Notes on the Jellinek-Berry Thermostated Ideal Gas

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Abstract

This note studies Hamiltonian systems which are thermostated using the Jellinek–Berry thermostat (J. Chem. Phys. 1988; Phys. Rev. A 1988). Jellinek & Jellinek and Berry propose an extension of Nosé's thermostat (J. Chem. Phys. 1984). They introduce multiple functional parameters in order to achieve ergodicity of the thermostatted dynamics. This family of Hamiltonian thermostats aim to simulate the macro canonical ensemble of a Hamiltonian H by coupling H to a 1-d heat reservoir with potential energy $v(s)$ and kinetic energy $p^2/2Q(s)$. Our note derives a normal form for the reservoir's potential energy; investigates when the Jellinek–Berry thermostated system admits a Nosé–Hoover reduction; and, we demonstrate that a Jellinek–Berry thermostated periodic ideal gas is completely integrable and satisfies a KAM twist condition called Rüssmann non-degeneracy. This is used to deduce that a thermostated, collision-less, non-ideal gas (i.e. one with a smooth potential energy) at sufficiently high temperatures of the reservoir has a positive measure set of invariant tori–hence, the thermostated dynamics are non-ergodic.

1 Introduction

A key concern in molecular dynamics is the computation of thermodynamical properties of a statistical-mechanical system. The landmark paper by Nosé [4] demonstrates a way that the NVT ensemble can be computed using an extended Hamiltonian. Recall that the NVT ensemble assumes constancy of the number, N, of particles; the volume, V, of the system; and the temperature, T, of the heat bath.

The Nosé thermostat introduces an additional state variable, s, with an associated potential energy $gkT\ln s$ and kinetic energy $p_s^2/2Q$. The parameter Q is called the *thermostat mass*. Given a smooth Hamiltonian $H : T^*M \to \mathbf{R}$, the Nosé thermostat is *coupled* to H via the momentum re-scaling:

$$p \to p/s. \tag{1}$$

From these ingredients, one obtains a new Hamiltonian $F : T^*(\mathbf{R}^+ \times M) \to \mathbf{R}$ defined by:

$$F(q,p,s,p_s) := H(q,p/s) + \underbrace{\frac{{p_s}^2}{2Q} + gkT\ln s}_{N_{Q,kT}(s,p_s)}, \tag{2}$$

where M is the configuration space of the system, $q \in M$ is a configuration, $p \in T_q^*M$ is a momentum vector, g is a constant the depends only on the number of degrees of freedom, k is Boltzmann's constant and T is the notional temperature of a heat bath in which the Hamiltonian is immersed.

Recall that the *micro-canonical ensemble* of a Hamiltonian F is determined by fixing N, V and the energy $F = E$ instead of the temperature T. A key motivation for the form of the Nosé thermostat and coupling is that, when $g = n + 1$, the micro-canonical ensemble of F projects to the canonical ensemble of H at temperature T, i.e. the NVT ensemble. Indeed, if one fixes an energy level E of F, then the expected value of a measurement $\psi : T^*M \to \mathbf{R}$ is proportional, up to a constant factor depending only on the parameters:

$$\mathbf{E}_T(\psi) \propto \int \mathrm{d}s\,\mathrm{d}p_s\,\mathrm{d}q\,\mathrm{d}p\,\psi\,(q,p/s)\,\delta(F-E), \qquad \beta = \frac{1}{kT} \tag{3a}$$

$$\propto \int \mathrm{d}q\,\mathrm{d}\rho\,\psi(q,\rho)\exp\left(-\beta H(q,\rho)\right), \qquad \rho = \frac{p}{s} \tag{3b}$$

which is the expected value of ψ according the Gibbs–Boltzmann distribution, i.e. the canonical ensemble of H in a heat bath with temperature T.

Early studies and numerical investigations reveal that the Nosé thermostat is not effective in producing a Hamiltonian F that is ergodic on fixed energy levels [5]. Legoll, Luskin and Moeckel subsequently prove, using KAM theory, that the Hamiltonian flow of F is not ergodic on energy levels when the thermostat mass Q is sufficiently large [14, 15]. Several Hamiltonian thermostats that extend Nosé's are in the literature, e.g. [11]. The most general form in the literature that preserves the simplicity of Nosé's thermostat, while introducing many additional functional parameters is due to Jellinek [6] and Jellinek & Berry [7].

The latter generalization is significant in many respects. For instance, the choice of coupling determines whether particular first integrals of the Hamiltonian H are inherited by F: Nosé's coupling implies that linear-in-momentum first integrals are inherited. With an extended range of possible couplings, one can study how different couplings affect the dynamics. Moreover, it is hoped that these couplings can be chosen to achieve desired dynamical properties, such as ergodicity or a specific energy distribution. It is also hoped that extending the range of possible thermostat potential functions will achieve similar goals.

