Abstract. Let \( H(q,p) = \frac{1}{2} \|p\|^2 + V(q) \) be an \( n \)-degree of freedom \( C^r \) mechanical Hamiltonian on \( T^n \) \( T^n \) where \( r > 2n + 2 \). When the metric \( \| \cdot \| \) is flat, the Nosé-thermostated system associated to \( H \) is shown to have a positive-measure set of invariant tori near the infinite temperature limit. This is shown to be true for all variable mass thermostats similar to Nosé’s, too. These results complement results of Legoll, Luskin & Moeckel and the author \([4, 5, 2]\).

1. Introduction

In equilibrium statistical mechanics, the mechanical Hamiltonian \( H(q,p) \) is the internal energy of an infinitesimal system \( S \) that is immersed in a heat bath \( B \) at the temperature \( T \). Nosé [6], based on earlier work of Andersen [1], introduced a simple model of this energy exchange. 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 \( N(s, p_s) = \frac{1}{2M} p_s^2 + nkT \ln s \), (1)

where \( n \) is the number of degrees of freedom of the system \( S \), \( M \) is the “mass” of the thermostat and \( k \) is Boltzmann’s constant. Nosé’s thermostated Hamiltonian \( F \) has two desirable properties: the orbit average of twice the kinetic energy, \( 2K = \| ps^{-1} \|^2 \), is \( T \) and the thermostated system is Hamiltonian.

Hoover’s reduction of Nosé’s thermostat eliminates the state variable \( s \) and rescales time \( t \) [3]:

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

The Nosé-Hoover thermostated simple harmonic oscillator reduces to the following “simple” system:

\[
\dot{q} = \rho, \quad \dot{\rho} = -q - \xi \rho, \quad \dot{\xi} = (\rho^2 - T) / M.
\]

(2)

Legoll, Luskin and Moeckel show in [4] that near the decoupled limit of \( M = \infty \) and \( \xi = 0 \), the thermostated harmonic oscillator (eq. 2) is non-ergodic. This is done via averaging, which reduces the thermostated equations to a non-degenerate twist map, that shows the existence of KAM tori. In a subsequent paper, the authors extend the averaging argument to thermostated integrable \( n \)-degree of freedom Hamiltonians [5]. It is shown that the averaged equations are integrable, which

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implies that near the decoupled limit the thermostated system’s orbits remain close to these invariant tori over a long, but finite, time horizon. This is a significantly weaker result than the 1-degree of freedom result.

1.1. Complete integrability & KAM sufficiency. Let \( \theta \in T^n = \mathbb{R}^n/\mathbb{Z}^n \) and \( I \in \mathbb{R}^n \equiv T^*_\theta T^n \) be coordinates on the cotangent bundle of \( T^n \) equipped with its canonical symplectic structure. Let \( H_c(\theta, I) = H_0(I) + \epsilon H_1(\theta, I; \epsilon) \) be a parameterized family of Hamiltonians that is \( C^r \) in all its variables where \( r > 2n \). For \( \epsilon = 0 \), the Hamiltonian is completely integrable with invariant tori \( T^n \times \{ I = C \} \) and the flow on these invariant tori is a translation-type flow with frequency vector \( \omega_0 = \left[ \partial H_0 / \partial I \right] \). The Hamiltonian \( H_0 \) (or, by abuse of terminology, \( H_c \)) is said to be Kolmogorov non-degenerate at \( I = C \) if (c.f. \[10\] §2.1, \[9\] §1.2):

\[
\det d\omega_0 |_{I = C} \neq 0, \quad \text{where} \quad d\omega_0 = \left[ \frac{\partial^2 H_0}{\partial I_i \partial I_j} \right]
\]  

(3)

or it is iso-energetically non-degenerate at \( I = C \) if:

\[
\det \begin{bmatrix} d\omega_0 & \omega_0 \\ \omega_0 & 0 \end{bmatrix} |_{I = C} \neq 0, \quad \text{where} \quad \omega_0 = \left[ \frac{\partial H_0}{\partial I} \right].
\]  

(4)

If \( H_0 \) is Kolmogorov non-degenerate, then, for all \( \epsilon \) sufficiently small, there is an open neighbourhood \( W \subset T^n \) containing \( C \), a measurable subset \( W_\epsilon \subset W \) and a symplectic diffeomorphism on \( T^n \times W \) that conjugates the Hamiltonian flow of \( H_{\epsilon=0} \) on \( T^n \times W_\epsilon \) to that of \( H_c \). The set \( W_\epsilon \) has a complement of measure \( O(\epsilon) \) and the conjugacy is as smooth as \( H_c \). In particular, the set of invariant tori that are “preserved” under perturbation has positive measure, which precludes ergodicity.

