uniquely expressed as $p_1 dq_1 + \cdots + p_m dq_m$ for some scalars $p_1, \ldots, p_m$. These “adapted” coordinates $(q_1, \ldots, q_m, p_1, \ldots, p_m)$ on $T^* M$ satisfy the properties

$$
\lambda = \sum_{i=1}^m p_i dq_i, \quad \{q_i, p_j\} = \delta_{ij}, \quad \{q_i, q_j\} = \{p_i, p_j\} = 0, \quad (4)
$$

where $\delta_{ij}$ is Kronecker’s delta-function. A **Darboux system of coordinates** is a coordinate system $(x_1, \ldots, x_m, y_1, \ldots, y_m)$ on $T^* M$ that satisfies the above Poisson
bracket relations. When \((x_1, \ldots, x_m, y_1, \ldots, y_m)\) is a Darboux system of coordinates, the 1-form \(\sum_{i=1}^m y_i dx_i\) equals the Liouville 1-form \(\lambda\) up to the addition of a closed 1-form.

The Poisson bracket endows the space of real-analytic (resp. smooth) functions on \(T^*M\) with the structure of a Lie algebra.

Recall the notion of complete integrability:

**Definition 2.1.** Let there exist a real-analytic map \(F : T^*M \to \mathbb{R}^m\), where \(m\) is the dimension of \(M\), such that

1. the components of \(F\) Poisson commute;
2. \(F\) has a regular value;
3. \(H = h \circ F\) is the pull-back of a real-analytic \(h : \mathbb{R}^m \to \mathbb{R}\).

Then, \(H\) is said to be **completely integrable** and \(F\) is a first-integral map for \(H\).

The significance of complete integrability is due to the following

**Theorem 2.1** (Liouville–Arnold–Duistermaat). Let \(H : T^*M \to \mathbb{R}\) be completely integrable with first-integral map \(F : T^*M \to \mathbb{R}^m\). The set of regular points of \(F, L \subset T^*M\), is an open and dense set that is fibred by Lagrangian tori and satisfies

\[
\begin{array}{ccc}
T & \xleftarrow{\lambda} & L \xleftarrow{\lambda} T^*M \\
\downarrow & & \downarrow \\
\pi & & \\
\downarrow & & \\
P & \xrightarrow{\delta} & T^*B \xrightarrow{\psi} \Sigma = T^*B/P \xrightarrow{\delta} \mathbb{R}^m \\
\end{array}
\]

where \(\cdots\) denotes a local isomorphism, \(P\) is a sub-bundle \(T^*B\) such that for each \(b \in B\), \(P_b\) is the set of pullbacks \(\pi^*(df)_b\) of locally periodic hamiltonians \(\pi^*f\). The quotient \(T_b^*B/P_b\) is a lagrangian torus so that \(L\) is locally isomorphic to \(\Sigma\). The obstruction to a global isomorphism is a 2-dimensional Chern class that was identified by Duistermaat [17] [14].

In the classical Liouville-Arnold theorem, the focus is on a neighbourhood of a single, regular Lagrangian torus \(L_b = \pi^{-1}(b)\) for some \(b \in B\). In that setting, there is a neighbourhood \(U \subset B\) of \(b\) with coordinates \((I_1, \ldots, I_n)\) where the functions \(\pi^*(I_j)\) generate periodic hamiltonian flows on \(\pi^{-1}(U) \subset L\) with unit primitive period. The tautological Liouville 1-form \(\lambda = \sum_{i=1}^n \theta_i dI_i\) is well-defined on \(T^*_U B\) and defines a local diffeomorphism \(T^*_U B \to \pi^{-1}(U)\) that induces a diffeomorphism \(T^*_U B/P_U \to \pi^{-1}(U)\) when the \(\theta_i\) are taken to be defined mod 1. This implies that the pull-back of the Poisson bracket \(\{,\}_U\) on \(\pi^{-1}(U)\) to \(T^*_U B/P_U\) satisfies

\[
\{I_i, \theta_j\}_U = \Delta_{ij}, \quad \{I_i, I_j\}_U = \{\theta_i, \theta_j\}_U = 0,
\]

where \(\Delta_{ij}\) is a constant, non-singular matrix. In fact, \(\Delta\) is an integer matrix with an integral inverse since the flows of the hamiltonian vector fields \(\{,\}_U\) and \(\{,I_j\}_U\) are periodic with unit primitive period. This implies that there are angle variable \(\varphi_i\) defined implicitly by \(\theta_i = \sum_{j=1}^m \Delta_{ij} \varphi_j\) for \(i = 1, \ldots, m\) and that satisfy \(\{I_i, \varphi_j\}_U = \delta_{ij}\).

In the sequel, the neighbourhood \(\pi^{-1}(U)\) will be suppressed in discussions involving action-angle variables.
2.1. Re-scalings. Let $\sigma \neq 0$ be a non-zero constant. The diffeomorphism $\varphi_\sigma : T^*M \to T^*M$ is defined by re-scaling $p$: $\varphi_\sigma(q,p) = (q, \sigma p)$. Let $f_\sigma = f \circ \varphi_\sigma$ be the composition of the map $f$ with $\varphi_\sigma$.

**Proposition 2.1.** If $H : T^* M \to \mathbb{R}$ is completely integrable with first-integral map $F : T^* M \to \mathbb{R}^m$, then $H_\sigma$ is completely integrable with first-integral map $F_\sigma$.

In addition, if $(I_1, \theta_1)$ are action-angle variables for $H$, then $(\sigma^{-1}I_1, \theta_{\sigma,1})$ are action-angle variables for $H_\sigma$.

**Proof.** An easy computation shows that if $f, g$ are analytic functions on $T^* M$ then

$$\{f_\sigma, g_\sigma\} = \sigma \{f, g\} \circ \varphi_\sigma.$$  \hfill (6)

This, coupled with (eq. 5), proves the proposition. \hfill $\square$

Let $I = (I_1, \ldots, I_m)$ be a local system of actions for $H$ and let $J_\sigma = \sigma^{-1} (I_{\sigma,1}, \ldots, I_{\sigma,m})$ be the actions for $H_\sigma$. Because $H$ is completely integrable, there is an analytic function $G$ such that $H = G \circ I$. Then $H_\sigma = G \circ I_\sigma$ and therefore

$$H_\sigma = G(\sigma J_\sigma),$$  \hfill (7)

where both $H_\sigma$ and $J_\sigma$ are functions of $(q, p)$.

**Proposition 2.2.** Let $R(\theta, I, \sigma) = H_\sigma - G(\sigma I)$. Then

$$R = O(\sigma - 1).$$  \hfill (8)

**Proof.** By the Taylor expansion about $\sigma = 1$, $J_\sigma = J_1 + O(\sigma - 1)$, and $J_1 = I$. Therefore, $I_\sigma = \sigma J_\sigma = \sigma I + O(\sigma - 1)$. The proposition follows from (eq. 7). \hfill $\square$

The hamiltonian function $G(\sigma I)$ is a truncation of $H_\sigma$ that is simple enough to analyze on a fixed system of action-angle coordinates. Unfortunately, it is not a good enough integrable truncation of $H_\sigma$ to be exploited when $H$ is coupled to a single thermostat via momentum re-scaling.

**Proposition 2.3.** Assume the hypotheses of Proposition 2.1. Then, for each toroidal cylinder $V \subset L$ with angle-action coordinates $(\theta, I) : V \to T^n \times B$, and $\sigma$ sufficiently close to 1, there is a generating function $\Sigma = \Sigma(\theta; J_\sigma; \sigma)$ of a symplectic map $f_\sigma : V \to \varphi_{\sigma^{-1}}(V)$ and a real-analytic function $\hat{G} = \hat{G}(I; \sigma)$ such that

$$(\theta_\sigma, J_\sigma) = f_\sigma(\theta, I)$$ \quad and \quad (9)

$$H_\sigma \circ f_\sigma(\theta, I) = \hat{G}(I; \sigma).$$  \hfill (10)

**Proof.** Define $f_\sigma$ by (eq. 9), where $\sigma$ is close enough to 1 so that $\varphi_{\sigma^{-1}}(V) \subset L$. The map $f_\sigma$ is symplectic because it is a canonical change of coordinates from one set of angle-action variables $(\theta, I)$ to another $(\theta_\sigma, J_\sigma)$. Moreover, such changes of angle-action variables are induced by a generating function, hence the existence of $\Sigma$. Finally, by Proposition 2.1 and (eq. 7), one obtains that the pullback of $H_\sigma$ by $f_\sigma$ is a real-analytic function of $I$ that is parameterized by $\sigma$. Hence (eq. 10) holds. \hfill $\square$

**Remark 2.1.** The diffeomorphism $\varphi_\sigma$ effects a momentum re-scaling, which is used in single thermostats following Nosé’s lead. On the other hand, Andersen’s barostat re-scales both momentum $p$ and spatial coordinates $q$, as does the classical version of Grilli & Tosatti’s thermostat. This is perfectly consistent with the framework
introduced here for momentum re-scaling, provided that the configuration manifold \( M \) is invariant under such a re-scaling of spatial coordinates (e.g. \( M \) is the complement of a finite number of hyperplanes in \( \mathbb{R}^m \)). Since the spatial and momentum re-scalings commute and (eq. 6) holds for each separately, it holds for the composition, too. That is, if \( \alpha, \beta \) are non-zero scalars and \( \sigma = (\alpha, \beta) \), then define the re-scaling diffeomorphism \( \varphi_\sigma(q, p) = (\alpha q, \beta p) \) of \( T^* M \). Then, (eq. 6) becomes

\[
\{ f_\sigma, g_\sigma \} = n(\sigma) \{ f, g \} \circ \varphi_\sigma
\]

(11)

where \( f_\sigma = f \circ \varphi_\sigma \), etc.. Propositions 2.1—2.3 hold with the appropriate replacement of the scalar \( \sigma \) by \( \sigma = (\alpha, \beta) \).

