Invariant tori for the Nosé thermostat near the high-temperature limit

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Abstract

Let $H(q,p) = \frac{1}{2}p^2 + V(q)$ be a 1-degree of freedom mechanical Hamiltonian with a $C^r$ periodic potential $V$ where $r > 4$. The Nosé-thermostated system associated to $H$ is shown to have invariant tori near the infinite temperature limit. This is shown to be true for all thermostats similar to Nosé’s. These results complement the result of Legoll, Luskin and Moeckel who proved the existence of such tori near the decoupling limit (Frederic et al 2007 Arch. Ration. Mech. Anal. 184 449–63, Frederic L et al 2009 Nonlinearity 22 1673–94).

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1. Introduction

The computation of equilibrium statistical properties of molecular systems is of great importance to applied subjects such as biology, chemistry, computational physics and materials science. These equilibrium statistical properties are phase space integrals like

$$\mathcal{F} = \int f(q,p) \, d\mu, \quad d\mu = \exp(-\beta H) \, dp \, dq / Z,$$

where $q$ is the position of the system and $p$ is its momentum, $H = H(q,p)$ is the total energy of the system, $\beta = 1/T$ is the reciprocal of the equilibrium temperature $T$ and $Z = Z(\beta)$ is a normalization constant, also called the partition function.

In practice, $f = f(q,p)$ is a ‘measurement’ or ‘observable’, such as the position of the first atom in the system. The computation of the integral (equation (1)) can be very expensive, so one often wants to replace that multi-dimensional average with the time average

$$\hat{f} = \lim_{T \to \infty} \frac{1}{T} \int_0^T f(q(t),p(t)) \, dt$$
where \((q(t), p(t))\) are the position and momenta of the system at time \(t\). In principle, \(\hat{f}\) depends on the initial condition \((q(0), p(0))\). When, for almost all initial conditions the average in equation (2)—called a Birkhoff average—converges to \(\overline{f}\) the system is ergodic. Ergodic systems have many interesting properties, but from the point-of-view here, they provide a means to an end: reduction of the multi-variable integral (equation (1)) to a single-variable integral.

In equilibrium statistical mechanics, the Hamiltonian \(H\) is the internal energy of an infinitesimal system \(S\) that is immersed in a heat bath \(B\) at the temperature \(T\). A simple model of the exchange of energy between the infinitesimal system \(S\) and heat bath \(B\) was introduced by Nosé [7]. This consists of adding an extra degree of freedom \(s\) and rescaling momentum by \(s\):

\[
F = H(q, ps^{-1}) + \frac{1}{2M}p_s^2 + nkT \ln s,
\]

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 \(T = \left|ps^{-1}\right|^2\) is \(T\) and the thermostated system is Hamiltonian. A drawback of the Nosé thermostat is the measure \(d\mu_N = \exp(-\beta F) dp dq ds ds\) is not normalizable (i.e. there is no partition function for \(F\)), so phase space averages with respect to the extended phase space variables \((q, p, s, ps)\) are undefined.

Hoover [3] introduced a non-symplectic reduction of Nosé’s thermostat by eliminating the state variable \(s\) and rescaling time \(t\):

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

This reduction has the desirable properties: when \(E = H(q, \rho) + \frac{1}{2M}\xi^2\), the measure \(d\mu_E = \exp(-\beta E) dq d\rho d\xi\) is finite and so has a partition function; it projects to \(d\mu\) (equation (1)); it is stationary for the reduced thermostat; and when the system is a simple harmonic oscillator, the equilibrium statistical mechanical model predicts the variates \(q, \rho\) and \(\xi\) are Gaussian.

Indeed, the Nosé–Hoover thermostated simple harmonic oscillator reduces to the following ‘simple’ system:

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

Legoll, Luskin and Moeckel show in [4] that near the decoupled limit of \(M = \infty\) and \(\xi = 0\), the thermostated harmonic oscillator (equation (4)) is non-ergodic. By means of an averaging argument, they reduce the thermostated equations to a non-degenerate twist map to show the existence of KAM tori. The result is generalized in a subsequent paper to 1-degree of freedom thermostats for which an associated potential function \(G\) (equation (33) of [5]) is not isochronous.