1.1 Jellinek–Berry and Brańka–Wojciechowski Thermostats

The point of departure of the Jellinek–Berry thermostat is the momentum-rescaling coordinate change $\rho = p/s$ in (1). Consider the simultaneous transformation of the configuration q and momentum p by invertible linear transformations that depend on s; in addition, let the Nosé mass Q depend on s, $Q = Q(s)$, and the Nosé potential, $\ln(s)$, be an arbitrary function $v = v(s)$. Let $x = (q, p)$ be the state vector of the Hamiltonian. One arrives at a generalized Jellinek-Berry thermostatted Hamiltonian (c.f. eqn. 12 of [12]):

$$G(x, s, p_s) := H(a(s) \cdot x) + \frac{p_s^2}{2Q(s)} + gkTv(s). \tag{4}$$

Here, a is an invertible linear transformation that depends on s and Q is a positive function. In the work of Jellinek, Jellinek–Berry it is assumed that $a(s)$ is diagonal in the given canonical coordinates and acts as the identity on the configuration coordinates q; in the work of and Brańka–Wojciechowski it is assumed that $a(s)$ acts as a scalar on p and as a distinct scalar on q. Those assumptions are not intrinsically necessary: this note proceeds without them.

It is necessary to formulate hypotheses on the various functional parameters in the Hamiltonian G (4). The following are based on analogies with the Nosé thermostat.

Assumption 1: The potential $v : \mathbf{R}^+ \to \mathbf{R}$ is a C^{r+1} diffeomorphism and $r > 2n+1$ where $n = \dim M$.

Assumption 2: The map $a : \mathbf{R}^+ \to GL(\mathbf{R}^{2n})$ is a C^r map.

Assumption 3: The Nosé mass $Q : \mathbf{R}^+ \to \mathbf{R}^+$ is a C^r map.

1.2 Ideal Gas

An ideal gas has only kinetic energy, so when that kinetic energy is defined by a flat metric (as it generally is), the Hamiltonian H is completely integrable. In this case, as Posch, Hoover and Vesely note [5], the Nosé Hamiltonian is completely integrable.[1] Holian, Voter and Ravelo [9] observe that the Nosé–Hoover equations can, when the thermostat mass Q is small, drive a many-body Hamiltonian system to have "persistent non-local oscillations." This observation is attributed to a Toda-like potential energy that is buried in the Nosé Hamiltonian. Indeed, this Toda-like potential energy is the potential energy of the Nosé Hamiltonian applied to an ideal gas. That is to say, the Toda-like demon of Holian, *et. al.* is the potential energy observed by Posch, *et. al.*. Similarly, the normal form that Legoll, *et. al.* derive in their study of the Nosé–Hoover thermostatted harmonic oscillator has that same Toda-like potential energy (see eqn. 27 and the following in [14]).

It seems appropriate, therefore, to begin the study of the dynamics and ergodic properties of the Jellinek-Berry thermostats with the study of a thermostatted ideal gas.

[1] The authors show the Nosé–Hoover equations are integrable [5, p. 4222], but this is equivalent to integrability of the Nosé Hamiltonian.

1.3 Outline

This note is organized as follows. Section 2 demonstrates that Assumption 1 implies a simple normal form for the Jellinek–Berry thermostat potential. This is used to determine sufficient conditions that imply the Jellinek–Berry thermostat has a reduction to a Nosé–Hoover-like thermostat. Section 3 studies the n-dimensional ideal periodic gas. We show that the Jellinek–Berry thermostatted system is completely integrable and, under two additional assumptions on the coupling map between the system and heat bath (see Assumptions 4 and 5 in §3.1), the frequency map satisfies a twist condition called Rüssman non-degeneracy. It is also shown that "almost all" coupling maps produce a frequency map that is Kolmogorov non-degenerate. In §3.4 these conditions are used to prove that, even when a sufficiently smooth potential energy is added, the thermostatted system is not ergodic on fixed energy levels when the temperature of the heat bath is sufficiently high. This note concludes in §5.

2 Normal forms

A *normal form* provides a reference point for a mathematical object. This section shows that the Assumption 1 implies that the thermostatic potential energy, v, can be transformed by a change of variables to either Nosé's form (a natural logarithm)[4] or to that of Dettmann & Morriss [10] (the identity). It also shows how, under several conditions, the transformation of the "virtual" state $x = (q, p)$ to a "physical" state $y = a(s) \cdot x$, when combined with a time reparameterization, can be used to reduce the Jellinek-Berry thermostatted Hamiltonian vector field to the form of a Nosé–Hoover vector field.

2.1 Universality of the Nosé potential

To remove some arbitrary functional parameters, let's investigate an implication of Assumption 1. By this Assumption, there is a C^r canonical change of coordinates

$$\sigma = e^{v(s)}, \qquad \Sigma = p_s / \left(v'(s) e^{v(s)} \right). \tag{5}$$

The transformed thermostatted Hamiltonian takes the form

$$G(x, \sigma, \Sigma) := H(b(\sigma) \cdot x) + \frac{\Sigma^2}{2R(\sigma)} + gkT \ln(\sigma), \tag{6}$$

where $R(\sigma) = Q(s)/(v'(s)e^{v(s)})^2$ and $b(\sigma) = a(s)$. That is, Assumption 1 implies that the Nosé potential can be assumed as given.