3. Single Thermostats

In [8], the following definition is introduced.

**Definition 3.1.** A \( C^r \), \( r > 2 \), function \( N_T(s, S) = \Omega(s)F(S) + T \ln s \) is a variable-mass thermostat of order 2 if \( \Omega > 0 \), \( F(0) = F'(0) = 0 \), \( F''(0) > 0 \) and \( F'' \) vanishes only at 0.

In the present paper, we will always assume that \( r = \omega \), i.e. the thermostat is real analytic. As noted in [8], order means the order of the first non-trivial term in the Maclaurin expansion of \( F \) and the thermostat mass is \( 1/\Omega(s) \). When \( \Omega \) is constant, the thermostat is called elementary. Higher-order thermostats are in the literature, but they present serious challenges for the techniques of this paper. The following are examples of real-analytic thermostats of order 2:

1. the Nosé-Hoover thermostat [50, 49, 27];
2. Tapias, Bravetti & Sanders logistic thermostat [58, 29];
3. Winkler’s thermostat and its generalization [64].

A note about Winkler’s thermostat: it appears in the form of (eq. 1) but with \( ps^{-1} \) replaced by \( ps^{-2} \) and more generally one may use the coupling \( ps^{-e} \) for any \( e > 0 \). By a change of variables, this is equivalent to a thermostat with the standard coupling \( ps^{-1} \) and controller \( N_T(s, S) = \frac{e}{2}(es^{-1}/S)^2 + T \ln s \). Such a thermostat is called a generalized Winkler thermostat.

One can extend the definition of a variable-mass thermostat of order 2 to include real-analytic hamiltonians of the form

\[
N_T(s, S) = T \ln s + \sum_{k=2}^{\infty} \frac{1}{k!} \Omega_k(s)S^k,
\]

(12)

where each \( \Omega_k \) is real-analytic on \( \mathbb{R}^+ \), \( F \) is non-negative, \( F_S = 0 \) only along \( \mathbb{R}^+ \times \{0\} \) and \( F_{SS} > 0 \) along \( \mathbb{R}^+ \times \{0\} \). These assumptions imply, in particular, that \( \Omega_2(s) > 0 \) for all \( s \).

**Definition 3.2.** A real-analytic function \( N_T \) satisfying the properties in the previous paragraph is called a generalized variable-mass thermostat of order 2.

One might be curious as to why the form of the potential is always \( T \ln s \) in the above definitions. In the non-hamiltonian setting, Jellinek, Jellinek & Berry and Ramshaw [32, 33, 34, 52] look at a general form for Nosé-Hoover-like thermostats and none of these authors make an equivalent assumption. However, those papers
do not attempt to derive a hamiltonian form for their non-hamiltonian thermostats and do not address the problem of a canonical form, which is a non-trivial problem since they are parameterized by several functional parameters. On the other hand, under fairly modest hypotheses—the thermostat acts via momentum re-scaling and the thermostatic equilibrium set projects to \( \{(s, S) \mid S = 0, s > 0\} \)—then it is known that, up to a symplectic change of variables in \((s, S)\), the potential can be taken to be \(T \ln s\) ([6] section 5.1, see also [49] part C]).

The cost, though, is that the function \(F\) takes a quite general form as in (eq. [12]).

4. Singly-Thermostated, Integrable Hamiltonians

Let \(N_T\) be a real-analytic, generalized variable-mass thermostat of order 2 and \(H\) be a real-analytically completely integrable hamiltonian.

4.1. An integrable truncation. An integrable truncation of \(H\), denoted by \(\mathbf{H}_0\) and the remainder \(R = H - \mathbf{H}_0\), are given by

\[
\mathbf{H}_0(I, s, S) = G(I/s) + N_T(s, S), \quad R(\theta, I, s, S) = R(1 - 1/s, \theta, I) \tag{13}
\]

where \(\sigma = 1/s\) in (eq. [7]) and \(R\) is defined in Proposition 2.2.

Proposition 4.1. The hamiltonian function \(\mathbf{H}_0\) is completely integrable.

The proof follows by virtue of the fact that the \(n\) components of \(I\) and \(\mathbf{H}_0\) are functionally independent, Poisson-commuting first integrals of the \(n + 1\)-degree of freedom hamiltonian \(\mathbf{H}_0\). The proposition justifies the description of \(\mathbf{H}_0\) as an **integrable truncation** of \(H\). In the ideal case, it would suffice to use \(\mathbf{H}_0\) to study the normal form of \(H\) in a neighbourhood of a \(\mathbf{H}_0\)-invariant torus. As it turns out, this does work when \(G\) is homogeneous in \(I\), but otherwise, one needs a finer truncation.

4.2. The temperature function and its Birkhoff average. Let us define a phenomenological temperature function for the hamiltonian \(H\).

**Definition 4.1.** Let \(H : T^*M \to \mathbb{R}\) be a real-analytic hamiltonian. For each \((q, p) \in T^*M\), and non-negative integer \(n\), define

\[
D^{(n)}H(q, p) = \frac{\partial^n}{\partial \sigma^n} \bigg|_{\sigma=1} H(q, \sigma p). \tag{14}
\]

The function \(D^{(1)}H(q, p)\), which equals \(\langle p, H_2(q, p) \rangle\), defined to be the **instantaneous temperature** of the system with state \(x = (q, p)\).

**Remark 4.1.** The functions \(D^{(n)}H\), for \(n \geq 1\), define a type of moment of momentum, while the ratios \(D^{(n+2)}H/D^{(n)}H\), define a type of “weighted temperature”. In 1-degree of freedom, the moments are used in the thermostats of Watanabe & Kobayashi [63] and in thermostats that target higher moments of temperature [28, 30, 31].

The function \(D^{(n)}H(q, p)\) is related to the \(n\)-th fibre derivative of \(H\), \(d^nH(q, p)\), via the identity

\[
D^{(n)}H(q, p) = \langle p^{(n)}, d^nH(q, p) \rangle \tag{15}
\]

where \(p^{(n)} = p \otimes \cdots \otimes p\) is the \(n\)-fold symmetric tensor product of \(p\) with itself.
Let $\varphi^t$ be the complete flow of the Hamiltonian $H$ and let $f : T^*M \rightarrow \mathbb{R}$ be a continuous function. The Birkhoff average of $f$, denoted by $\overline{f}$, is

$$\overline{f}(q, p) = \lim_{T \rightarrow \infty} \frac{1}{2T} \int_{-T}^{T} f(\varphi^t(q, p)) \, dt.$$  \hspace{1cm} (16)

**Definition 4.2.** The orbit mean temperature is the function $\kappa(q, p)$ that is the Birkhoff average of $D^{(1)}H$; more generally, the orbit mean moment of momentum is the function $\kappa_n(q, p)$ that is the Birkhoff average of $D^{(n)}H$ for $n \geq 1$.

**Proposition 4.2.** Let $H$ be completely integrable. If $(q, p) \in L$ (the union of regular Liouville tori), then

$$\kappa = \langle I, dG(I) \rangle = \frac{\partial}{\partial \sigma} \bigg|_{\sigma = 1} G(\sigma I),$$  \hspace{1cm} (17)

where $H = G \circ I$.

Proof. Let $\gamma(t) = (q(t), p(t)) = \varphi^t(q, p)$ be the integral curve through the point $(q, p) \in L$. Then, the closure of $\gamma(R)$ is contained in a Lagrangian torus and so there are angle-action coordinates $(\theta, I)$ defined in a neighbourhood $U$ of the orbit $\gamma(R)$, as described in the Liouville–Arnol’d–Duistermaat theorem 2.1. Then, since $\sum_{i=1}^n \frac{dI_i}{dt} \wedge d\theta_i = \sum_{i=1}^n q_i \frac{d\theta_i}{dt}$ there is an analytic function $S : U \rightarrow \mathbb{R}$ such that $dS + \sum_{i=1}^n I_i d\theta_i = \sum_{i=1}^n p_i dq_i$.