If \( H_0 \) is iso-energetically non-degenerate, then similar conclusions hold: for all \( \epsilon \) sufficiently small, there is an open neighbourhood \( W \subset T^n \) containing \( C \), a measurable subset \( W_\epsilon \subset W \) and an energy-preserving diffeomorphism \( H_{\epsilon=0}(c) \rightarrow H_{\epsilon=1}(c) \) that conjugates the Hamiltonian flow of \( H_{\epsilon=0} \) restricted to \( T^n \times W_\epsilon \subset H_{\epsilon=0}(c) \) to a time-change of the Hamiltonian flow of \( H_\epsilon \) restricted to \( H_{\epsilon=1}(c) \). The complement of \( W_\epsilon \) in \( W \) has measure \( O(\epsilon) \), which precludes ergodicity on the energy level \( c \).

These two forms of non-degeneracy are independent, see e.g. \[9\] §1.2.

1.2. The Thermostated Free Particle. In Andersen’s paper on his barostat, a simplifying assumption is made: the mechanical system is periodic, or in other words, the configuration space is a torus \([1]\). The present paper starts by proving the following results about thermostated free particles on flat tori. Specifically, let \( T^n = \mathbb{R}^n/\mathbb{Z}^n \) be the \( n \)-dimensional torus and say that the set of thermostatic equilibria of the thermostat \( F \) (eq. \[\ref{5}\]) is the set of points where \( s = 0 = \dot{p} \) (it is assumed this set is invariant).

\textbf{Theorem 1.1.} Let \( V : T^n \rightarrow \mathbb{R} \) be \( C^r \) for some \( r > 2n+2 \), \( \|v\|^2 \) a flat Riemannian metric on \( T^n \) and let \( H_\epsilon : T^*T^n \rightarrow \mathbb{R} \) be the family of mechanical Hamiltonians

\[
H_\epsilon(q, p) = \frac{1}{2} \|p\|^2 + \epsilon V(q).
\]  

(5)

Fix the thermostat mass \( M > 0 \), temperature \( T > 0 \) and let \( F_\epsilon \) be the Nosé-thermostated Hamiltonian (eq. \[\ref{1}\]) associated to \( H_\epsilon \). There is an open neighbourhood of the set of thermostatic equilibria of \( F_0 \) on which \( F_0 \) is both Kolmogorov and iso-energetically non-degenerate.
The Hamiltonian $H_0$ is purely kinetic, so the Nosé-thermostated Hamiltonian $F_0$ can be thought of as describing the thermostated free particle on a flat $n$-torus; in this case, the set of thermostatic equilibria is invariant. Moreover, by the real analyticity of $F_0$ and consequently the real analyticity of the change of coordinates to action-angle variables, each open set on which the non-degeneracy condition holds is dense in the extended phase space of the thermostated free particle. It follows from these facts and the remarks about KAM theory in subsection 1.1, that for all $\epsilon$ sufficiently small, the Hamiltonian flow of the Nosé thermostat $F$ is not ergodic on any energy level. The proof of Theorem 1.1 appears in section 4.1.

1.3. The high-temperature limit. Theorem 1.1 allows us to investigate the dynamics of Nosé’s thermostat near the high-temperature limit $T = \infty$ with the thermostat mass $M$ held constant. It proves non-degeneracy, in both of the above senses, of a suitably rescaled thermostat at the $T = \infty$ limit, thereby establishing the existence of positive measure sets of KAM tori for thermostated mechanical systems on the $n$-torus at sufficiently high temperatures.

**Theorem 1.2.** Let $V : \mathbb{T}^n \rightarrow \mathbb{R}$ be $C^r$ for some $r > 2n+2$, $\|\cdot\|^2$ a flat Riemannian metric on $\mathbb{T}^n$ and let $H : T^*\mathbb{T}^n \rightarrow \mathbb{R}$ be the mechanical Hamiltonian
\[
H(q,p) = \frac{1}{2} \|p\|^2 + V(q).
\] (6)

Fix the thermostat mass $M > 0$. The rescaled Nosé-thermostated Hamiltonian $F$ (eq. 1) associated to $H$ is both Kolmogorov and iso-energetically non-degenerate in the $T = \infty$ limit.

The rescaled thermostat is explained in more detail in section 3. Theorem 1.2 is, in fact, a corollary of Theorem 1.1 where the role of the small parameter $\epsilon$ is played by the inverse temperature $\beta$. The proof of Theorem 1.2 appears in section 4.1.

These results are stronger than those obtained in [5] largely because multi-dimensional averaging is not needed to prove Theorem 1.1. Instead, we are able to use the complete integrability of the Nosé-thermostated free particle to verify the Kolmogorov and iso-energetic non-degeneracy conditions.

A corollary of Theorem 1.1 (resp. 1.2) is that if $\|\cdot\|_1$ is a Riemannian metric that is $C^r$-sufficiently close to the flat metric $\|\cdot\|$, then the conclusion of the Theorem 1.1 (resp. 1.2) holds for the Nosé-thermostated Hamiltonian $F_1$ associated to $H_1(q,p) = \frac{1}{2} \|p\|^2_1$ (resp. $H_1(q,p) = \frac{1}{2} \|p\|^2_1 + V(q)$).