1.1. The high-temperature limit

The present paper examines the dynamics of Nosé’s thermostat near the high-temperature limit \(T = \infty\) with the thermostat mass \(M\) held constant. It presents a proof of the existence of KAM tori based on the integrability of suitably rescaled equations at the \(T = \infty\) limit. Specifically,
Theorem 1.1. Let $V : \mathbb{R}/2\pi \mathbb{Z} \to \mathbb{R}$ be $C^r$, $r > 4$, and let $H : T^* \mathbb{R}/2\pi \mathbb{Z} \to \mathbb{R}$ be
\[ H(q, p) = \frac{1}{2} p^2 + V(q). \] (5)
Fix the thermostat mass $M > 0$. The Nosé-thermostated Hamiltonian $F$ (equation (3)) associated to $H$ possesses invariant KAM tori for all $T > 0$ sufficiently large.

The intuition behind this theorem is the following: for large temperatures, because the potential $V$ is bounded, most of the energy must be kinetic. Therefore, the dynamics should look like a perturbation of the purely kinetic hamiltonian (where $V \equiv 0$). While this picture is not exactly correct, it is accurate in that the high-temperature thermostated system resembles a perturbation of an integrable system.

1.2. Alternative 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. Let’s say that a Nosé-like thermostat is one which involves momentum rescaling and the thermodynamic equilibrium (where $\dot{s} = 0 = \dot{p}_s$) is independent of that rescaling. This paper proves that

Theorem 1.2. Let $(N, u) = (N_T(s, p_s), u(s))$ be a thermostat that satisfies

1. $N$ is homogeneous quadratic and increasing in $p_s$;
2. $u : \mathbb{R}^+ \to \mathbb{R}^+$ is an increasing diffeomorphism;
3. for all Hamiltonians $H = H(q, p)$, if $F = H(q, pu(s)) + N_T(s, p_s)$ has a thermodynamic equilibrium then it is independent of $s$.

Then, up to a rescaling and change of variables, $u = s$ and there is a smooth positive function $\Omega_T = \Omega_T(u)$ such that
\[ N = \frac{1}{2} \Omega_T p_s^2 + nkT \ln u. \] (6)

In addition, if $\Omega_T(u / \sqrt{T}) \not\to \Omega(u)$ in $C^r(\mathbb{R}^+, \mathbb{R}^+)$ for some $r > 4$, then the Nosé-thermostated Hamiltonian $F$ associated to $H$ (equation (5)) possesses invariant KAM tori for all $T > 0$ sufficiently large.

This theorem is proven in a manner similar to that of theorem 1.1. Indeed, theorem 1.1 can be viewed as a special case of theorem 1.2.

1.3. A Hamiltonian proof of non-ergodicity of the thermostated harmonic oscillator
It is common in the analysis of the Nosé–Hoover thermostat to fix the temperature $T = 1$ and let the thermostat mass $M \to \infty$ (the weak-coupling limit). This is not equivalent to fixing the thermostat mass $M = 1$ and letting $T \to \infty$ (the high-temperature limit), see equation (8) below, but the method used in the proof of theorem 1.1, along with first-order averaging, yields a proof of the following theorem, first proven in [4].

Theorem 1.3. Let $\omega > 0$ and
\[ H(q, p) = \frac{1}{2} p^2 + \frac{1}{2} (\omega q)^2. \] (7)
Fix the temperature $T > 0$. The Nosé-thermostated Hamiltonian $F$ (equation (3)) associated to $H$ possesses KAM tori for all $\epsilon = 1/\sqrt{M} > 0$ sufficiently small.

2. Terminology and notation

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

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 $x_i$.