If we define $\gamma_T = \gamma([-T, T])$ to be a centred orbit segment and $\kappa_T$ to be the mean instantaneous temperature over this segment, then

$$2T\kappa_T(q, p) = \int_{-T}^{T} \langle \dot{q}(t), H_2(q(t), p(t)) \rangle \, dt = \int_{-T}^{T} \langle \dot{q}(t), \dot{p}(t) \rangle \, dt,$$  \hspace{1cm} (18)

$$= \int_{-T}^{T} p \cdot dq = \int_{-T}^{T} I \cdot d\theta + S(\gamma(T)) - S(\gamma(-T)),

= \int_{-T}^{T} \langle \omega(I), I \rangle \, dt + S(\gamma(T)) - S(\gamma(-T)),

= 2T\langle \omega(I), I \rangle + S(\gamma(T)) - S(\gamma(-T)),$$

where $\omega(I) = dG(I)$. Since $S$ is continuous on $U$, it is bounded on a neighbourhood of $\gamma(R)$, and $\kappa = \lim_{T \rightarrow \infty} \kappa_T$, so the result follows. \hfill \Box

**Remark 4.2.** Let $U, V \subset T^*M$ be open sets; a map $f : U \rightarrow V$ is exact symplectic if the pull-back of the tautological Liouville 1-form $\lambda|V$ under $f$ equals $\lambda|U$ up to the derivative of a scalar function. That is, $f$ is exact symplectic if $f^* (\lambda|V) = (\lambda + dS)|U$ for some $S : U \rightarrow \mathbb{R}$. The preceding proof makes use of a single property of the transformation to action-angle coordinates: it is exact symplectic. Indeed, the following is true:

If $f : U \rightarrow V$ is exact symplectic, and $\kappa = \kappa_H$ is the orbit mean temperature function of the Hamiltonian $H$ on $V$, then the orbit mean temperature function $\kappa_{H \circ f}$ of the Hamiltonian $H \circ f$ on $U$ equals $\kappa \circ f$.

In short, the orbit mean temperature function is an invariant of exact symplectic changes of coordinates.

**Remark 4.3.** The Birkhoff average is used because it provides a very natural proof of proposition 4.2. On the other hand, the regularity of the function $\overline{f}$ is generally quite low (just $L^1$) even when $f$ is real analytic. The low regularity stems from the
denseness of the “resonant tori” where the frequency vector $\omega(I)$ enjoys non-trivial integral linear relations: $\exists k \in \mathbb{Z} - \{0\}$ such that $\langle k, \omega(I) \rangle = 0$. These resonances mean the functions $\exp(i \langle k, \theta \rangle)$ do not average to 0. On the other hand, the set of “non-resonant tori” is of full measure, and on each such torus, the Birkhoff average converges to the mean value over the torus.

It follows that the Birkhoff average $\overline{f}$, of a real-analytic function $f$, is an equivalence class of integrable functions that contains a real-analytic representative, namely the fibre average of $f$. This latter is the average of $f$ on each Lagrangian torus, the average being computed with respect to the unique Haar measure on that torus.

In the sequel, we prefer to identify $f$ with this real-analytic fibre average.

4.3. Thermostatic equilibria and iso-thermal non-degeneracy.

Definition 4.3. Fix $T > 0$ and let $\kappa$ be the orbit mean temperature function (def. 4.2). The set

$$\mathcal{T} = \{(\theta, I, s, S) \mid \kappa(I/s) = T, \ s > 0, \ S = 0\}$$

is the set of thermostatic equilibria at temperature $T$ for the integrable truncated hamiltonian $H_0$ (eq. 13).

Proposition 4.3. Assume that $T$ is a regular value of $\kappa$. Then, the thermostatic equilibrium set $\mathcal{T}$ is an invariant, real-analytic submanifold for the hamiltonian flow of $H_0$.

Remark 4.4. The closure of $\mathcal{T} \subset T^* M$ is, in general, an intractable object. However, in case the Liouville foliation of the integrable hamiltonian $H$ is well-behaved (such as when the first integral map $F$ is non-degenerate [18] [16] [15]), then $\kappa$ extends continuously to the closure of $\mathcal{T}$. In this situation, it is useful to regard the $\overline{\mathcal{T}}$ as the set of thermostatic equilibria. The utility of this point of view is highlighted by section 5 where a periodic orbit $\Gamma$ in $\mathcal{T} \setminus \mathcal{T}$ is used to compute the normal form of $\overline{H}$ in a neighbourhood of $\Gamma$ in order to apply KAM theory.

4.4. A normal form. Let $T^*(T^n \times \mathbb{R}^+)$ be the cotangent bundle of $T^n \times \mathbb{R}^+$ and let $X_0 \subset T^*(T^n \times \mathbb{R}^+)$ be the zero section of that bundle and, for $0 < c < 1$, let $X_c \subset X_0$ be the privileged subset

$$X_c = \{ (\theta, I, s, S) \mid \theta \in T^n, \ s \in (c, 1/c), \ I = 0, \ S = 0 \}.$$ 

Lemma 4.1. Let $H$ be the Nosé-thermostated hamiltonian (eq. 1) and let $\mathcal{T}$ be the thermostatic equilibrium set (eq. 19). Then, there are neighbourhoods $W \supset \mathcal{T}$, $X \supset X_c$, $X \subset T^*(T^n \times \mathbb{R})$, a submanifold $\hat{\mathcal{T}} \subset W$ that is a graph over $\mathcal{T}$ and a real-analytic symplectomorphism $\varphi$ such that

$$(\theta_1, I_1, s, S) = \varphi(\theta, I, v, V), \quad X \xrightarrow{\varphi} W \xleftarrow{\varphi} \hat{\mathcal{T}}, \quad X_c \xrightarrow{\varphi} \hat{\mathcal{T}}.$$
and

\[ H \circ \varphi = \hat{G}(I; 1/s_o(I)) + T \ln s_o(I) + \frac{1}{2} \epsilon \alpha(I) \left( \nu^2 + V^2 \right) + \epsilon^2 \mathbf{P}_e \circ \varphi. \]  

(20)

where \( \hat{G}(I; \sigma) \) is the pullback of \( H_\sigma \) in action-angle coordinates, \( \alpha \) is defined in (eq. 31), \( \epsilon = \sqrt{\alpha}, s_o \) is defined in (eq. 25), \( \mathbf{H} \) is an integrable truncation of \( H \) and \( \mathbf{P}_e \) is a remainder term that is real analytic in \( \epsilon \) for \( \epsilon > 0 \) and continuous at \( \epsilon = 0 \).

**Proof.** Let \( V \subset L \) be a toroidal cylinder with angle-action variables \((\hat{\theta}, \hat{I}) : V \rightarrow T^n \times B \) for \( H \). By proposition 2.3 for each such \( V \subset L \) and each \( \sigma \) sufficiently close to 1, there is a symplectic map \( f_\sigma : V \rightarrow L \) such that \( H_\sigma \circ f_\sigma \) is a real-analytic function of the action variables \( \hat{I} \) and the parameter \( \sigma \), i.e. \( H_\sigma \circ f_\sigma(\hat{\theta}, \hat{I}) = \hat{G}(\hat{I}; \sigma) \) where \( \hat{G} \) is real-analytic in both the action variable and parameter \( \sigma \) and \( f_1 \) is the identity. It follows that there is a real-analytic generating function \( \hat{\theta} \cdot \hat{I} + \Sigma(\hat{\theta}, \hat{I}; \sigma) \) of the symplectomorphism \( f_\sigma \) that satisfies

\[ (\hat{\theta}, \hat{I}) = f_\sigma(\hat{\theta}, \hat{I}) \quad \text{iff} \quad \hat{I} = I + \frac{\partial \Sigma}{\partial \hat{\theta}}, \quad \hat{\theta} = \hat{\theta} + \frac{\partial \Sigma}{\partial \hat{I}}. \]

(21)

and \( \Sigma(\hat{\theta}, \hat{I}; \sigma) = O(\sigma - 1) \).

Let us use the symplectomorphism \( f_\sigma \) to define a symplectomorphism \( f \) of \( V \times T^* \mathbb{R}^+ \) as follows: the generating function of \( f \) is defined by

\[ \nu(\hat{\theta}, \hat{I}, s, \hat{S}) = \hat{\theta} \cdot \hat{I} + \Sigma(\hat{\theta}, \hat{I}; 1/s) + \hat{S}s. \]

(22)

Hence,

\[ (\theta, I, s, S) = f(\hat{\theta}, \hat{I}, \hat{s}, \hat{S}) \quad \text{iff} \quad S = \hat{S} - \frac{1}{s^2} \frac{\partial \Sigma}{\partial \hat{S}}, \quad \hat{s} = s, \]

(23)

and (eq. 21) holds. Therefore,

\[ H \circ f(\hat{\theta}, \hat{I}, \hat{s}, \hat{S}) = \hat{G}(\hat{I}; 1/\hat{s}) + \frac{a}{2} \left( \hat{S} - \frac{1}{s^2} \hat{S}_3 \right)^2 + T \ln \hat{s} \]

(24)

where \( \hat{S}_3 \) is \( \Sigma \) evaluated at \( (\hat{\theta}, \hat{I}; \sigma) \) with \( I \) a function of \( \hat{\theta} \) and \( \hat{I} \) by (eq. 21) and \( \hat{S}_3 = \frac{\partial \Sigma}{\partial \hat{S}} \) is the partial derivative with respect to the third variable.