1.4. Variable-Mass Thermostats. A natural question that arises in light of the above results on the existence of invariant tori is whether there are thermostats like Nosé’s that do not possess these invariant KAM tori in the large temperature limit. A Nosé-like, or variable-mass, thermostat is one which involves momentum rescaling and the thermostatic equilibrium (where $\dot{s} = 0 = \dot{\rho}_s$) is independent of that rescaling. [2, Theorem 1.2] proves that in such a case the thermostat $N$ is characterized by a smooth positive function $\Omega_T = \Omega_T(s)$, possibly parameterized by the temperature $T$, such that
\[
N = \frac{1}{2} \Omega_T \rho_s^2 + nkT \ln s.
\] (7)

The function $1/\Omega_T$ might be viewed as a variable thermostat mass.

With this characterization of variable-mass thermostats, this paper proves
Theorem 1.3. Assume the Hamiltonian $H_\varepsilon$ satisfies the hypotheses of Theorem 1.1, fix $T > 0$ and let $\Omega = \Omega_T \in C^r(\mathbb{R}^+, \mathbb{R}^+)$ and $N$ be the Nosé-like thermostat (eq. 7). Then there is an open set, whose closure contains the set of thermo-
static equilibria of the thermostated Hamiltonian $F_0$ (eq. 7), on which $F_0$ is both
Kolmogorov and iso-energetically non-degenerate.

The infinite temperature limit corollary of Theorem 1.3 is

Theorem 1.4. Assume the hypotheses of Theorem 1.2, let $N$ be the Nosé-like
thermostat (eq. 7) and let $\Omega_T \in C^r(\mathbb{R}^+, \mathbb{R}^+)$ be such that
$R_T(s) = \Omega_T(s/\sqrt{T})$ converges to a limit $\Omega \in C^r(\mathbb{R}^+, \mathbb{R}^+)$ as $T \to \infty$. Then the thermostated Hamiltonian $F_0$ (eq. 1) with the variable-mass thermostat
$N$ (eq. 7) determined by $\Omega_T$ is both Kolmogorov and iso-energetically non-degenerate in the $T = \infty$ limit.

These two theorems are proven in a similar manner to their constant-mass coun-
terparts. Of course, the constant-mass theorems are special cases, but because the
variable-mass case is more involved, we have elected to present proofs of each. The
proofs appear in section 4.2.

2. Terminology and Notation

Generating functions are a classical and convenient way to create canonical trans-
formations. To explain, let $(q', p') = f(q, p)$ be a canonical transformation, so that
$q' \cdot dp' + p' \cdot dq = d\phi$ is closed and therefore locally exact. That is, there is a locally-defined function $\phi = \phi(p'; q)$ of the mixed coordinates $(p'; q)$ such that $q' = \partial \phi / \partial p'$ and $p = \partial \phi / \partial q$. The transformation $f$ is implicitly determined by $\phi$. The identity
transformation has the generating function $\phi = q \cdot p'$.

In the sequel, a canonical system of coordinates $(x, X) = (x_1, \ldots, x_n, X_1, \ldots, X_n)$
are denoted using the capitalization convention: the Liouville 1-form equals $\sum_{i=1}^n X_i dx_i$
and $X_i$ is the momentum conjugate to the coordinate $x_i$.

In practice, construction of action-angle coordinates for a particular Hamiltonian
is a very difficult problem. However, approximate action-angle coordinates may be
constructed by methods similar to their construction in the Birkhoff normal form:
by means of a sequence of generating functions that transform the Hamiltonian into
a near-integrable form. In this case, one verifies non-degeneracy for the integrable
approximation.

3. The Rescaled Thermostat

The parameters $n, k, T$ that enter the thermostat may have physical significance,
but for the purposes here, it suffices to amalgamate $nkT$ into a single parameter,
which is denoted by $T$. Let us rescale the variables in the Nosé thermostat
$q = \sqrt{M} w \mod \mathbb{Z}^n, \quad p = W/\sqrt{M}, \quad s = \sigma/\sqrt{MT}, \quad p_s = \sqrt{MT} \Sigma$. (8)

With this canonical change of variables, the thermostated Hamiltonian for $H$ (eq. 6)
is, where $\beta = 1/T$,

$$F = T \times \left[ \frac{1}{2} \|W/\sigma\|^2 + \frac{1}{2} \Sigma^2 + \beta V(w\sqrt{M}) + \ln \sigma \right]_{F_\beta} - \frac{1}{2} T \ln(MT). \quad (9)$$

The coordinates $(W, \Sigma)$ are canonically conjugate, so up to a constant
rescaling of time, the Hamiltonian flow of $F$ equals that of $F_\beta$. Additionally, when
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\( M = 1, F_\beta \) is the Nosé-thermostated Hamiltonian for the Hamiltonian \( H_\beta \) (eq. 5) of Theorem 1.1 with \( \epsilon = \beta \).