The KAM theorem gives sufficient conditions which imply that a sufficiently smooth perturbation (say $C^r$ for $r > 2n$) of an integrable $n$-degree of freedom Hamiltonian has invariant tori. A Hamiltonian which satisfies one of these sufficient conditions is said to be KAM sufficient.

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 KAM sufficiency for the integrable approximation.

3. The rescaled thermostat

Let us rescale the variables in the Nosé thermostat so that the Boltzmann constant $k = 1$ and

$$q = \sqrt{M} \mod 2\pi, \quad p = W \sqrt{M}, \quad s = \sigma \sqrt{MT}, \quad p_s = \sqrt{MT} \Sigma. \quad (8)$$

With this canonical change of variables, the thermostated Hamiltonian for $H$ (equation (5)) is

$$(\epsilon = 1/\sqrt{M})$$

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

Since the coordinates $(w, \sigma)$ and $(W, \Sigma)$ are canonically conjugate, up to a rescaling of time by the factor $T$, the Hamiltonian flow of $F$ equals that of $F_{\beta}$.

4. KAM tori in the high-temperature limit

Because the timescale of the thermostat, $\epsilon$, enters into the rescaled thermostated Hamiltonian $F_{\beta}$ only through the bounded potential $V$, and the analysis of this section focuses on the high-temperature limit $\beta \rightarrow 0^+$, the convention is adopted that

$$M = 1 \quad (\implies \epsilon = 1). \quad (10)$$

The analysis below is altered in insignificant ways by this additional hypothesis.
Lemma 4.1. Let $\beta = 0$. Under the canonical change of coordinates induced by introducing cartesian coordinates,

$$(a, b) = (\sigma \cos w, \sigma \sin w),$$

the rescaled thermostated Hamiltonian equals

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

That is, $F_0$ is a mechanical hamiltonian with a rotationally invariant potential.

The proof is a simple computation. With the interpretation that $F_0$ is the Hamiltonian of the thermostated free particle ($V \equiv 0$), Hoover [3] observed this integral, or rather its reduced form, and the reduced integral appears in the work of Legoll, Luskin and Moeckel [4, 5].

There is a family of periodic orbits of $F_0$ along the variety

$$\Xi = \{(\sigma, w, \Sigma, W) | \sigma = |W| = 0, \Sigma = 0\},$$

with each periodic orbit parameterized by the angular momentum integral $\mu = W$. Ideally, one would like to apply a theorem of Rüssmann and Sevryuk [8, 9]. In this context the theorem says that if the ratio of periods $T_1/T_2$ of the periodic orbit and the linearized reduced hamiltonian is not constant, then $F_0$ is KAM-sufficient, i.e. invariant KAM tori survive for $F_0$ for all $\beta$ sufficiently small. Unfortunately, the potential functions $U(\sigma) = \sigma^4/\alpha$ (including the degeneration, $U = \ln$, at $\alpha = 0$) are characterized by constancy of this ratio.

Instead, we compute an approximate change of coordinates to action-angle variables using a succession of generating functions.

As noted above, $F_0$ has an invariant family of periodic orbits along the variety $\Xi$, with each periodic orbit $\Xi_\mu = \{(\mu, w, 0, \mu) | w \in \mathbb{R}/2\pi \mathbb{Z}\}$ parameterized by angular momentum $\mu = 0$. On the other hand, let $T^*T^2$ have the canonical coordinates $\{(\theta, \eta, I, J) | \theta, \eta \in \mathbb{R}/2\pi \mathbb{Z}, \ I, J \in \mathbb{R}\}$ and let $Z \subset T^*T^2$ be the zero section $\{(\theta, \eta, 0, 0)\}$.