Let us define the set of thermostatic equilibria, \( \hat{T} \), for the function \( \hat{G} \). Let

\[ \hat{T} = \left\{ (\hat{\theta}, \hat{I}, \hat{s}, \hat{S}) \mid \hat{G}_2(\hat{I}; 1/\hat{s}) = \hat{s}T, \hat{s} > 0, \hat{S} = 0 \right\}, \]

where \( \hat{G}_2 \) is the partial derivative of \( \hat{G} \) with respect to the second variable. The function \( \hat{\kappa} := \hat{G}_2(\hat{I}; 1/\hat{s})/\hat{s} \) is the orbit mean temperature of \( H \) in this system of coordinates. By hypothesis and since the map \( f \) is exact symplectic, by remark 4.2 when \( a = 0 \) the function \( \hat{\kappa} \) equals \( \kappa \circ f \) and \( T \) is a regular value. Hence, for all \( a \) sufficiently small there are neighbourhoods \( \hat{J} \ni 1 \) and \( \hat{W} \ni \hat{\kappa}^{-1}(T) \) and a real-analytic function \( \hat{s}_o : \hat{W} \rightarrow \hat{J} \) such that

\[ (\hat{I}, \hat{s}) \in \hat{W} \times \hat{J}, \quad \hat{\kappa}(\hat{I}; 1/\hat{s}) = T \iff \hat{s} = \hat{s}_o(\hat{I}). \]

(25)

Define a generating function \( \hat{\nu} \) by

\[ \hat{\nu}(\hat{\theta}, \hat{I}, \hat{u}, \hat{S}) = \hat{\theta} \cdot \hat{I} + \frac{\hat{S}\hat{s}_o(\hat{I})}{1 - \hat{u}} \]

(26)
and symplectomorphism \( \hat{f} \) by
\[
(\hat{\theta}, \hat{I}, \hat{s}, \hat{S}) = \hat{f}(\hat{\theta}, \hat{I}, \hat{s}, \hat{S}) \quad \text{iff} \quad \hat{S} = \hat{U}(1 - \hat{\nu})^2/\hat{s}_o(\hat{I}), \quad \hat{s} = \hat{s}_o(\hat{I})/(1 - \hat{\nu}) \quad (27)
\]
\[
\hat{I} = \hat{I}, \quad \hat{\theta} = \hat{\theta} + \frac{\partial \hat{\nu}}{\partial \hat{I}}.
\]

This produces
\[
H \circ f \circ \hat{f}(\hat{\theta}, \hat{I}, \hat{s}, \hat{S})
\]
\[
= \hat{G}(\hat{I}; (1 - \hat{\nu})/\hat{s}_o(\hat{I})) + \frac{a}{2} \left( \hat{U}(1 - \hat{\nu})^2/\hat{s}_o(\hat{I}) - \left( \frac{1 - \hat{\nu}}{\hat{s}_o(\hat{I})} \right)^2 \hat{\Sigma}_3 \right)^2
\]
\[
+ T \ln \hat{s}_o(\hat{I}) - T \ln(1 - \hat{\nu}), \quad (28)
\]
\[
= \hat{G}(\hat{I}; 1/\hat{s}_o) + T \ln \hat{s}_o + \frac{1}{2} \hat{\nu}^2 \left( \frac{\hat{G}_22(\hat{I}; 1/\hat{s}_o)}{\hat{s}_o^2} + T \right) + \frac{a}{2\hat{s}_o^2} \hat{\nu}^2 + TO_3(\hat{\nu})
\]
\[
+ \frac{a}{2} \left( \frac{1 - \hat{\nu}}{\hat{s}_o} \right)^4 \hat{\Sigma}_3 \left( -2\hat{U}\hat{s}_o + \hat{\Sigma}_3 \right), \quad (29)
\]

where \( TO_3(\hat{\nu}) = T(\hat{\nu}^3/3 + \cdots) \) is the collection of terms of degree 3 and higher coming from last term in (eq. 28).

Next, define a generating function
\[
\hat{\nu}(\hat{\theta}, \hat{I}, \hat{v}, \hat{U}) = \hat{\theta} \cdot \hat{I} + \gamma(\hat{I})\hat{v}\hat{U}, \quad \text{where}
\]
\[
\gamma(\hat{I}) = \sqrt{\frac{a}{\hat{G}_{22} + \hat{s}_o^2T}}, \quad \alpha(\hat{I}) = \frac{\sqrt{\hat{G}_{22} + \hat{s}_o^2T}}{\hat{s}_o}, \quad (31)
\]

The resulting symplectomorphism, \( \hat{f} \), transforms (eq. 29) into the Hamiltonian
\[
G = G_{\epsilon,T} \quad \text{where (with } \epsilon = \sqrt{a} \text{ and dropping the } \hat{\text{ decoration on the variables})}
\]
\[
G = \hat{G}(\hat{I}; 1/\hat{s}_o) + T \ln \hat{s}_o + \frac{1}{2} \epsilon \alpha(\hat{I}) \left( \nu^2 + V^2 \right) + \epsilon^{3/2} P(I, \theta, v, V; \epsilon), \quad (32)
\]

where \( P \) is real-analytic in its arguments, real-analytic in \( \epsilon \) for \( \epsilon > 0 \) and continuous at \( \epsilon = 0 \).

The remainder of the proof of the lemma follows from defining \( \varphi = f \circ \hat{f} \circ \hat{f} \), whence \( G = H \circ \varphi \) and \( P = P \circ \varphi \).

**Remark** 4.5. The reason the proof of Lemma 4.1 works is ultimately due to the fact that each \( H_\sigma \) is completely integrable, or in somewhat less precise terms, the Nosé-thermostat “vibrates” an integrable hamiltonian within a family of integrable hamiltonians. One can see that the preceding lemma readily admits the following generalization:

Let \( N_T(s, S) = F(s, S) + T \ln s \) be a generalized variable-mass thermostat of order 2 (definition 3.2) and define \( N_{a,T}(s, S) = a^{-2}N_T(s, aS) \) for \( a > 0 \). If \( H \) is thermostated by \( aN_{a,T} \), then the conclusions of Lemma 4.1 hold as stated with the only exception that \( \alpha \) equals \( \sqrt{\Omega S(\hat{s}_o)} \) times the \( \alpha \) appearing in (eq. 31).

In this case, one sees that the remainder term \( P \), absorbs all but the lowest degree term \( (\frac{1}{2} a \Omega S(s)S^2) \) in the thermostat, and when we expand around the thermostatic
equilibrium set, only the lowest degree term \( \frac{1}{2} a \Omega_2(\hat{s}_o)(\hat{U}/\hat{s}_o)^2 \) is not absorbed in the remainder.

**Remark 4.6.** To lowest order, the frequency of the normal oscillations of \( \mathbf{H}/\hat{r} \) is \( \epsilon \alpha(I) \) where \( \epsilon = \sqrt{\alpha} \). In [50, eq. 2.29], Nosé derives an approximation to the frequency of the oscillations of the thermostat state \( s \). In his solution, one finds the approximation to this frequency to be, in the notation of the current paper,

\[
\epsilon \left( \frac{2nT}{(n + 1)s_o^2} \right)^{\frac{1}{2}},
\]

In comparison to (eq. 31), Nosé’s approximation imputes the value \( \hat{G}_{22} = nT/(n + 1)s_o^2 \) along the thermostatic equilibrium set. On the other hand, it follows from the calculations in remarks 4.7 & 4.8, that \( \hat{G}_{22} = (\lambda - 1)T s_o^2 \) on that same set when \( H = G(I) \) is positively homogeneous of degree \( \lambda \) in \( I \), so Nosé’s approximation is only correct when the degree of homogeneity \( \lambda = 2 - 2/(n + 1) \). Leimkuhler & Sweet [42, p. 190] use Nosé’s approximation to determine an “optimal” choice of mass \( Q = 1/a \) to thermostat a single harmonic oscillator, but they find that it produces an unsatisfactory distribution of the thermostat state and need to make \( Q \) almost an order of magnitude smaller to produce a satisfactory distribution.

Figures 1 & 2 show the ratio of the frequencies of the normal and internal oscillations of a 1-degree of freedom hamiltonian of the form of (eq. 33) that is thermostated with the Nosé thermostat with \( a = 10^{-2} \) and \( 10^{-1} \), respectively, and \( T = 1 \). It is clear from the graphs that Nosé’s approximation is only accurate for the thermostated harmonic oscillator, while the present paper’s approximation is accurate in all the examples considered.

**Remark 4.7.** Let us compute an example to illustrate Lemma 4.1. Let the number of degrees of freedom be \( n \geq 1 \), let \( \xi, \eta > 0 \) be even integers and \( \lambda > 0 \) satisfy the identity \( 1/\lambda = 1/\xi + 1/\eta \). Define

\[
H(q, p) = h(q_1, p_1) + \cdots + h(q_n, p_n), \quad h(x, p_x) = \frac{1}{c} (p_x^\xi + x^\eta).
\]

(33)

(the constant \( c > 0 \) is a normalization constant chosen below). The hamiltonian \( H \) is separable and a simple computation shows that in action-angle variables

\[
H = G \circ I = I_1^\lambda + \cdots + I_n^\lambda,
\]

(34)

where the normalization constant \( c \) is chosen so that \( c = (\pi\eta/(2B(1 + 1/\xi, 1/\eta)))^\lambda \) and \( B \) is the Beta function [1, Chapter 6].