Because the thermostat mass, \( M \), is fixed and enters into the rescaled thermostated Hamiltonian \( F_\beta \) only through the bounded potential \( V \), the convention is adopted that

\[ M = 1. \] (10)

The analysis below is altered in insignificant ways by this additional hypothesis.

4. The Nosé Thermostat

In the 1-degree of freedom case, the following lemma illuminates the nature of the Hamiltonian \( F_\beta \) (eq. 9).

Lemma 4.1 ([2]). Let \( n = 1 \) and \( \beta = 0 \). Under the canonical change of coordinates induced by introducing cartesian coordinates, \( (a, b) = (\sigma \cos w, \sigma \sin w) \), the rescaled thermostated Hamiltonian equals

\[ F_0 = \frac{1}{2} [A^2 + B^2] + \frac{1}{2} \ln (a^2 + b^2). \] (11)

That is, \( F_0 \) is a mechanical Hamiltonian with a rotationally invariant logarithmic potential.

In the \( n \)-degree of freedom case, the Hamiltonian \( F_\beta \) is the average of \( n \) such Hamiltonians, under the constraint that the radial distance from the origin (\( \sigma \)) and radial momentum (\( \Sigma \)) coincide for each.

The Hamiltonian \( F_0 \) is completely integrable. In particular, there is a family of normally elliptic invariant tori of \( F_0 \) along the variety \( \{ \sigma = \| W \| \neq 0, \Sigma = 0 \} \), parameterized by the angular momentum integral \( \mu = W \). To deduce the existence of a positive-measure set of invariant KAM tori, one would like to apply a theorem of Rüssmann and Sevryuk [7, 8]. The potential functions \( U(\sigma) = \sigma^\alpha / \alpha \), and the degeneration \( U = \ln \) frustrate this.

Instead of this straightforward route, we are obliged to compute action-angle variables for \( F_0 \) and verify non-degeneracy directly. The computation of action-angle variables is a difficult problem for most integrable systems, due to the problems involved in computing the necessary integrals (quadratures). However, in order to apply KAM theory, it suffices to compute approximate action-angle variables, or rather action-angle variables for an approximation to the given integrable Hamiltonian—this is most commonly done in a neighbourhood of an elliptic critical point via the Birkhoff normal form. We pursue a similar strategy in a neighbourhood of the above-mentioned normally elliptic invariant tori. As in the case of the Birkhoff normal form, one postulates the form of the Hamiltonian in action-angle variables up to a given order and attempts to solve for the generating function of the canonical change of variables. This is the strategy of the following lemma.

4.1. Constant Temperature Thermostat. In order to state the following lemma, let us recall that a flat Riemannian metric on the \( n \)-torus induces an inner product on \( \mathbb{R}^n \) which will be denoted by \( \langle \cdot, \cdot \rangle \). By means of this inner product, \( \mathbb{R}^n \) and its dual vector space are identified. The identification will be denoted by \( v \mapsto v' = \langle v, \cdot \rangle \). The dual inner product on the dual of \( \mathbb{R}^n \) will be denoted by \( \langle \cdot, \cdot \rangle \), also, so the inverse of the map \( v \mapsto v' \) is \( v'' \mapsto v \).
The point \( P \in \mathbb{R}^+ \times \mathbb{T}^n \times \mathbb{R} \times \mathbb{R}^n \equiv T^*(\mathbb{R}^+ \times \mathbb{T}^n) \) is denoted by \( P = (\sigma, w, \Sigma, W) \), which gives a coordinate system. Similarly, a point \( Q \in T^*(\mathbb{T}^1 \times \mathbb{T}^n) \) is denoted by \( Q = (\theta, \eta, I, J) \). The zero section of \( T^*X \) is denoted by \( Z(X) \).

**Lemma 4.2.** Let \( C \) be a unit co-vector and let \( \lambda \subset T^*(\mathbb{R}^+ \times \mathbb{T}^n) \) be the isotropic graph of \( w \rightarrow (1, w, 0, C) \). There are neighborhoods \( \mathcal{O} \supset \lambda \) and \( \mathcal{P} \supset Z(\mathbb{T}^1 \times \mathbb{T}^n) \) and a canonical transformation \( \Phi : \mathcal{P} \rightarrow \mathcal{O} - \lambda, (\sigma, w, \Sigma, W) = \Phi(\theta, \eta, I, J) \), that transforms the Hamiltonian \( F_0 \) (eq. 15) to the sum \( G_0 + G_1 \) where

\[
G_0 = \frac{I}{4} \left( 1 - \frac{11}{24} I + \langle C, J \rangle \right) + O(5) \tag{12}
\]

\[
G_1 = -\langle C, J \rangle - \langle C, J \rangle^2 + \frac{1}{2} \| J \|^2 + (\| J \|^2 - \frac{4}{3} \langle C, J \rangle^2) \langle C, J \rangle \tag{13}
\]

where \( I \) has degree 2, \( J \) has degree 1 and \( O(5) \) is a remainder term containing terms of degree \( \geq 5 \).