2.2 The linear thermostat potential

An alternative to Nosé's logarithmic thermostat potential is due to Dettmann & Morriss [10], who introduce the form in their study of the Nosé–Hoover thermostat. From our point of view, a linear thermostat potential offers computational advantages when analyzing normal forms and non-degeneracy conditions like the Rüssman and Kolmogorov non-degeneracy conditions (see §3).

By Assumption 1, there is a C^r canonical change of coordinates

$$\nu = v(s), \qquad \mathrm{N} = p_s / v'(s). \tag{7}$$

The transformed thermostatted Hamiltonian takes the form

$$G(x, \nu, \mathrm{N}) := H(b(\nu) \cdot x) + \frac{\mathrm{N}^2}{2R(\nu)} + gkT\nu, \tag{8}$$

where $R(\nu) = Q(s)/(v'(s))^2$ and $b(\nu) = a(s)$. That is, Assumption 1 implies that this linear potential can be assumed as given.

In the remainder of this note, it is assumed that the Assumption 1 holds and that the thermostatted Hamiltonian is in the form of (8).

2.3 The *Physical* transformation

The standard interpretation of the canonical coordinates $x = (q, p)$ is that they are *virtual*. The *physical* coordinates y are related to the virtual coordinates by the transformation:

$$y = a(s) \cdot x = b(\sigma) \cdot x. \tag{9}$$

Let's call this the *physical transformation*. This is consistent with the terminology in the literature on the Nosé–Hoover thermostat, where p is regarded as a "virtual" momentum and $\rho = p/s$ is regarded as a "real" or "physical" momentum.

The Hamiltonian G (6), and its associated Hamiltonian vector-field, are transformed to:

$$\hat{G}(y, \sigma, \Sigma) = H(y) + \frac{\Sigma^2}{2R(\sigma)} + gkT \ln(\sigma), \tag{10a}$$

$$\dot{y} = b(\sigma) J b(\sigma)^* \mathrm{d}H(y) + \frac{\Sigma}{R(\sigma)} \varphi(\sigma) \cdot y, \tag{10b}$$

$$\dot{\sigma} = \frac{\Sigma}{R(\sigma)}, \tag{10c}$$

$$\dot{\sigma} = \frac{R'(\sigma)}{2R(\sigma)^2} \Sigma^2 + \langle dH(y), \varphi(\sigma) \cdot y \rangle - gkT/\sigma, \tag{10d}$$

where b^* is the transpose of b, J is the symplectic matrix and $\varphi(\sigma) = -b'(\sigma) \cdot b(\sigma)^{-1}$.

Since the physical transformation is not necessarily symplectic, the vector field is not canonical; but, it does preserve $\hat{G}$. Since the volume form $\mathrm{d}x\, \mathrm{d}s\, \mathrm{d}p_s$ is invariant for the Hamiltonian vector field of G (4), the transformed volume form $\mathrm{d}y\, \mathrm{d}\sigma\, \mathrm{d}\Sigma \times (\det b(\sigma))^{-1}$ is invariant for this vector field in physical coordinates.

2.4 The independence transformation

A final, non-canonical, coordinate transformation transforms the total energy $\hat{G}$ (10a) into a sum of three independent terms:

$$\nu = \sigma / \sqrt{R(\sigma)}, \tag{11a}$$

$$\widehat{G}(y, \sigma, \nu) = H(y) + \frac{1}{2}\nu^2 + gkT \ln(\sigma), \tag{11b}$$

and the vector field to:

$$\dot{y} = b(\sigma) J b(\sigma)^* dH(y) - \frac{\nu}{\sqrt{R(\sigma)}} \varphi(\sigma) \cdot y, \tag{12a}$$

$$\dot{\sigma} = \frac{\nu}{\sqrt{R(\sigma)}}, \tag{12b}$$

$$\dot{\nu} = \frac{1}{\sigma \sqrt{R(\sigma)}} \left(\langle \mathrm{d}H(y), \sigma \cdot \varphi(\sigma) \cdot y \rangle - gkT \right). \tag{12c}$$

The volume form $\mathrm{d}y\, \mathrm{d}\sigma\, \mathrm{d}\nu \times \sqrt{R(\sigma)} / \det(b(\sigma))$ is invariant for this vector field.

Note that if $b(\sigma)$ is symplectic, then $b(\sigma) J b(\sigma)^* = J$, so the equation for $\dot{y}$ (12a) assumes the form of a Hamiltonian vector field plus a friction-like term where the coefficient of friction depends on thermostat state through the variables σ, ν. Also, note that in the equation for $\dot{\nu}$ (12c), the first term–$\langle \mathrm{d}H(y), \sigma \cdot \phi(\sigma) \cdot y \rangle$–has the form of an instantaneous temperature.