It is easy to see that \( H_\sigma(q, p) = \sigma^\lambda H(Q, P) \) when \( q = Q\sigma^\chi, p = P/\sigma^\chi \) and \( \chi = \lambda/\xi \). The generating function

\[
\nu(Q, p, s, \hat{S}) = Q \cdot p \cdot s^{-\chi} + \hat{S}s
\]

(35)

induces the symplectomorphism \( (q, p, s, S) = f(Q, P, \hat{s}, \hat{S}) \)

\[
(q, p, s, S) = (Qs^{-\lambda}, Ps^\lambda, \hat{s}, \hat{S} - \chi \hat{s}^{-1}QP).
\]

(36)

Therefore, the Nosé-thermostated hamiltonian is transformed to

\[
\mathbf{H} \circ f(Q, P, \hat{s}, \hat{S}) = \hat{s}^{-\lambda} H(Q, P) + a \frac{1}{2} \left( \hat{S} - \chi \hat{s}^{-1}QP \right)^2 + T \ln \hat{s}.
\]

(37)
Figure 1. (T) The ratio of the frequencies of the normal (thermostat) and internal oscillations of a weighted homogeneous, single degree-of-freedom hamiltonian. The upper curve (blue) is that implied by Lemma 4.1 while the lower curve (red) is implied by Nosé’s approximation (see Remark 4.6). The dots are determined by integrating the Nosé-thermostated weighted-homogeneous hamiltonians (eq. 33) with even integer exponents $2 \leq \xi, \eta \leq 10$. The computation of the error bar is described in figure 4. The orbits are started at $x = 0, S = 0, s = 1$ and $p_x$ is determined from the condition that $H = T/\lambda$ (see remark 4.7). A stepsize of $h = 2^{-5}$ and time interval of length $2^{10}$ is used; $a = 10^{-2}$ and $T = 1$ are the fixed thermostat parameters. (ML+R) The Fourier transforms of $x, p_x, \sqrt{a}S$ and $s$ (ignoring the mean value of $s$) for the Nosé-thermostated harmonic oscillator ($\xi = 2 = \eta$). (BL+R) As above, with $\xi = 10 = \eta$. 
Figure 2. (T,ML+R) As for figure 1, but with $a = 10^{-1}$. (BL+R) As above, with $\xi = 10, \eta = 6$. The dominant frequency of the oscillations in $x$ (and $p_x$) is visible at $k = 235$ while there are “beats” at $k = 134, 335$; the secondary peak at $k = 702$ is surrounded by two pair of beat frequencies at $k = 803, 904$ and $k = 601, 500$. The dominant frequency in $S$ is at $k = 468$ and is driven by the internal oscillations of $x$ and $p_x$. It is surrounded by two pair of beats at $k = 569, 670$ and $k = 266, 367$. The frequency of the normal oscillations of $S$ ($k = 102$) is responsible for the beating.
With the convenient notation that \( I^\lambda = \sum_{i=1}^n I_i^\lambda = G(I) \), one sees that the function \( \hat{G} \) equals
\[
\hat{G}(\hat{I}; 1/\hat{s}) = G(\hat{I}/\hat{s}) = (\hat{I}/\hat{s})^\lambda.
\]
The thermostatic equilibrium set \( \hat{T} = \hat{G}^{-1}(T/\lambda) \) and so
\[
\hat{s}_o(\hat{T}) = \left( \frac{\lambda G(\hat{I})}{T} \right)^{1/\lambda}.
\]

4.5. Main Theorem. The re-scaled frequency map of \( \mathbf{G} = \mathbf{H} \circ \varphi \) (eq. [32]) from Lemma 4.1 is computed to be
\[
\Omega(I) = (\hat{G}_1(I; 1/\hat{s}_o), \alpha(I)), \quad \alpha(I) = \frac{\sqrt{\Omega_2(\hat{s}_o)} (\hat{G}_2 + \hat{s}_o^2 I)}{\hat{s}_o^2},
\]
using equation (eq. [25]) and remark 4.5.

**Theorem 4.1.** Assume that for some \( T > 0 \), the re-scaled frequency map \( \Omega \) of the function \( \mathbf{G}_{s,T} \) (eq. [32]) is R-non-degenerate when \( \epsilon = 0 \). Then, there exists a function \( \epsilon_o(T) \) such that \( \epsilon_o(T) \) is positive for all but countably many values of \( T > 0 \) and for all \( 0 < \epsilon < \epsilon_o(T) \), there exists a neighbourhood of the thermostatic equilibrium set \( \hat{T} \) and a positive-measure, \( \mathbf{G}_{s,T} \)-invariant set \( \mathbf{K}_{s,T} \) in this neighbourhood. In particular, the Hamiltonian flow of \( \mathbf{G}_{s,T} \) is not ergodic for \( 0 < \epsilon < \epsilon_o(T) \).

**Proof.** By Lemma 4.1 and Theorem 6.1 the theorem follows. \( \square \)

**Remark 4.8.** (Continuation of remark 4.7). It is straightforward to verify that, when \( \lambda \neq 1 \), the re-scaled frequency map \( \Omega(I) \) (eq. [40]) is R-non-degenerate for this example. Indeed, one can verify that the map \( I \rightarrow \hat{G}_1(I; 1/\hat{s}_o) \) is a diffeomorphism onto its image: This is because it equals the diffeomorphism \( I \rightarrow dG(I) \) multiplied by a positive scalar \((1/\hat{s}_o^\lambda)\) and the degree of homogeneity of their product is \(-1\). Therefore, if the image of \( \Omega \) is contained in a linear subspace, there is a normal vector to the subspace of the form \( v = (w, -1) \) and so \( \alpha(I) = \langle w, \hat{G}_1(I; 1/\hat{s}_o) \rangle \) for a fixed vector \( w \). In this case, \( \alpha(I) = \sqrt{\Omega_2(\hat{s}_o)} \sqrt{T/\hat{s}_o} \) so the subspace condition implies the identity in \( I \):
\[
\sqrt{\Omega_2(\hat{s}_o)} = \sqrt{T/\lambda} \frac{1}{G(I)} \sum_{i=1}^n w_i I_i^{\lambda - 1}.
\]

Evaluation of each side at the points \( I^{(i)} = \delta_{ij} \) (\( \delta \) is Kronecker’s delta function), implies that \( w_i = w_o = \sqrt{\Omega_2(\hat{s}_o)} (\lambda/T)^{\frac{1}{2} + 1/\lambda} \) where \( \hat{s}_o = (\lambda/T)^{1/\lambda} \). Substituting this into (eq. [41]) implies
\[
\sqrt{\Omega_2(\hat{s}_o)} = \sqrt{\Omega_2(\hat{s}_o)} \cdot \lambda^{2/\lambda} \cdot T^{-2} \cdot \sum_{i=1}^n I_i^{\lambda - 1}.
\]
Let \( I = bs^{1/\lambda} \) for \( b = (T/\lambda)^{1/\lambda} \). Then \( G(I) = (bs)^\lambda \) and \( \hat{s}_o(I) = s \) so (eq. [42]) implies that
\[
\Omega_2(s) = \Omega_2(\hat{s}_o) \cdot (\lambda/T)^{2(1+1/\lambda)} \cdot s^{2(\lambda - 1)} = cs^{2\lambda - 2}.
\]
On the other hand, if \( I = bs \sum_{i=1}^k I^{(i)} \) for \( k \leq n \), then \( G(I) = k(bs)^\lambda \) and \( \hat{s}_o(I) = k^{1/\lambda} s \), which implies that \( \Omega_2(s) = k^{1+2/\lambda} \cdot c \cdot s^{2\lambda - 2} \). Thus, when \( n > 1 \), there is no solution to (eq. [42]), hence the re-scaled frequency map \( \Omega \) is R-non-degenerate.
This demonstrates R-non-degeneracy for the thermostated Hamiltonian except when \( \lambda = 1 \) (the thermostated harmonic oscillator) or \( n = 1 \). When \( n = 1 \) and \( \lambda \neq 1 \), an R-degenerate generalized variable-mass thermostat of order 2 must have the variable mass function \( \Omega_2 \) described by (eq. 43). In particular, the Nosé and logistic thermostats are R-non-degenerate in this case, too, while the generalized Winkler thermostat is R-non-degenerate unless \( \lambda = 2 - \frac{1}{c} \) (see p. 8).

4.6. Main Corollary. Let \( X \) be a real-analytic manifold and \( C^k(X) \) be the space of real-valued functions \( f : X \rightarrow \mathbb{R} \) which are continuous with \( k \geq 0 \) continuous derivatives; \( C^\infty(X) = \bigcap_{k \geq 0} C^k(X) \) and \( C^\omega(X) \subseteq C^\infty(X) \) is the set of real-analytic functions. Besides the intrinsic direct limit topology, there are many topologies on the space of real-analytic functions \( C^\omega(X) \) since \( C^\omega \subset C^\infty \subset C^k \) for all \( k \geq 0 \). Let us use the subspace topology from the uniform \( C^k \) topology. In this case, a basic open set consists of a compact set \( K \subset X \) and an open set \( U \subset \bigcup_{i=0}^k \mathbb{R}^{d_i} \) such that the map \( x \mapsto J_k(x) \), \( J_k(x) = (f(x), df_x, \ldots, d^k f_x) \), maps \( K \) into \( U \) (\( d_i \) is the dimension of the linear space of symmetric tensors of degree \( i \) on \( \mathbb{R}^n \)). When \( X \) is symplectic, there is a distinguished subset \( \mathfrak{J} \) of completely integrable Hamiltonian functions and \( \mathfrak{J}^k = \mathfrak{J} \cap C^k(X) \) for \( k \in \{2, \ldots, \infty, \omega \} \). We can equip \( \mathfrak{J}^\omega \) with the \( C^k \) subspace topology.