**Remark 4.1.** A few points on the statement of Lemma 4.2

1. The variables \((\theta, \eta, I, J)\) are angle-action variables, to leading order, for the Hamiltonian \( F_0 \).

2. It may seem odd that \( I \) and \( J \) do not both have degree 1 in the expansions.

3. The reason is revealed in the proof: the expressions in eq.s 12, 13 or 14 originate from degree 4 Taylor polynomials in coordinates on \( \mathcal{O} \) and in these coordinates, \( I \) is a quadratic function and \( J \) is linear. This reflects the fact that the regular Liouville tori in \( \mathcal{O} - \lambda \) limit onto the isotropic torus \( \lambda \).

**Proof.** The generating function \( \varphi(\Sigma, W; u, v) = (1 - u) \| W \| + \langle C - W, v \rangle \) induces the canonical transformation \((\sigma, w, \Sigma, W) = f(u, v, U, V)\) where

\[
\sigma = (1 - u) \| C - V \|, \quad \Sigma = U/\| C - V \|, \quad W = C - V.
\]

This transforms the Hamiltonian \( F_0 \) in variables \((\sigma, w, \Sigma, W)\) to

\[
F_0 = \frac{1}{2} (1 - u)^{-2} + \frac{1}{2} \| C - V \|^{-2} U^2 + \ln(1 - u) + \ln \| C - V \|. \tag{15}
\]

The symplectic map \( f \) is singular along the set \( \{ V = C \} \) (which should be mapped to the zero section of \( T^*\mathbb{T}^n \), \( \{(w, W) \mid W = 0\} \)), and it transforms \( \{ u = 0, U = 0 \} \) to the variety \( \{ \sigma = \| W \| \neq 0, \Sigma = 0 \} \) which consists of quasi-periodic and periodic invariant tori.

The determination of a further coordinate change is independent of the final term in \( F_0 \), which involves only \( V \), so we let \( G_0 = F_0 - \ln \| C - V \| \) as indicated in (eq. 15). With the fourth-order Maclaurin expansion of \( G_0 \), one obtains

\[
G_0 = \left( 2 \langle C, V \rangle^2 - \frac{1}{2} \| V \|^2 + \langle C, V \rangle + \frac{1}{2} \right) U^2 + \left( \frac{9u^2}{4} + \frac{5u}{3} + 1 \right) u^2 + O(5), \tag{16}
\]

where \( O(5) \) is the remainder term that contains terms of degree 5 and higher.
Because $G_0$ is independent of $v$, one postulates a second symplectic transformation $(x, y, X, Y) \rightarrow (u, v = y, U, V)$ with the generating function
\[
\nu = \nu(U, V; x, y) = xU + \langle y, V \rangle + \sum_{i,k,l} \nu_{ijkl} x^i U^k V^l + O(5),
\]
where $l$ is a multi-index, $V^l = \prod_{i=1}^n V_i^l$, the degree of the terms in the sum are 3 or 4 and $O(5)$ is the remainder of terms of degree at least 5. In addition, a transformed Hamiltonian is postulated
\[
G_0 = \left( x^2 + \frac{X^2}{2} \right) \left( \alpha \left( x^2 + \frac{X^2}{2} \right) + \langle \gamma Y, Y \rangle + \langle \beta, Y \rangle + 1 \right) + O(5),
\]
where $\alpha$ is a scalar, $\beta$ is a co-vector and $\gamma$ is a symmetric linear map. One solves for the generating function $\nu$ and $G_0$ simultaneously, and arrives at
\[
\nu = \langle y, V \rangle + U \left[ x \left( 1 + \frac{1}{2} \langle C, V \rangle - \frac{1}{4} \|V\|^2 + \frac{5}{8} \langle C, V \rangle \right) - \frac{5}{6} x^2 \left( 1 + \langle C, V \rangle \right) + \frac{55}{144} x^3 \right] + O(5),
\]
and
\[
\alpha = -\frac{11}{24}, \quad \beta = C, \quad \gamma = \frac{1}{2} \left( 3CC' - 1 \right).
\]
Note that when $n = 1$ and $C = 1$, the above results simplify to those found in [2].

To complete the proof, let $I = (x^2 + X^2/2)$, $\theta$ be the conjugate angle (mod $2\pi$), and $\eta = y \mod \mathbb{Z}^n$, $J = Y$. The composition of the sequence of above-defined canonical coordinate changes defines the canonical coordinate change $\Phi^{-1}: (\sigma, w, \Sigma, W) \rightarrow (\theta, \eta, I, J)$. The transformed Hamiltonian $G_0$ (eq. 18) is congruent mod $O(5)$ to that in eq. 19.

The form of the function $G_1$ (eq. 19) in these coordinates is determined by the Maclaurin expansion of $\frac{1}{2} \ln(1 - t)$ to fourth order, combined with the substitution $t = 2\langle C, J \rangle - \|J\|^2$. This yields the stated expansion of $G_1$ to $O(5)$.