2.5 Time rescaling

As stressed by Jellinek, the rescaling of time can be chosen independent of the already-mentioned functional parameters in the thermostat, provided that one is willing to use a *weighted* micro-canonical measure. A weighted micro-canonical measure is of the form

$$\mathbf{E}_{T,w}(\psi) = \int \mathrm{d}x\, \mathrm{d}s\, \mathrm{d}p_s\, \psi(a(s) \cdot x) \times \delta(F - f)/w, \tag{13}$$

where $w = w(x, s, p_s) > 0$ is a C^r function. In the rescaled time τ, where $d/d\tau = w \times d/dt$, the weighted micro-canonical measure is invariant. In order to reproduce the canonical ensemble of H, Jellinek chooses $w = c \times \sqrt{R(\sigma)}\sigma^l / \det(b(\sigma))$, where $c = \exp(f/gkT) \times \sqrt{2\pi gkT}$. By routine calculations, one obtains that the expected value of ψ is:

$$\mathbf{E}_{T,w}(\psi) = \int \mathrm{d}y\, \psi(y) \times \exp\left(-r\beta H(y)\right) / Z(r\beta), \qquad \text{where} \qquad r = \frac{l+1}{g}, \beta = \frac{1}{kT} \tag{14}$$

and $Z(\beta)$ is the normalization constant to ensure the expected value of unity is unity. By inspection, g should be chosen to be $l + 1$ in order to reproduce the canonical ensemble of H at temperature T.

Let's note that Jellinek's choice of weighting function is not unique. For example, the weighting function

$$w(y, \sigma, \nu) = c \times \sqrt{R(\sigma)} / \det(b(\sigma)) \times \sigma^l \times \exp(a\beta(H(y) + \frac{1}{2}\nu^2)) \tag{15}$$

leads to a similar result for $\mathbf{E}_{T,w}(\psi)$ as in (14), with r replaced by $r + a$ and a similar change made to c. This observation implies that there is a one-parameter family of weighted micro-canonical ensembles that all marginalize to yield the canonical ensemble of H at constant β.

2.6 The Nosé–Hoover reduction

Nosé and Hoover show how to reduce the Hamiltonian equations of the Nosé thermostatted Hamiltonian by means of a change state and re-parameterization of time. Let's say that a transformation of state and re-parameterization time is a **Nosé–Hoover reduction** of the Jellinek–Berry thermostatted equations if it transforms the equations into a form in which the state variable σ is redundant (12).

Consider the Jellinek–Berry thermostatted vector field in the coordinates (y, σ, ν), (12). In order to reduce the equations to a system that is independent of σ for all Hamiltonians H via a time change that depends only on σ, $\mathrm{d}t = w(\sigma)\mathrm{d}\tau$, it is clear from equation (12c) that there are two sufficient conditions:

1. $w(\sigma) = \sigma \cdot \sqrt{R(\sigma)}$; and
2. $\sigma \cdot \varphi(\sigma) = \xi$, a constant element in $\mathrm{gl}(\mathbf{R}^n)$, the vector space of $n \times n$ real matrices.

Inspection of equation (12a) shows that there is a third condition:

3. $\Lambda(\sigma) = w(\sigma) \times b(\sigma) J b(\sigma)^* = \Lambda$, a fixed skew symmetric matrix that is congruent to the symplectic matrix J.

From (2), it follows that $-\sigma \cdot b'(\sigma) = \xi \cdot b(\sigma)$. Then, $b(\sigma) = \exp(-\rho(\sigma) \cdot \xi) \cdot b(1)$ and so $\rho(\sigma) = \ln(\sigma)$. From (3), it follows that $w(1) \times b(1) J b(1)^* = \Lambda$ and then $w(\sigma) \cdot \exp(-\ln(\sigma)\xi) \cdot \Lambda \cdot \exp(-\ln(\sigma)\xi^*) = w(1) \cdot \Lambda$. The determinant of each side then implies that $w(\sigma) = w(1) \times \sigma^{2\kappa}$, where $\kappa = \frac{1}{2n}\mathrm{Tr}(\xi)$. It follows from (1) that $R(\sigma) = w(\sigma)^2/\sigma^2 = w(1)^2 \times \sigma^{4\kappa-2}$ and that $R(1) = w(1)^2$. Finally, (3) implies that if $c(\sigma) = b(1)^{-1}b(\sigma)$, then $w(1) \times J = w(\sigma) \times c(\sigma) J c(\sigma)^*$. That is, $c(\sigma)$ is a conformally symplectic matrix with conformality factor $w(1)/w(\sigma) = \sigma^{-2\kappa}$. Since $c(\sigma) = \exp(-\ln(\sigma) b(1)^{-1} \xi b(1))$, it follows that $\eta = b(1)^{-1}(\xi - \kappa 1)b(1)$ is infinitesimally symplectic. This completes the proof of the following theorem:

Theorem 1. *If, for all C^r Hamiltonians H, there is a Nosé–Hoover reduction of the vector field* (12) *via a time change* $\mathrm{d}t = w(\sigma)\mathrm{d}\tau$, *so that* (12a) *&* (12c) *are independent of σ, then*