Lemma 4.2. There are open sets $A \subset T^*T^2, B \subset T^*(\mathbb{R}^2 \times T^4)$ such that $Z \subset A, \Xi_i \subset B$ and a canonical transformation

$$\Phi : A \rightarrow Z \rightarrow B \rightarrow \Xi_i \quad (\sigma, w, \Sigma, W) = \Phi(\theta, \eta, I, J)$$

that transforms the Hamiltonian $F_0$ (equation (9)) to

$$F_0 = I \left( \frac{11}{24} I + J + J^2 \right) - J(1 + J/2 + J^2/3 + J^3/4) + O(5)$$

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. The transformation $\Phi$ extends continuously over the zero section $Z$. The extension blows down the 2-torus $Z$ to the 1-torus (periodic orbit) $\Xi_i$ by collapsing the $\theta$-cycle on $Z$. In addition, the non-standard choice of degrees for the action variables $I$ and $J$ is because they are determined by the pullback of the degrees of $\sigma, w, \Sigma$ and $W$ (all of degree 1) by $\Phi$.

Proof. The generating function $\phi(W, \Sigma; u, v) = (1 - u)W\Sigma + (1 - W)v$ induces the canonical transformation $(\sigma, w, \Sigma, W) = f(u, v, U, V)$ where

$$\sigma = (1 - u)(1 - V), \quad w = -v - U(1 - u)(1 - V) \mod 2\pi, \quad \Sigma = U(V - 1), \quad W = 1 - V.$$
This transforms the Hamiltonian $F_0$ to

$$F_0 = \frac{1}{2}(1-u)^{-2} + \frac{1}{2}(1-V)^{-2}u^2 + \ln(1-u) + \ln(1-V).$$

(16)

The symplectic map $f$ is singular along the set $\{V = 1\}$ (which should be mapped to the zero angular momentum locus $\{W = 0\}$), and it transforms $\{u = 0, U = 0\}$ to the variety of periodic points $\Xi$. By design, $f$ maps an open neighbourhood of $\{u, v, U, V\} | u = U = V = 0\}$ onto an open neighbourhood of the periodic locus $\Xi$.

The determination of a further coordinate change is independent of the final term in $F_0$, which involves only $V$, so let $G_0 = F_0 - \ln(1-V)$ as indicated in equation (16). With the fourth-order Maclaurin expansion of $G_0$, one obtains

$$G_0 = \left(\frac{3V^2}{2} + V + \frac{1}{2}\right)U^2 + \left(\frac{9u^2}{4} + \frac{5u}{3} + 1\right)u^2 + O(5),$$

(17)

where $O(5)$ is the remainder term that contains terms of degree 5 and higher.

One postulates a second generating function

$$\nu = \nu(U, V; x, y) = xU + yV + \sum_{3 \leq i+j+k+l \leq 4} \nu_{ijkl} x^i y^j U^k V^l + O(5),$$

(18)

and a transformed Hamiltonian

$$G_0 = \left(\frac{x^2 + \frac{X^2}{2}}{2}\right)\alpha\left(\frac{x^2 + \frac{X^2}{2}}{2}\right) + \gamma Y^2 + \beta Y + 1 + O(5).$$

(19)

One solves for the generating function $\nu$ and $G_0$ simultaneously, and arrives at

$$\nu = yV + \frac{55UX^3}{144} - \frac{5UVx^2}{6} - \frac{5UX^2}{6} + \frac{3UY^2x}{8} + \frac{UVx}{2} + \frac{233UV^3}{288} + xU - \frac{5UV^3}{9} - \frac{5U^3}{18} + O(5)$$

(20)

and $\alpha = -11/24, \beta = \gamma = 1$.

Finally, let $I = (x^2 + X^2/2), \theta$ be the conjugate angle (mod $2\pi$), and $\eta = y \bmod 2\pi, J = Y$. Then the transformed Hamiltonian $F_0$ is congruent mod $O(5)$ to that in equation (14).