**Proof of Theorem 1.1.** The thermostated Hamiltonian $F_\epsilon = F_0 + \epsilon V(w) = F_0 + O(\epsilon)$ where $O(\epsilon) = \epsilon V(w)$ is $C^r$ and $\mathbb{Z}^n$-periodic in $w$. Under the sequence of canonical transformations in lemma 4.2, $w = -\eta + \rho(\theta, \eta, I, J) + O(5) \mod \mathbb{Z}^n$ where $\rho$ is a real-analytic map, and $O(5)$ is a remainder in $I, J$. So the perturbation in the approximate angle-action variables $(\theta, \eta, I, J)$ is $C^r$ and $O(\epsilon)$.

The Hessian of $F_0$ in the action variables $(I, J)$ is
\[
A = \begin{bmatrix}
-\frac{11}{24} & C' \\
C & 1 - 2CC'
\end{bmatrix}
\]
when $I = 0, J = 0$.

When restricted to the invariant subspace $V$ spanned by $(1,0)$ and $(0, C)$, $A$ is non-singular; and the restriction of $A$ to the invariant subspace $V^\perp$ is also non-singular. Thus, $F_0$ is Kolmogorov non-degenerate in a neighbourhood of the invariant isotropic torus $\lambda$. Since $\lambda$ is determined by the arbitrary unit co-vector $C$, $F_0$ is Kolmogorov non-degenerate in a neighbourhood of $\{1\} \times \mathbb{T}^n \times \{0\} \times S^{n-1} \subset T^* (\mathbb{R}^+ \times \mathbb{T}^n)$. 
The proof of iso-energetic non-degeneracy follows from Kolmogorov non-degeneracy. When \( I = 0, J = 0 \), the derivative of \( F_0 = G_0 + G_1 \) is \( dI - \langle C, dJ \rangle \equiv (1, -C) \). Therefore, the determinant of the bordered Hessian (eq. 4) is \(-1/12\). □

4.2. The High-Temperature Limit.

Proof of Theorem 1.2. The rescaled thermostated Hamiltonian \( F_\beta = F_0 + \beta V(w) = F_0 + O(\beta) \) where \( O(\beta) = \beta V(w) \) is \( C^r \) and \( Z^n \)-periodic in \( w \) (eq. 9). Therefore, we can apply Theorem 1.1 to deduce the result. □

5. Nosé-like Thermostats

This section proves theorems 1.3 and 1.4.

5.1. Constant Temperature Thermostats. Assume that the temperature \( T > 0 \) is fixed, so by the rescaling (eq. 8) it can be assumed \( T \) is unity. Without loss of generality, it can be assumed that the rescaled inverse thermostat mass \( \Omega \) maps 1 to 1. In this case, the Nosé-like variable-mass thermostat for the Hamiltonian \( H_\epsilon \) (eq. 6) is

\[
F_\epsilon = \frac{1}{2} \|W/\sigma\|^2 + \frac{1}{2} \Omega(\sigma) \Sigma^2 + \epsilon V(w) + \ln \sigma. \tag{22}
\]

The set of thermostatic equilibria \( T \) of a variable mass thermostat coincides with the set of thermostatic equilibria for the constant mass thermostat. Given this, the notation and terminology of lemma 4.2 are used in the following lemma.

Lemma 5.1. Let \( C \) be a unit co-vector and let \( \lambda \subset T^*(R^+ \times T^n) \) be the isotropic graph of \( w \rightarrow (1, w, 0, C) \). Assume that \( r > 2n + 2, \Omega \in C^r(R^+, R^+) \) and \( \Omega(\sigma) = 1 + a(\sigma - 1) + b(\sigma - 1)^2/2 + O((\sigma - 1)^3) \). If

1. \( \beta = (1 - a/2)C; \)
2. \( b = 16\alpha + 3a^2/2 - 5a + 22/3; \) and \( b = 16\alpha + 3a^2/2 - 5a + 22/3; \) and
3. \( \gamma = (a - 2)/4 + (4\alpha + a^2/2 - 2a + 10/3) CC' \),

then there are neighborhoods \( \mathcal{O} \supset \lambda \) and \( \mathcal{P} \supset Z(T^1 \times T^n) \) and a canonical transformation \( \Phi : \mathcal{P} \rightarrow \mathcal{O} - \lambda, (\sigma, w, \Sigma, W) = \Phi(\theta, \eta, I, J) \) that transforms the Hamiltonian \( F_0 \) (eq. 22) into the sum \( G_0 + G_1 \) where

\[
G_0 = I(1 + \alpha I + \langle \beta, J \rangle + \langle \gamma J, J \rangle) + O(5), \tag{23}
\]

\( G_1 \) is given in eq. 12 and \( I \) has degree 2, \( J \) has degree 1 and \( O(5) \) is a remainder term containing terms of degree \( \geq 5 \).

Remark 5.1. In the case \( a = b = 0 \), one finds that \( \alpha, \beta \) and \( \gamma \) are determined by eq. 20. If one sets \( a = 2 \) and \( \alpha = -1/3 \), then \( \beta = 0, \gamma = 0 \) and \( G_0 = I(1 - I/3) + O(5) \).