1. *conditions 1–3 above hold; and*
2. $b(\sigma) = \exp(-\ln(\sigma) \cdot \xi)$;
3. $w(\sigma) = w(1)\sigma^{2\kappa}$ *where* $\kappa = \frac{1}{2n}\,\mathrm{tr}(\xi)$;
4. $\eta = b(1)^{-1}(\xi - \kappa 1)b(1)$ *is an infinitesimally symplectic matrix:* $\exp(\eta) J \exp(\eta^*) = J$;
5. $R(\sigma) = R(1)\sigma^{4\kappa-2}$ *and* $R(1) = w(1)^2$;
6. $b(\sigma) = \sigma^{-\kappa} \times b(1) \exp(-\ln(\sigma)\eta) b(1)^{-1}$ *is conjugate to a conformally symplectic group.*

The conditions of Theorem 1 are, perhaps, more comprehensible when stated in terms of the coordinate $\nu = \ln \sigma$. To simplify the exposition, let's write $b(\nu)$ instead of $b(e^\nu)$, etc. The conditions become:

2. $b(\nu) = \exp(-\nu \cdot \xi)$;

3. $w(\nu) = w(1)e^{2\kappa\nu}$;

and

5. $R(\nu) = R(1)e^{(4\kappa-2)\nu}$ and $R(1) = w(1)^2$;

6. $b(\nu) = e^{-\kappa\nu} \times b(1)\exp(-\nu\eta)b(1)^{-1}$.

2.6.1 Application: the Nosé thermostat

Theorem 1 implies that if the thermostat vector field (12) admits a Nosé–Hoover reduction, then system's functional parameters are highly determined. Let's examine the case of the Nosé thermostat. In this case,

$$b(\sigma) = \begin{bmatrix} 1 & 0 \\ 0 & \sigma^{-1} \end{bmatrix}, \qquad \xi = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}. \tag{16}$$

This implies that $\kappa = \frac{1}{2}$, whence $R(\sigma) = R$ is constant, and $w(\sigma) = \sqrt{R} \times \sigma$. The reduced vector field is

$$y' = \sqrt{R}J\mathrm{d}H(y) - \nu \cdot \xi \cdot y, \tag{17a}$$
$$\sigma' = \sigma\nu, \tag{17b}$$
$$\nu' = \langle \mathrm{d}H(y), \xi \cdot y\rangle - gkT. \tag{17c}$$

This form differs from the usual Nosé–Hoover reduction only due to the additional factor $\sqrt{R}$ in the time reparameterization. The parameter $\sqrt{R}$ is frequently used to "tune" the thermostat.

If one changes the matrix ξ, one obtains a family of thermostats where the instantaneous temperature function $\kappa(y) = \langle \mathrm{d}H(y), \xi \cdot y\rangle$ may mix configuration and momentum variables. For example, if ξ is the identity matrix, then the instantaneous temperature κ combines both kinetic and potential energies.

2.6.2 Application: Winkler-type thermostats

Winkler [8] proposes an analogue of the Nosé thermostat with the re-scaling matrix

$$b(\sigma) = \begin{bmatrix} 1 & 0 \\ 0 & \sigma^{-e} \end{bmatrix}, \qquad \xi = e \times \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \tag{18}$$

where e is a constant. In all cases, $\kappa = e/2$. Theorem 1 implies that if the thermostat vector field (12) admits a Nosé–Hoover reduction, then $R(\sigma) = R(1) \times \sigma^{2(e-1)}$. So, the thermostat mass $R(\sigma)$ is constant only in the Nosé thermostat.

In Winkler's case, he chooses $e = 2$ and a constant R.

2.6.3 Application: generalized Nosé thermostats

3 The Ideal Periodic Gas

Let us consider an ideal gas–whose potential energy is identically zero–with periodic boundary conditions. The configuration space of this system is the n-dimensional torus, $\mathbf{T}^n = (\mathbf{R}/2\pi\mathbf{Z})^n$, where n equals the product of the number of spatial dimensions and the number of bodies. The kinetic energy is a quadratic form in the momentum, so the total energy is

$$H(q,p) = \frac{1}{2} \times \langle p, p\rangle, \tag{19}$$

where $q \in \mathbf{T}^n$, $p \in T_q^*\mathbf{T}^n \equiv \mathbf{R}^n$. The thermostatted Hamiltonian, with the linear thermostat potential is

$$G(q,p,\nu,N) = \frac{1}{2} \times \langle b(\nu) \cdot p, b(\nu) \cdot p\rangle + \frac{1}{2}r(\nu)N^2 + gkT\nu, \tag{20}$$

where $r = 1/R$ and, since b must fix q, notation is abused and used to denote the transformation of just the momentum, p.

The following theorem is clear, since p and G provide $n+1$ functionally independent first integrals of motion.

Theorem 2. *The thermostatted ideal gas Hamiltonian G, (20), is Liouville completely integrable.*

Due to the presence of so many functional parameters, the computation of action-angle variables for this completely-integrable Hamiltonian is not possible. However, under suitable conditions, one can derive a normal-form expansion of the G in the neighbourhood of a family of invariant, isotropic, tori. This family of tori is interesting in its own right, because it can be understood in terms of an equilibrium between the system and heat bath.