Proof of theorem 1.1. The rescaled thermostated Hamiltonian $F_\beta = F_0 + \beta V(q) = F_0 + O(\beta)$ where $O(\beta) = \beta V(w)$ is $C^r, r > 4,$ and $2\pi$-periodic in $w$. Under the sequence of canonical transformations in lemma 4.2, $w = -\eta + \rho(\theta, \eta, I, J) + O(5) \bmod 2\pi$ where $\rho$ is an analytic real-valued function, and $O(5)$ is a remainder in $I, J$. So the perturbation in the approximate angle-action variables $(\theta, \eta, I, J)$ is $C^r, r > 4,$ and $O(\beta)$.

Since $F_0$ (equation (14)) has a non-vanishing Hessian determinant in the action variables $(I, J)$, the KAM theorem applies [1, 2, 6, 10].

1 A reader who is familiar with the Birkhoff normal form may wonder why $G_0$ includes cubic terms. These computations mirror those for the Birkhoff normal form, but our Hamiltonian is not being expanded in a neighbourhood of an isolated critical point.
5. Nosé-like thermostats

This section proves theorem 1.2. This section employs the convention that $G_i$ denotes the partial derivative of the function $G$ with respect to the $i$th variable.

5.1. The thermostat’s normal form

To prove the normal form for a Nosé-like thermostat in theorem 1.2, observe that Hamilton’s equations for the Hamiltonian $F(q,p,s,p_s) = H(q,p,u) + N(s,p_s)$ are

\[ \dot{q} = u^{-1}H_z, \quad \dot{p} = -H_z, \]
\[ \dot{s} = N_z, \quad \dot{p}_s = \frac{u'}{u}E(H) - N_z, \]  

(21)

where $H_i (N_i)$ is the partial derivative of $H (N)$ with respect to the $i$th argument, $E(H(q,p)) = p \cdot H_z(q,p)$ is the fibre derivative of $H$ and $H$ and its derivatives are evaluated at $(q,p,u)$.

In thermodynamic equilibrium, $\dot{s} = 0 = \dot{p}_s$. Solving $\dot{p}_s = 0$ yields $E(H) = N_i/(\ln u)$. Since the right-hand side is independent of $(q,p)$, the left-hand side must be depend only on $s$ and therefore it must be constant. Following convention, let $nkT$ be this constant. Then, since $\dot{s} = 0$ and $N$ is increasing and homogeneous of degree 2 in $p_s$,

\[ N(s,p_s) = \frac{1}{2} A p_s^2 + nkT \ln u, \]  

(22)

where $A = A(s) > 0$. Because $T$ is constant, the function $A$ may be parameterized by $T$ so: $A = A_T$. Since $u$ is a diffeomorphism, the change of variables $s \rightarrow u$ gives

\[ N(u,p_u) = \frac{1}{2} \Omega_T p_u^2 + nkT \ln u, \]  

(23)

where $\Omega_T = A_T \cdot (u')^2$. This proves the normal form for the thermostat under the hypotheses of theorem 1.2.

Remark 5.1. In the general case where $N_z$ vanishes along $p_s = 0, A = A(s, p_s)$ is a smooth function of both variables. This added generality introduces the possibility of multiple thermodynamic equilibria at the same temperature, which differ only in the value of the momentum $p_s$. It is difficult to understand the significance of this.

5.2. KAM-tori in the high-temperature limit

By means of the rescaling in equation (8), with $M = 1$, the thermostated Hamiltonian is transformed to

\[ F = T \times \left[ \frac{1}{2} (W/\sigma)^2 + \frac{1}{2} \Omega_T (\sigma/\sqrt{T}) \Sigma^2 + \beta V(w/\epsilon) + \ln \sigma \right] - \frac{1}{2} T \ln(T). \]  

(24)

By the hypothesis of theorem 1.2, as $T \rightarrow \infty$, $\Omega_T (\sigma/\sqrt{T})$ converges in $C'(\mathbb{R}^+, \mathbb{R}^+)$ to a limit $\Omega(\sigma)$ for some $r > 4$.  