Proof of Lemma 5.1. The proof is similar to that of Lemma 4.2 so only the highlights are sketched.
One utilizes the change of coordinates in eq. (14). The Maclaurin expansion of $G_0$ in the coordinates $(u, v, U, V)$ is (c.f. eq. (16)):

$$
G_0 = U^2 \left[ \frac{b}{4} u^2 - \frac{1}{2} (a + (b - a) \langle C, V \rangle) u \\
+ \frac{1}{4} (8 + b - 5a) \langle C, V \rangle^2 - \frac{1}{4}(2 - a) \|V\|^2 + \frac{1}{4}(2 - a) \langle C, V \rangle + \frac{1}{2} \right] \\
+ u^2 \left[ \frac{9u^2}{4} + \frac{5u}{3} + 1 \right] + O(5).
$$

One postulates a generating function $\nu$ and form of $G_0$ as in equations (17–18) and solves for $\nu$ and the parameters $\alpha, \beta$ and $\gamma$. One determines that

$$
\nu = \langle \langle y, V \rangle \rangle + \langle \langle \gamma J, J \rangle \rangle + \frac{1}{6} (2 - a) \langle \langle C, V \rangle \rangle x \\
+ U^3 \left[ \frac{1}{36} (3a - 10) - \frac{1}{72} (96a + 9a^2 - 56a + 84) \langle \langle C, V \rangle \rangle + \frac{1}{144} (100 - 36a - 9a^2) x \right] + O(5),
$$

and $\alpha, \beta$ and $\gamma$ are given in terms of $a$ and $b$ by (13–15) above.

Proof of Theorem (1.3). We verify iso-energetic and then Kolmogorov non-degeneracy. One computes the derivative, up to $O(4)$, to be

$$
dG_0 = (1 + 2\alpha I + \langle \langle \beta, J \rangle \rangle + \langle \langle \gamma J, J \rangle \rangle) dI + I \langle \langle \beta + 2\gamma J \rangle \rangle, dJ
$$

$$
dG_1 = (-\langle \langle J, J \rangle \rangle + 4\langle \langle C, J \rangle \rangle^2 + 2\langle \langle C, J \rangle \rangle + 1) \langle \langle J, dJ \rangle \rangle + \\
(4\langle \langle C, J \rangle \rangle \langle \langle J, J \rangle \rangle + \langle \langle J, J \rangle \rangle - 8\langle \langle C, J \rangle \rangle^3 - 4\langle \langle C, J \rangle \rangle^2 - 2\langle \langle C, J \rangle \rangle - 1) \langle \langle C, dJ \rangle \rangle
$$

and the Hessian of $G_0$ and $G_1$, up to $O(3)$, to be

$$
d^2G_0 = \begin{bmatrix}
2\alpha \\
(\beta + 2\gamma J)
\end{bmatrix}
\begin{bmatrix}
\beta + 2\gamma J
\end{bmatrix}
\text{ and } d^2G_1 = \begin{bmatrix}
0 & 0 \\
0 & Q
\end{bmatrix}
$$

where

$$
Q = (1 - \|J\|^2 + 2\langle \langle C, J \rangle \rangle + 4\langle \langle C, J \rangle \rangle^2) 1 - 2JJ' \\
+ (4\|J\|^2 - 8\langle \langle C, J \rangle \rangle - 24\langle \langle C, J \rangle \rangle^2 - 2) CC' + (2 + 8\langle \langle C, J \rangle \rangle) (CJ' + JC')
$$

Assume that there exists parameters $a$ and $b$ and a unit co-vector $C$ such that $F_0$ does not satisfy the iso-energetic non-degeneracy condition in a neighbourhood of $I = 0$ and $J = 0$. Let the bordered Hessian (eq. (4)) of $F_0$, mod $O(3)$, be denoted by $B$. Let $I = 0$ and $J = \rho C$ for a real scalar $\rho$. Let $W$ be the subspace with orthonormal basis...
(1, 0, 0), (0, C, 0) and (0, 0, 1). W is invariant mod $O(\rho^3)$ by $B$. A calculation yields

$$B|W = \begin{bmatrix} 2\alpha & 2\gamma\rho + \beta & \gamma\rho^2 + \beta\rho + 1 \\ 2\gamma\rho + \beta & -3\rho^2 - 2\rho - 1 & -\rho^2 - \rho - 1 \\ \gamma\rho^2 + \beta\rho + 1 & -\rho^2 - \rho - 1 & 0 \end{bmatrix} + O(\rho^3) \quad (29)$$

$$\det(B|W) = 1 - 2\alpha - 2\beta + (-4\gamma - 2\beta^2 - 4\alpha + 2) \rho + (-6\beta\gamma - 2\gamma - \beta^2 + 2\beta - 6\alpha + 3) \rho^2 + O(\rho^3) \quad (30)$$

where we have abused notation and let the scalar $\beta$ (resp. $\gamma$) denote the inner product of the vector $\beta$ with $C$ (resp. matrix $\gamma$ with $CC^t$). The determinant $\det(B|W) = O(\rho^3)$ with real $\alpha, \beta$ and $\gamma$ iff $\alpha = 1/2, \beta = 0$ and $\gamma = 0$. If $\beta = 0$, then lemma [5.1] implies that $a = 2$. The same lemma implies that if $a = 2$ and $\alpha = 1/2$, then $\gamma \neq 0$. Therefore, $\det(B|W)$ has, at worst, a quadratic zero at $\rho = 0$ (a more detailed calculation shows the vanishing is at worst linear).