3.1 Thermostatic equilibria

The Hamiltonian vector field of G, (20), is

$$\dot{q} = G_p = c(\nu)p, \qquad \dot{p} = -G_q = 0, \tag{21a}$$

$$\dot{\nu} = G_N = r(\nu)N, \qquad \dot{N} = -G_\nu = -\frac{1}{2}r'(\nu) \times N^2 + \left(-\frac{1}{2}\langle c'(\nu)p, p\rangle - gkT\right), \tag{21b}$$

$$c(\nu) = b(\nu)^* b(\nu). \tag{21c}$$

A *thermostatic equilibrium* occurs at a point where $\dot{\nu} = \dot{N} = 0$. By inspection, this occurs when

$$N = 0, \qquad \langle c'(\nu)p, p\rangle = -2gkT. \tag{22}$$

Let's formulate some reasonable assumptions about the rescaling map $b(\nu)$ and the induced map $c(\nu)$. In order to formulate these assumptions, recall that the *co-norm* of an endomorphism ϕ of a normed linear space, $m(\phi)$, is defined to be

$$m(\phi) = \inf\{|\phi(v)| \mid |v| = 1\}.$$

The *norm* of ϕ, $|\phi|$, is defined with the infimum replaced by the supremum.

In the Winkler-type thermostat, which includes Nosé's, $b(\nu) = \exp(-e\nu)$ and so $c(\nu) = \exp(-2e\nu)$ for $e > 0$. Therefore, c and c' satisfy the following assumptions:

Assumption 4: $c(\nu)$ and $-c'(\nu)$ are positive definite;

Assumption 5: $m(c'(\nu)) \to \infty$ as $\nu \to -\infty$ and $|c'(\nu)| \to 0$ as $\nu \to \infty$;

Let's define

Definition 1. *The function $\kappa = -\dfrac{1}{2gk}\langle c'(\nu)p, p\rangle$ is the instantaneous temperature of the thermostatted ideal gas.*

Assumptions 4 & 5 imply the following, whose proof is straightforward:

Proposition 3. *There exists a C^r smooth function $\nu_0(p; gkT)$ defined for all non-zero p such that equation (22) is satisfied iff $N = 0, \nu = \nu_0(p; gkT)$.*

In light of this proposition, let's define the following:

Definition 2. *The set*

$$\mathscr{T}_T = \{(q, p, \nu, N) \mid q \in M, p \neq 0, \nu = \nu_0(p; gkT), N = 0\}$$

is called the set of thermostatic equilibria.

It is clear that $\mathscr{T}_T$ is a C^r submanifold of $T^*(\mathbf{R}^n \times \mathbf{R})$ for all $T > 0$. It is invariant under the Hamiltonian flow of the Hamiltonian G and it is fibred by invariant, isotropic n tori.

3.2 The normal form of G near the thermostatic equilibrium submanifold

As noted, although the Hamiltonian G is completely integrable, the computation of action-angle variables is essentially impossible. What can be done, though, is to determine action-angle variables for a suitable expansion of G in a neighborhood of the thermostatic equilibrium submanifold. Equivalently, these action-angle variables determine a normal form for G.

To determine the normal form, let us introduce a canonical change of coordinates:

$$\nu = \nu_0(p) + u, \qquad N = U, \qquad q = \hat{q} + U \cdot \mathrm{d}\nu_0, \qquad \hat{p} = p. \tag{23}$$

The Hamiltonian G is transformed to:

$$G = \left\{ \begin{array}{c} \overbrace{\frac{1}{2}c_0 + gkT\nu_0(p)}^{G_0} + \overbrace{\frac{1}{4}c_2u^2 + \frac{1}{2}r_0U^2}^{\omega_1 I} + \\ \frac{1}{2}r_1uU^2 + \frac{1}{4}r_2u^2U^2 + \frac{1}{12}c_3u^3 + \frac{1}{48}c_4u^4 + O(5), \end{array} \right\} \quad \text{where} \quad \left\{ \begin{array}{rcc} c_k & = & \langle c^{(k)}(\nu_0(p)) \cdot p, p \rangle, \\ r_k & = & r^{(k)}(\nu_0(p)) \\ \omega_1 & = & \sqrt{r_0c_2/2} \end{array} \right\} \tag{24}$$

and $O(5)$ denotes a remainder that vanishes to fifth order in (u, U) and $f^{(k)}$ denotes the k-th derivative of the function f.

The Birkhoff normalization algorithm is based on a sequence of canonical coordinate changes such that the Hamiltonian G, (24), is transformed to a Hamiltonian that Poisson commutes with the components of $J = (p, I)$. Because G is completely integrable, this sequence of transformations converges to the transformation to action-angle variables.