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The Hamiltonian $F_0$ has the invariant variety $\Xi$ (equation (13)) of periodic points and the invariant periodic set $\Xi_1$, as in the constant thermostat mass case.

**Lemma 5.1.** Assume that $\Omega(\sigma) = 1 + a(\sigma - 1) + b(\sigma - 1)^2 + \cdots$. If $b = (96\alpha + 9a^2 - 30a + 44)/6$, $\beta = (2 - a)/2$ and $\gamma = (48\alpha + 3a^2 - 21a + 34)/12$, then there are open sets $A \subset T^*T^2$, $B \subset T^*(\mathbb{R}^4 \times \mathbb{T}^4)$ such that $Z \subset A, \Xi_1 \subset B$ and a canonical transformation $\Phi : A \rightarrow B - \Xi_1$ $(\sigma, w, \Sigma, W) = \Phi(\theta, \eta, I, J)$ that transforms the Hamiltonian $F_0$ (equation (24)) to

\[
F_0 = I(\alpha I + 1 + \beta J + \gamma J^2) - J(1 + J/2 + J^2/3 + J^3/4) + O(5)
\]

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

**Remark 5.2.** In the case $a = b = 0$, one finds that $\alpha = -11/24$ and $\beta = 1 = \gamma$, which is the result of lemma 4.2. Similar to the assumption that $M = 1$ in the Nosé-thermostat case, the assumption that the inverse mass $\Omega(1) = 1$ simplifies the statement of lemma 5.1 and the proof of theorem 1.2, but the latter theorem holds for any value of $\Omega(1) > 1$.

The proof of lemma 5.1 is similar to that of lemma 4.2 and is omitted. The relations between the parameters $a$ and $b$ of the thermostat’s inverse mass $\Omega$ and $\alpha, \beta, \gamma$ of the normal form in approximate action-angle variables arise from the attempt to force the normal form to be $I$.

**Proof of theorem 1.2.** By lemma 5.1, the determinant of the Hessian of $F_0$ with respect to the action variables $I, J$ is

\[-(2\alpha + \beta^2) + 4\alpha \gamma I - 4(\beta \gamma + \alpha)J - (4\gamma^2 + 6\alpha)J^2 + O(3),\]

which equals $O(3)$ iff $\alpha = \beta = \gamma = 0$. However, if $\alpha = 0 = \gamma$, then $a = 2$ and so $\beta \neq 0$. \square

6. The harmonic oscillator in the weak-coupling limit

**Proof of theorem 1.3.** After applying the change of variables in equation (8), and a rescaling of $(W, w)$ the rescaled thermostated harmonic oscillator Hamiltonian is

\[
G_\epsilon = \frac{1}{2}(W/\sigma)^2 + \frac{1}{2}w^2 + \kappa \left(\frac{1}{2}\Sigma^2 + \ln \sigma\right),
\]

where $\kappa = \epsilon \omega \sqrt{\beta}$. In the following, it will be assumed that $\omega = \beta = 1$ so that $\kappa = \epsilon$. The generating function $\varphi = wW\sqrt{\sigma} + \sigma U$ induces the canonical change of variables

\[
\sigma = u, \quad w = v/\sqrt{u}, \quad \Sigma = U + \frac{1}{2}vW/\sqrt{u}, \quad W = V\sqrt{u}.
\]

When composed with the canonical transformation $u \rightarrow 1 - u, U \rightarrow -U$, the Hamiltonian $G_\epsilon$ transforms to
This Hamiltonian weakly couples the variables \((v, V)\) with \((u, U)\) when \(\kappa \ll 1\), with \((v, V)\) evolving on a fast time-scale and \((u, U)\) evolving on a slow timescale. Averaging the Hamiltonian \(G_k\) in \((v, V)\) over a period gives

\[
\bar{G}_k = - \frac{E}{2(1-u)} + \kappa \left[ \frac{1}{2} \left( \frac{U^2}{2} + \frac{E^2}{2\kappa} + \ln(1-u) \right) \right] + O(\kappa^2) \tag{29}
\]