**Corollary 4.1.** Let \( H \in \mathfrak{J}^\omega \) be completely integrable and \( N = N_{n,T} \) be a generalized variable-mass thermostat of order 2. Assume that

1. \( T \) is a regular value of the orbit mean temperature function \( \kappa \) of \( H \);
2. The function \( G_{22} \) is non-negative.

Then, there is a set \( \mathfrak{U} \subset \mathfrak{J}^\omega \) that is relatively open in the uniform \( C^2 \) topology such that

1. \( H \) is in the closure of \( \mathfrak{U} \);
2. If \( H' \in \mathfrak{U} \), then the re-scaled frequency map \( \Omega' \) of \( H' \) is R-non-degenerate.

**Proof.** The proof of this corollary is straightforward. Consider a “semi-global” perturbation of \( \hat{G} \) on \( W \times \mathbb{R}^+ \) that is of the form \( \hat{g}(I, s) = \frac{1}{2}(s - \hat{s}_o)^2\Phi(I) \) where \( \Phi \) is a non-negative, real-analytic function and let \( \hat{G}^{(\eta)} = \hat{G} + \eta \hat{g} \) where \( \eta \) is a parameter. Assume that \( \Phi \) does not satisfy any linear equation with coefficients in the ring over \( \mathbb{R} \) generated by \( \Omega_2(\hat{s}_o) \) and the components of \( G_1 \). The functions \( \hat{G}^{(\eta)} \) share the same thermostatic equilibrium scaling function \( \hat{s}_o \) by construction. By choosing \( \Phi \) appropriately, it is clear that one may assume that \( \hat{G}^{(\eta)}_{11} \) is non-degenerate at some point in \( \mathcal{T} \) for all \( \eta > 0 \) sufficiently small. Thus, suppose that for each \( \eta \) there is a vector \( v_\eta = (w_\eta, -1) \) such that the perturbed, re-scaled frequency map \( \Omega^{(\eta)} \) lies in the linear subspace orthogonal to \( v_\eta \). Then

\[
\Omega_2(\hat{s}_o) = \frac{\hat{s}_o^4}{G_{22}/\eta + \hat{g}_{22} + \hat{s}_o^2 T/\eta},
\]

must hold identically for \( \eta > 0 \). This implies that, as \( \eta \rightarrow \infty \), \( \langle w_\eta/\eta, \hat{G}_1 \rangle \) must converge to a function of \( I \); and so, since \( \hat{G}_1 \) is a local diffeomorphism, \( w_\eta/\eta \) converges to a fixed vector \( r \) as \( \eta \rightarrow \infty \). Therefore,

\[
\Phi = \frac{\Omega_2(\hat{s}_o)}{\langle r, \hat{G}_1 \rangle^2}.
\]
Thus \( \Phi \) satisfies a linear equation in the ring over \( \mathbb{R} \) generated by \( \Omega_{2}(s_{0}) \) and the coefficients of \( \hat{G}_{1} \). Contradiction.

Finally, it has been shown that there are specific perturbations that are “semi-global” and \( \mathbb{R} \)-non-degenerate. For a global perturbation of \( H \), one can take \( H + \psi(F \circ \varphi_{1}/s) \) where \( \psi \) is real-analytic, \( F \) is the first-integral map of \( H \), and \( \psi \) is chosen as a sufficiently close approximation to a \( \hat{g} \) from the preceding paragraph.

\[ \square \]

5. An example: rotationally-symmetric potentials

Let’s consider examples of rotationally-symmetric mechanical Hamiltonians on a surface \( \Sigma = \mathbb{R}^{2} \) or \( S^{2} \). In [41, section 4], Legoll, Luskin and Moeckel consider the case where the hamiltonian is

\[ H(r, p_r, \theta, p_{\theta}) = \frac{1}{2} \left( p_r^2 + \frac{r^{-2} p_{\theta}^2}{s^2} \right) + v(r) + F(s, aS)/a + T \ln s, \]

(46)

in symplectic polar coordinates on \( T^{*}\mathbb{R}^{2} \).

In addition to the general result on the existence of integrals for the averaged Nosé-Hoover thermostat (see Theorem 1.1 above), for the specific potential \( v(r) = r^2 + r^4 \), they show numerical evidence that, for “small” \( a \sim 10^{-2} \) and \( T = 1 \), the Nosé-Hoover thermostated system (eq. 2) is nearly integrable and the averaged system has 2 independent integrals, which corresponds to 3 independent integrals for the Nosé-thermostated hamiltonian \( H \) (eq. 1).

5.1. The case of \( \mathbb{R}^{2} \). Let’s consider the case where \( H \) (eq. 46) is a rotationally-invariant, real-analytic mechanical hamiltonian. Thermostat \( \hat{H} \) with a real-analytic generalized, variable-mass thermostat of order 2, to get:

\[ H(r, p_r, \theta, p_{\theta}, s, S) = \frac{1}{2} \left( p_r^2 + \frac{r^{-2} p_{\theta}^2}{s^2} \right) / s^2 + v(r) + F(s, aS)/a + T \ln s, \]

(47)

where \( F(s, S) \) is described in (eq. 12).

Recall the two hypotheses from the statement of Theorem 1.2 about the potential \( v \) that are assumed to hold on some open interval in \( \mathbb{R}^{+} \):

H1. The function \( v'(r) > 0 \);
H2. The function \( rv''(r) + v'(r) > 0 \).

Lemma 5.1. Assume H1 and H2 hold on an open interval \( J \subset \mathbb{R}^{+} \).

Let \( r_o = r_o(p_\theta/s; T) \) and \( s_o = s_o(p_\theta; T) \) be real-analytic, scalar functions of a single variable parameterized by the temperature \( T \). Define the generating function

\[ \nu(\rho, p_r, \theta, p_{\theta}, u, S) = \rho \cdot r_o \cdot (1 + \rho) + \theta \cdot p_{\theta} + S \cdot s_o / (1 - u), \]

(48)

which generates the symplectic map \( f \)

\[ r = r_o \cdot (1 + \rho), \quad p_r = p_\rho / r_o, \quad \theta = \hat{\theta} + \xi, \]

\[ p_{\theta} = p_\theta, \quad s = s_o / (1 - u), \quad S = (1 - u)^2 U / s_o \]

\[ - p_\rho \cdot r_o' \cdot (1 + \rho) \cdot (1 - u)^2 / (r_o \cdot s_o^2), \]

where \( \xi \) is a real-analytic function and \( r_o \) and its derivative are evaluated at \( p_\theta(1 - u) / s_o \).

\[ ^{3} \text{Recall that } a \text{ in the present paper is } 1/Q \text{ in [41] and } \epsilon^2 \text{ in (eq. 2).} \]
Then, \( G = H \circ f \) has a relative critical point at \( \rho = u = p_\rho = U = 0 \) if there is an \( r_o \in J \) such that the following hold:

\[
T = r_o \cdot v'(r_o), \quad \tau = |p_\theta|/s_o, \quad \text{and} \quad \tau^2 = r_o^3 \cdot v'(r_o). \tag{50}
\]

Proof. Let \( U = p_\rho = u = \rho = 0 \). Since both \( p_r \) and \( S \) are linear in \( p_\rho \) and \( U \) and \( H \) is quadratic in \( p_r \) and \( S, \dot{u} = 0 = \dot{\rho} \). Assume that \( \tau = p_\theta/s_o \) and \( p_\theta > 0 \) (in case \( p_\theta < 0 \), one takes \( \tau = -p_\theta/s_o \)). Then one computes:

\[
\dot{p}_\rho = -G_\rho = (\tau/r_o)^2 - r_o \cdot v'(r_o),
\]

\[
\dot{U} = -G_u = (\tau \cdot r_o^3 \cdot r_o' \cdot v'(r_o) - \tau^3 \cdot r_o' - Tr_o^3 + \tau^2 \cdot r_o)/s_o^3.
\tag{51}
\]

The first equation implies the last equation of (eq. 50) given the middle one. By hypotheses \( H1 \) & \( H2 \), the function \( r \mapsto r^3 \cdot v'(r) \) is increasing on \( J \) and therefore the function \( \tau = \sqrt{r^3 \cdot v'(r)} \) is increasing on \( J \). Hence, there is a local inverse \( r_o = r_o(\tau) \).

The second equation of (eq. 51) implies that

\[
T = (\tau^2 \cdot r_o - \tau^3 \cdot r_o' + \tau \cdot r_o^3 \cdot r_o' + v'(r_o))/r_o^3 = \tau^2/r_o^2 = r_o \cdot v'(r_o),
\]

where the inverse function theorem has been applied to \( r_o = r_o(\tau) \) to simplify the expression in parentheses. This proves the lemma.