Lemma 4. *There is a canonical change of variables,*

$$q = \theta + \chi(\hat{p}, \phi, I),\ \hat{p} = p,\ u = v(p, \phi, I),\ U = \Upsilon(p, \phi, I),$$

that is defined on a neighborhood of $\mathscr{T}_T$ such that

$$G = G_0 + \omega_1 I + \omega_2 I^2 + O(I^3), \tag{25}$$

where

$$\omega_2 = \frac{3\,r_0^2\,c_2\,c_4 - 5\,r_0^2\,c_3^2 - 6\,r_0\,r_1\,c_2\,c_3 + \left(6\,r_0\,r_2 - 9\,r_1^2\right)\,c_2^2}{48\,r_0\,c_2^2}, \tag{26}$$

and the remaining terms are defined in (24).

Proof. Let $\psi = \psi_2(U, p; v) + Uv + p \cdot \tilde{q}$ be the generating function of the symplectic transformation $(q, p, u, U) = \psi(\tilde{q}, \tilde{p}, v, V)$. A routine calculation shows that when

$$\begin{aligned} \psi_2 = &-\frac{vU^3r_2}{16c_2} - \frac{5vU^3r_1^2}{32c_2r_0} + \frac{vU^3c_3r_1}{16c_2^2} - \frac{vU^3c_4r_0}{32c_2^2} + \frac{47vU^3c_3^2r_0}{288c_2^3} - \frac{U^3r_1}{3c_2} - \frac{2U^3c_3r_0}{9c_2^2} \\ &+ \frac{v^3Ur_2}{32r_0} - \frac{3v^3Ur_1^2}{64r_0^2} - \frac{v^3Uc_3r_1}{32c_2r_0} - \frac{5v^3Uc_4}{192c_2} + \frac{25v^3Uc_3^2}{576c_2^2} - \frac{v^2Uc_3}{6c_2} \end{aligned} \tag{27}$$

then G is transformed to (25), where $\omega_1 I = \frac{1}{4}c_2v^2 + \frac{1}{2}r_0V^2$, and the remaining terms are defined in (24) and (26). A second symplectic transformation $v = \lambda\sqrt{2I}\sin(\phi), V = \lambda\sqrt{2I}\cos(\phi)$ completes the transformation to normal form when $\lambda^4 = 2r_0/c_2$. □

3.3 Rüssmann non-degeneracy

There are several flavours of KAM theory for Hamiltonian systems. All share some assumption about the "non-degeneracy" of the frequency map of an integrable Hamiltonian system. The weakest form of non-degeneracy features prominently in the work of Rüssmann.

Definition 3. *[13] Let $U \subset \mathbf{R}^n$ be an open set. A C^r map $f : U \to \mathbf{R}^n$ is* R-degenerate *if there is a proper subspace that contains $f(U)$; it is* R-non-degenerate *if it is not R-degenerate.*

Assume that $f : U \to \mathbf{R}^n$ extends continuously to the closure $\bar{U} \supset U$. If f is R-degenerate, then there is a proper subspace $P \subset \mathbf{R}^n$ such that $f(U) \subset P$. Since P is closed, this implies that $f(\bar{U}) \subset P$, too. This proves the proposition:

Proposition 5. *The frequency map of the integrable Hamiltonian G,* (20)*, is R-non-degenerate.*

Proof. Let $F : T^*(M\times\mathbf{R}) \to \mathbf{R}^{n+1}$ be the first-integral map of G, defined by $F(q,p,\nu,N) = (p, G(q,p,\nu,N))$. The thermostatic equilibrium submanifold $\mathscr{T}_T$ lies in the closure of the set of regular values of the first-integral map F. The frequency map, Ω, of G extends continuously to $\mathscr{T}_T$ by the normal form lemma 4. The singular set of F is the disjoint union of $\mathscr{T}_T$ and the zero momentum set $Z = \{(q,p,\nu,N) \in T^*(M\times\mathbf{R}) \mid p = 0\}$. Since Z is closed, for each open set U of regular points of F whose closure is disjoint from Z, Ω extends continuously to $\bar{U}$.

Let Z_ε be the open neighbourhood of Z consisting of all points (q,p,ν,N) such that $|p| < \varepsilon$; let U be the interior of Z_ε^c intersected with the regular point set of F, so that $\bar{U} = Z_\varepsilon^c$. Assume that $\Omega|U$ is R-degenerate. Since $\omega_1 \not\equiv 0$, there is a non-zero η such that either:

1. $\langle \eta, c(\nu_0(p))\cdot p\rangle \equiv 0$; or
2. $\omega_1(p) \equiv \langle \eta, c(\nu_0(p))\cdot p\rangle$,

for all p with $|p| \geq \varepsilon$.

In case 1, it can be assumed without loss that $|\eta| > \varepsilon$. In particular, when $p = \eta$, one concludes that $\langle \eta, c(\nu_0(\eta))\cdot\eta\rangle = 0$. Since $c(\nu)$ is positive definite for all ν and $\eta \neq 0$, this implies that $\nu_0(\eta)$ is undefined. But, by assumption 4, ν_0 is defined for all non-zero arguments. Contradiction.