On the other hand, a calculation shows that $B|W^\perp = 1 + O(\rho)$. Therefore, $B = B(\rho)$ is non-degenerate in a deleted neighbourhood of $\rho = 0$. Since $F_0$ is $C^r$ the iso-energetic non-degeneracy condition holds in an open set that contains the torus $\lambda_C$ in its closure. Since $C$ is arbitrary, there is an open set on which the iso-energetic non-degeneracy condition holds and this set contains the set of thermostatic equilibria in its closure.

Let us now assume that there exist parameters $a, b$ and a unit co-vector $C$ such that $F_0$ fails to be Kolmogorov non-degenerate on a neighbourhood of $I = 0, J = 0$.

Let $A$ be the Hessian of $F_0$, mod $O(3)$, and let $V$ be the subspace spanned by $(1, 0)$ and $(0, C)$. When $J = \rho C$ for some real scalar $\rho$, then the subspace $V$ is $A$-invariant mod $O(3)$. In this case, $A|V$ is the upper left $2 \times 2$ corner of $B|W$ (eq. 29) so

$$\det(A|V) = -2\alpha - \beta^2 + (-4\beta\gamma - 4\alpha) \rho + (-4\gamma^2 - 6\alpha) \rho^2 + O(\rho^3). \quad (31)$$

On the other hand, $A|V^\perp = 1 + O(\rho)$, so if $A$ is singular in a neighbourhood of $I = 0, \rho = 0$, then $\det(A|V) = O(\rho^3)$ so $A = -\beta^2/2$ and $\gamma = -\beta/2$ and $\gamma^2 = -3\alpha/2$ (where we use the same abuse of notation as we did above). The only solution is $\alpha = \beta = \gamma = 0$.

When $\alpha, \beta$ and $\gamma$ are determined by Lemma [5.1] then $\alpha = \beta = 0$ implies that $a = 2$ and $\gamma \neq 0$. Therefore, $A$ is non-degenerate in some deleted neighbourhood of $\rho = 0$. This proves that, for any choice of $a, b$ and unit co-vector $C$, any neighbourhood of the isotropic torus $\lambda = \lambda_C \subset T^* (\mathbb{R}^+ \times T^n)$ contains points where $F_0$ is Kolmogorov non-degenerate. \hfill \square

Remark 5.2. It follows from the above proof that if $F_0$ is both Kolmogorov and iso-energetic degenerate at $I = 0, J = 0$, then $a = 0, b = -8$ and so $\alpha = -1/2, \beta = C$ and $\gamma = -1/2 + 4/3CC^t$. Moreover, $F_0$ is degenerate in both senses along the entire set of thermostatic equilibria. On the other hand, if $\Omega(\sigma) \neq -4(\sigma - 1)^2 + O((\sigma - 1)^3)$, then $F_0$ is non-degenerate in one of the two senses along the set of thermostatic equilibria.

5.2. The high-temperature limit. Let $\Omega_T$ be the unscaled inverse thermostat mass as assumed in the statement of Theorem [1.4]. By means of the rescaling (eq.
with $M = 1$, the thermostated Hamiltonian is transformed to

$$F = T \times \left[ \frac{1}{2} \|W/\sigma\|^2 + \frac{1}{2} \beta \Sigma^2 + \beta V(w) + \ln \sigma \right] - \frac{1}{2} T \ln(T), \quad (32)$$

where $R_T(\sigma) = \Omega_T(\sigma/\sqrt{T})$. By the hypotheses of Theorem 1.4, $\Omega = \lim_{T \to \infty} R_{T,1}$ exists in $C^1(\mathbb{R}^+, \mathbb{R}^+)$. The proof of Theorem 1.4 now follows from Theorem 1.3.

6. Conclusion

This paper has shown that $n$-degree of freedom Nosé-like thermostats “suffer” from persistence of invariant tori near suitable completely integrable limits, extending the results of [2] which deals with the $n = 1$ case. A central role is played here by the flat (or free) limit and hence the assumption that the configuration space is an $n$-torus. It remains unclear if these results extend to other configuration spaces, such as the $n$-sphere with a round metric; possibly not. More likely is that the results do extend to $n$-dimensional ellipsoids with distinct axes, or more generally, Liouville metrics on spheres or products of spheres.

Of equal interest is to study how (topological) entropy or Arnol'd diffusion is generated in these thermostats near the infinite temperature limit.

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