By virtue of the previous lemma, one can define the functions \( \tau(r) = \sqrt{r^3 \cdot v'(r)} \) and \( T(r) = r \cdot v'(r) \) for \( r \in J \). By \( H1 \), \( T(r) > 0 \) and by \( H2 \), \( T'(r) > 0 \). Hence, there is a single-valued inverse \( r(T) \) for \( T \in T(J) \). This implies that the equations (eq. 50) determine a unique value for \( r_o = r(T) \) and a unique value \( \tau = \tau(T) \). So, the middle equation defines

\[
s_o(p_\theta; T) = \frac{|p_\theta|}{\tau(T)}, \tag{52}
\]

and \( r_o = r_o(\tau(T); T) \), also.

Henceforth, it is assumed that \( r_o, s_o \) and \( \tau \) are determined as in lemma 5.1.

5.1.1. Symplectic reduction. Let’s fix the value \( p_\theta = \mu \neq 0 \) and reduce the hamiltonian \( G \) modulo the rotational action by translation of \( \theta \). The symplectic reduction of \( \{p_\theta = \mu \} \subset T^\ast(\mathbb{R}^2 \times \mathbb{R}^+) \) by this free action of \( \text{SO}(2) \) is a symplectic manifold \( X_\mu \) that is symplectomorphic to \( T^\ast(\mathbb{R}^+ \times \mathbb{R}^+) \). The Darboux coordinates \( (\rho, p_\rho, u, U) \) are defined on a neighbourhood of the reduced critical point \( (r = r_o, p_r = 0, s = s_o, S = 0) \) of the reduced hamiltonian \( G_\mu \) (obtained from \( G \) by fixing \( p_\theta = \mu \)).

Lemma 5.2. The linearized hamiltonian vector field of \( G_\mu \) at the critical point \( \rho = u = p_\rho = U = 0 \) is

\[
\dot{X} = A X = \begin{pmatrix}
A & B \\
-C & 0 \\
0 & -D
\end{pmatrix} X, \tag{53}
\]

where \( X = [\rho, u, p_\rho, U] \) and (with \( r = r_o, W = (rv'' + 3v') \))

\[
C = rW, \quad D = 2rv'(W - 2v')/W, 
\]

\[
A = \frac{1}{(rs_o)^2} + 4a\Omega_2(s_o)(v')^2/s_o^2W^2, \quad B = -2a\Omega_2(s_o)v'/s_o^2W, \quad E = a\Omega_2(s_o)/s_o^2.
\]


The characteristic polynomial of $A$ is
\[ p(x) = x^4 + (DE + AC)x^2 + CD(AE - B^2). \] (55)
For $a > 0$, the hessian of $G_\mu$ at the critical point is positive definite, by H1 & H2. Therefore, let $\pm i\omega_1, \pm i\omega_2$ be the purely imaginary roots of $p$, with $\omega_2 \geq \omega_1 > 0$, and let $\eta = \omega_1/\omega_2$. The function $\eta = \eta(\mu; a, T)$ is continuous everywhere and real-analytic except at the points where $\eta = 1$.

Lemma 5.3. The following hold:

1. If, for fixed $a, T > 0$, $\eta = \eta(\mu; a, T)$ is a non-constant function of $\mu = p_\theta$, then there exists a full-measure set, $\mathcal{M}$, of $\mu$ and a neighbourhood $O$ of the critical point of $G_\mu$ such that for each $\mu \in \mathcal{M}$, there exists a positive-measure set of invariant tori $\mathcal{T}_\mu \subset O$; or

2. For each $T > 0$ and $\mu \neq 0$, there exists a full-measure set $\mathcal{A} \subset \mathbb{R}^+$ such that if $a \in \mathcal{A}$, then there is a neighbourhood $O$ of the critical point of $G_\mu$ and a positive-measure set of invariant tori $\mathcal{T}_a \subset O$.

To prove this lemma, one needs to recall a classic result of Russmann. Recall that a vector $\omega \in \mathbb{R}^n$ is Diophantine with constant $\gamma > 0$ and exponent $\tau > 0$ if
\[ |\langle k, \omega \rangle| \geq \gamma |k|^{-\tau}, \quad \forall k \in \mathbb{Z}^n \setminus \{0\}. \]
It is well-known that the set of Diophantine vectors is of full measure in $\mathbb{R}^n$.

Russmann, in [54, p. 56], proves that if the Hamiltonian $H$ has a critical point with first Birkhoff invariant $H_2 = \langle \omega, I \rangle$ where $\omega$ is a Diophantine vector and the Birkhoff normal form of $H$ is $B = \sum_{k=1}^{\infty} a_k H_k^2$ (with $a_1 = 1$), then this formal power series actually converges on a neighbourhood of the critical point and there is a real-analytic symplectic map $\varphi$ defined on the same neighbourhood such that $H \circ \varphi = B$. In two degrees of freedom, this implies the following.

Theorem 5.1 (Russmann [54]; Churchill, Pecelli, Sacolick and Rod [13]).
Let $H(x_1, x_2, p_1, p_2) = H_2(I_1, I_2) + O(3)$ where $H_2 = \omega_1 I_1 + \omega_2 I_2$ and $I_i = \frac{1}{2} (x_i^2 + p_i^2)$, be a real-analytic hamiltonian defined on a neighbourhood of $0 \in \mathbb{R}^4$. Assume that $\omega = (\omega_1, \omega_2)$ is a Diophantine vector in $\mathbb{R}^2$. One of the two possibilities holds:

1. for some $k > 1$, the Birkhoff normal form of $H$ of degree $k$ is non-zero modulo polynomials of degree $k$ in $H_2$; or

2. for all $k > 1$, the Birkhoff normal form of $H$ of degree $k$ is a polynomial in $H_2$.

In the second case, there is a real-analytic symplectic map $\varphi$ defined on a neighbourhood of $0$ and real-analytic function $G$ such that $H \circ \varphi = G \circ H_2$.

Remark 5.1. It follows that if a two-degree-of-freedom hamiltonian $H$ has a critical point with $H_2 = \langle \omega, I \rangle$ and $\omega$ Diophantine, then there is a neighbourhood of the critical point that contains a positive measure set of invariant tori. In case (1), this follows from the fact that there is a $k > 0$ such that the Birkhoff polynomial $B_k$ of degree $k$ has a Hessian that is non-degenerate for some $(I_1, I_2)$ near $(0, 0)$. In case (2), it is clear since $H$ is integrable.

Proof of Lemma 5.3. In case (1), $\eta$ is a non-constant function of $\mu$, so the frequency map $\mu \rightarrow (\omega_1, \omega_2)$ is R-non-degenerate and real-analytic (except for at most countably many values of $\mu$). It follows that the pre-image of the full-measure set of Diophantine vectors is a set of full measure.
Remark 5.2. If $\Omega_2$ is constant, then for fixed $a, T$, the coefficient $DE + AC \propto s_0^{-2}$ while $CD(AE - B^2) \propto s_0^{-4}$, so the roots of the characteristic polynomial (eq. 55) lie on a line through 0 when $p_\theta = \mu$ varies. Thus, $\eta$ is constant as a function of $\mu$. In addition, it is easy to see that when $\Omega_2$ is non-constant, then $\eta$ is, too. On the other hand, case (2) of lemma 5.3 holds independent of whether $\Omega_2$ is constant or not. Figure 3 graphs the function $T \mapsto \eta(1; a, T)$ for the Nosé-thermostated planar system with potential energy $v(r) = r^2 + r^4$ and selected values of $a$.

5.2. The case of surfaces of revolution. Let us study the more general class of surfaces with a rotational symmetry. A standard construction of a surface of revolution, $M$, is to fix a unit-speed “profile” curve $\gamma(\xi) = (r(\xi), 0, z(\xi))$ in the $x$–$z$ plane and to rotate that curve about the $z$-axis. A rotationally-invariant mechanical hamiltonian $H : T^* M \rightarrow \mathbb{R}$ has the form

$$H(\xi, p_\xi, \theta, p_\theta) = \frac{1}{2} \left( p_\xi^2 + (p_\theta/r(\xi))^2 \right) + w(\xi),$$

where $\theta$ is the angle of rotation and $w : M \rightarrow \mathbb{R}$ is a rotationally-invariant potential energy.