The Hamiltonian \(\kappa^{-1} \bar{G}_k\) has a second-order Maclaurin expansion of

\[
\frac{1}{2} U^2 + \left( \frac{3 E^2}{16} + \frac{E}{\kappa} - \frac{1}{2} \right) u^2 + \left( \frac{E^2}{8} + \frac{E}{\kappa} \right) u + \frac{E^2}{16} + \frac{E}{\kappa} + O(\kappa). \tag{30}
\]

When \(E = \kappa + O(\kappa^2)\), \(\kappa^{-1} \bar{G}_k\) has a critical point at \(u = U = 0\) and the fourth-order Maclaurin expansion is

\[
\frac{1}{2} (U^2 + u^2) + \frac{2}{3} u^3 + \frac{3}{4} u^4 + 1 + O(\kappa) \tag{31}
\]

Computations similar to those in lemma 4.2 show that the Birkhoff normal form is

\[
\tilde{G}_k = \kappa I (1 - 3 I/24) + O(\kappa^2, 5), \tag{32}
\]

where \(I = \frac{1}{2}(U^2 + u^2)\). Since the averaged system is KAM sufficient, the unaveraged Hamiltonian \(G_k\) is an \(O(\kappa^2)\) perturbation of a KAM sufficient Hamiltonian system.

**Remark 6.1.** One may attempt to apply the Birkhoff normal form to the Hamiltonian \(\hat{G}_k = G_k - \kappa H/(1 - u)\). The generating function

\[
\nu = U x - 2 U x^2/3 + 65 U x^3/288 + 295 U x/288 - 4 U^3/9 + V y + U (x - 2)(y^2 + V^2)/4 + U^2 V y/2 \tag{33}
\]

induces a canonical transformation \((u, v, U, V) = f(\theta, \eta, I, J)\) that transforms \(\hat{G}_k\) to normal form:

\[
\tilde{G}_k = \kappa I + \alpha I^2 + \beta I J + \gamma J^2 + O(5), \tag{34}
\]

where \(\alpha = -13 \kappa/24, \beta = -1, \gamma = -1/2\kappa\) and \(I = (x^2 + X^2)/2, J = (y^2 + Y^2)/2\). Note that when \(J = 0, \tilde{G}_k\) in equation (34) coincides with the averaged Hamiltonian \(\bar{G}_k\) in equation (32).

If the total energy is fixed at \(\bar{G}_k = \kappa h\), then

\[
J = \kappa (h + h^2/2 - I + I^2/24 + O(5)) \tag{35}
\]

is the Hamiltonian of the reduced system \(d\hat{\theta}/dh = -\partial J/\partial I, dI/d\eta = 0\) on the isoenergy level \(\tilde{G}_k = \kappa h\). This implies that the Hamiltonian \(\tilde{G}_k\) is KAM sufficient [10, pp 46–7].

\(^2\)The first line of equation (33) provides the generating function to transform equation (31) to equation (32).
The final step in this line of proof would be to prove that in the limit at $\kappa = 0$ of a suitably renormalized $\hat{G}_\kappa$ is KAM sufficient and $G_\kappa$ is a suitably small perturbation.

7. Conclusion

This note has demonstrated the existence of KAM tori near the high-temperature limit of a Nosé-thermostated 1-degree of freedom system with a periodic potential, along with similar thermostats that are scale-invariant. It has also given a 'Hamiltonian' proof of Legoll, Luskin and Moeckel's result on the existence of KAM tori in the Nosé–Hoover thermostated harmonic oscillator in the weak-coupling limit.

It is expected that the techniques of this paper may be used to demonstrate similar results for $n$-degree of freedom Nosé-thermostated systems. Potentially more fruitful, however, is that the techniques of this paper might be useful to create thermostats with the desired properties. Of course, some features of the Nosé-type thermostat must be abandoned in the process.

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