Remark 5.3. The simplest examples of profile curves and the associated surfaces of revolution are:

$$\gamma(\xi) = \begin{cases} 
(c, 0, \xi), & \xi \in \mathbb{R}, \quad \text{a cylinder of radius } c > 0; \\
(\xi, 0, 0), & \xi > 0, \quad \text{the } x$–$y \text{ plane; } \\
(C + \cos(\xi), 0, \sin(\xi)), & \xi \in [0, 2\pi], \quad \text{a torus when } C > 1; \\
(\sin(\xi), 0, -\cos(\xi)), & \xi \in [0, 2\pi], \quad \text{the unit sphere.}
\end{cases}$$

If $r'(\xi) \neq 0$ for $\xi$ in an interval $K$, then there is the inverse function $\xi(r)$ defined on the interval $J = r(K)$. One can equally use $(r, \theta)$ as a local coordinate system on $M$, in which case the mechanical hamiltonian is transformed to:

$$H(r, p_r, \theta, p_\theta) = \frac{1}{2} \left( (c(r)p_r)^2 + (p_\theta/r(r))^2 \right) + v(r),$$

where $v(r) = w(\xi(r))$ and $c(r) = 1/\xi'(r)$. The thermostated hamiltonian $H$ is

$$H(r, p_r, \theta, p_\theta, s, S) = \frac{1}{2} \left( (c(r)p_r)^2 + (p_\theta/r(r))^2 \right) / s^2 + v(r) + F(s, aS)/a + T \ln s,$$

i.e. the planar case (eq. 47) has the same form with $c \equiv 1$. It follows that lemma 5.1 holds verbatim, while lemma 5.2 holds with one change: in the expression for the coefficient $A$, $1/(r s_0)^2$ becomes $(c(r)/rs_0)^2$ (recall that $r = r_0$ in that lemma). Finally, lemma 5.3 holds for the frequency ratio function $\eta$, in this case, too.
5.3. Numerical calculations. To illustrate Theorem 1.2 and Corollary 1.1, figures 4–7 display a panel of data obtained by integrating the thermostated planar mechanical system with a Lennard-Jones (12,6) potential at a temperature of $T = 1/2$ and varying values of $a$. The 4-th order Candy–Rozmus–Forest–Ruth algorithm is utilized [9, 22]. This technique is based on splitting the Hamiltonian $H$ into $H_1 + H_2$ where each $H_i$ is trivially integrable. Because the kinetic energy is euclidean, this is accomplished by treating $s$ as a momentum variable and $S$ as a configuration variable. Interestingly, the proof of the normal-form Lemma used a similar trick (see eq. 22).

6. Properly Degenerate KAM Theory

Arnol’d [5], in his attempt to prove the stability of the $n$-body problem, formulated an important extension of his work on the stability of quasi-periodic motions [4]. In that work, one considers a Hamiltonian on $T^m \times D^m \times R^2l$ of the form

$$H_\epsilon(\theta, I, x, y) = H_0(I) + \epsilon H_1(\theta, I, x, y; \epsilon),$$

(60)

where the perturbation $H_1$ itself is decomposed as

$$H_1(\theta, I, x, y) = P_1(I; \epsilon) + \sum_{|k| \leq d} \alpha_k(I; \epsilon) J^k + O(|x, y|^{2d+1}).$$

(61)

The coordinates $x_i, y_i$ are canonically conjugate, $J_i = \frac{1}{2} (x_i^2 + y_i^2)$ for $i = 1, \ldots, l$ and $J^k = J_1^{k_1} \times \cdots \times J_l^{k_l}$. The decomposition of $H_1$ is obtained by averaging over the fast variables $\theta$ to a sufficiently high degree and then computing the Birkhoff polynomial of the resulting function of $(x, y)$ (parameterized by $I$).

Arnol’d used the case where $d = 3$, while Chierchia & Pinzari obtain Arnol’d’s results with only $d = 2$ [10, 11]. On the other hand, Chierchia & Pusateri prove the following theorem for $d = 1$ (see [19] for the $C^\infty$ case):

**Theorem 6.1.** Assume that the real-analytic Hamiltonian $H_\epsilon$ as in (eq. 60) and (eq. 61), which depends $C^1$ on $\epsilon$, has a re-scaled frequency map at $\epsilon = 0$,

$$\Omega(I) = (dH_0(I), \alpha_1(I), \ldots, \alpha_l(I)),$$

that is $R$-non-degenerate. Then, for all $\epsilon$ sufficiently small, there exists a positive-measure set of phase space that belongs to $H_\epsilon$-invariant Lagrangian tori. These tori are $O(\epsilon)$-close to the Lagrangian tori $\{I = \text{const.}, J = O(\epsilon)\}$. The flow on each such torus is quasi-periodic with Diophantine frequencies.

Note that [12, Theorem 4] as stated is not the theorem used to prove the existence of real-analytic KAM tori for the spatial $n$-body system in that paper—see [12, p. 870]. Instead, the authors use theorem 6.1 which allows for the Hamiltonian and its decomposition to depend in non-trivial ways on $\epsilon$—but it must be at least continuous in $\epsilon$. It is this theorem that is needed to prove Theorem 1.3 of the present paper.

7. Conclusions

This paper has demonstrated that, in a weakly-coupled regime, the generalized, variable-mass thermostats of order 2—including the Nosé, logistic and Winkler thermostats—cannot force most integrable systems to sample from the Gibbs-Boltzmann distribution. It has also shown that for some integrable systems (rotationally-invariant mechanical systems on surfaces), these same thermostats never force...
the system to be ergodic (at least for a full-measure set of coupling parameters/thermostat masses).

A number of questions remain, though. Here are a select few.

1. **Effective bounds for $Q_o$:** Theorem 1.3 proves the existence of some positive lower bound $Q_o$ for the thermostat mass (equivalently, a positive upper bound for the coupling coefficient $a$) beyond which there are positive-measure sets of KAM tori for the thermostated system. The theoretical values for the bounds are generally incredibly small—see, for example, the discussion in [26, Section 4.4]. It is desirable to have a better understanding of this bound, if only for some particular thermostats and Hamiltonians.

2. **The Thermostated Harmonic Oscillator:** Theorem 1.3 does not apply to the 1-d harmonic oscillator coupled to a generalized, variable-mass thermostat of order 2 (remark 4.8). Of course, Legoll, Luskin & Moeckel prove the existence of invariant tori in a neighbourhood of the thermostatic equilibrium set, for all $a$ sufficiently small, by different means [40]. On the other hand, there is an abundance of numerical evidence that suggest KAM tori persist for $a \cong 1$. Is it true that the “perturbation” term $P_\epsilon$ in (eq. 20) contains terms that stabilize the system, even for $\epsilon \cong 1$?

3. **Extensions of Theorem 1.3:** There are several directions to extend the theorem. Beyond the previous point, it is desirable to have a generally effective means to determine if the theorem applies to a particular thermostated Hamiltonian. In addition, order-2n single thermostats appear in the literature, so it is desirable to extend the theorem to encompass such thermostats [59, 63]. A further direction to extend the theorem is to reversible thermostats that do not necessarily have a Hamiltonian reformulation. The thermostat of Kusnengov, Bulgac & Bauer is one such example, while the generalized Nosé-Hoover is a second [39, 38, 57].

**Acknowledgments**

Computations in this paper have been done with Maxima CAS [45].

This research has been partially supported by the Natural Science and Engineering Research Council of Canada grant 320 852.

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Figure 3. The frequency ratio $\eta = \omega_1/\omega_2$ v. the natural logarithm of the temperature $T$ for selected values of $a$. The potential energy is $v(r) = r^2 + r^4$ and the thermostat is Nosé’s. The value of $\eta$ at $a = 0$ is $T = 0$ in all cases.
Figure 4. Nosé Thermostat. (TL) The frequency ratio function \( \eta = \omega_1/\omega_2 \) for the Lennard-Jones 12-6 potential \( v(r) = r^{-12} - r^{-6} \) as a function of the parameter \( a \) for the Nosé thermostat at temperature \( T = 1/2 \) (in blue) and the "empirical" frequency ratio as measured by a numerically-integrated orbit segment on the interval \([0, B]\), with \( B = 2^8 \), stepsize = \( 2^{-4} \), and a displacement \( \delta = 10^{-6} \) from the relative equilibrium. The error bars are (conservative) estimates of the uncertainty in the estimated ratios whose height is \((k_1 + 1)/((k_2 - 1) - (k_1 - 1))/((k_2 + 1)\) when \( \omega_i = 2\pi k_i/N \) and \( N \) is the sample size. (TR) As in (TL) with \( B = 2^{10} \); the decrease in uncertainty is notable. (ML) As in (TL) with \( \delta = 10^{-2} \). (MR) As in (TR) with \( \delta = 10^{-2} \). (BL+R) Selected amplitude vs. frequency number of the Fourier transform of \( x \) and \( p_x \) (dark grey and black, left axis); \( y \) and \( p_y \) (dark blue and blue, left axis) and \( s \) and \( S \) (light red and red, right axis). The mean value of \( s \) is ignored to highlight the oscillatory modes.
Figure 5. Nosé Thermostat. Top panel: (TL) Projection of an orbit segment onto the $sSx$ 3-space seen from an oblique angle; (TR) The same orbit segment projected onto the $sS$ plane. (BL) Change in energy from its initial value. (BR) Change in angular momentum from its initial value.

Bottom panel: Same as for top panel with different value of $a$ and $\delta$. 

$a = 1, T = 1/2, \lambda = 1/16, B = 1024, \delta = 10^{-6}$

$a = 1, T = 1/2, \lambda = 1/16, B = 1024, \delta = 10^{-6}$

$a = 19, T = 1/2, \lambda = 1/16, B = 1024, \delta = 10^{-2}$

$a = 19, T = 1/2, \lambda = 1/16, B = 1024, \delta = 10^{-2}$
Figure 6. Logistic Thermostat. For a description, see figure 4.
Figure 7. Logistic Thermostat. For a description, see figure 5.

- $a = l, T = 1/2, b = 1/16, B = 1024, \delta = 10^{-6}$

- $a = l, T = 1/2, b = 1/16, B = 1024, \delta = 10^{-6}$

- $a = 19, T = 1/2, b = 1/16, B = 1024, \delta = 10^{-4}$

- $a = 19, T = 1/2, b = 1/16, B = 1024, \delta = 10^{-4}$