In case 2, one observes that both ω_1 and ν_0 are even in p. Hence, the left-hand side is even in p and the right-hand side is odd. Thus, both sides are identically zero. Hence, case 1 holds. Contradiction.

Therefore, $\Omega|U$ must be R-non-degenerate. □

3.4 Kolmogorov non-degeneracy

Kolmogorov introduced the non-degeneracy condition in [1].

Definition 4. *Let $U \subset \mathbf{R}^n$ be an open set. A C^r map $h : U \to \mathbf{R}$ is* Kolmogorov-nondegenerate *if the map*

$$U \to \mathbf{R}^n, \qquad x \mapsto \nabla h(x)$$

is a local diffeomorphism. If h is not Kolmogorov-nondegenerate, then it is said to be Kolmogorov-degenerate. *If h is Kolmogorov-degenerate everywhere, then it is said to be* totally Kolmogorov-degenerate.

This definition is equivalent to the requirement that the Hessian matrix $\nabla^2 h$ be invertible at all $x \in U$. If h is totally Kolmogorov-degenerate and $\nabla^2 h$ extends continuously to the closure $\bar{U}$, then $\nabla^2 h$ is singular on $\bar{U}$.

Proposition 6. *If the frequency map of the integrable Hamiltonian G,* (20)*, is totally Kolmogorov-degenerate on the regular-value set of the first integral map, then there exists an open set $W \subset \mathscr{T}_T^c$ and a function $\psi \in C^{r-1}(W)$ such that:*

1. *G_{0pp} is non-singular;*
2. *$d\omega_1 = G_{0pp}\cdot d\psi$;*
3. *$\omega_2 = \langle d\psi, G_{0pp}\cdot d\psi\rangle = \langle d\omega_1, (G_{0pp})^{-1}\cdot d\omega_1\rangle$.*

Proof. Assume that the Hamiltonian G is totally Kolmogorov-degenerate. By the normal-form lemma, the frequency map Ω and its derivative, $d\Omega$, extend to a continuous map on the set Z defined in the proof of Lemma 4. By the same normal-form lemma, in a neighbourhood of $\mathscr{T}_T$, the Hessian of $G = G(p,I)$ is

$$\nabla^2 G = \mathrm{d}\Omega = \underbrace{\begin{bmatrix} G_{0pp} & \nabla\omega_1 \\ \nabla\omega_1^* & \omega_2 \end{bmatrix}}_{\mathcal{G}} + O(I). \tag{28}$$

If G is totally Kolmogorov-degenerate, then $\mathcal{G}$ has a non-trivial kernel for all $p \neq 0$. Let $w = (w_1, w_2)$ be in the kernel of $\mathcal{G}$ for all $p \neq 0$: so, $\mathcal{G}\cdot w = 0$. Let us prove that w_2 is not identically zero: Assume the contrary, that $w_2 \equiv 0$. Then, $G_{0pp}\cdot w_1 \equiv 0$, $w_1 \neq 0$ for all $p \neq 0$. But,

$$G_{0pp} = c - 2(c'p)(c'p)^*/c_2 \tag{29}$$

where c, c' and c'' are evaluated at $\nu = \nu_0(p)$. It is clear from Assumption 4 that $\nu_0^{-1}(\nu)$ is diffeomorphic to the unit sphere via a radial transformation $p \mapsto \lambda(p;\nu)p$. One concludes from the zero-homogeneity in p of the right-hand side of equation (29) that the right-hand side is singular for all $p \neq 0$. This implies that $c(\nu)$ is a scalar multiple of the identity, say $c(\nu) = \gamma(\nu)1$, and that

$$\gamma = 2(\gamma')^2/\gamma'' \tag{30}$$

for all ν. The general solution to this differential equation is $\gamma(\nu) = a/(\nu - \nu_0)$ for arbitrary $a, \nu_0 \in \mathbf{R}$. But c is defined for all real ν. Contradiction.

Therefore, w_2 is non-zero for some p. Moreover, there is an open set of p such that G_{0pp} is non-singular, that is, the frequency map $p \mapsto G_{0p}$ is a local diffeomorphism. Since $\mathcal{G} \cdot w \equiv 0$ and $w_2 \neq 0$, one can assume without loss that $w_2 = -1$. Thus, $0 = G_{0pp} \cdot w_1 - \nabla\omega_1$ and $0 = \langle \nabla\omega_1, w_1 \rangle - \omega_2$. The first equation implies, since the frequency map is a local diffeomorphism, that w_1 is a gradient and this proves the second part of the proposition. The second equation implies the third part. □

Remark 1. Let's note that property 3 of Proposition 6 is not satisfied identically. Indeed, consider a variable-mass generalization of the Nosé–Hoover system: let $\kappa > 0, \rho$ be constants and choose $b(\nu)$ so that

$$c(\nu) = e^{-2\kappa\nu}\, 1, \qquad\qquad r(\nu) = e^{2\kappa\rho\nu}. \tag{31}$$

When $\kappa = 1, \rho = -2$, this yields the Nosé–Hoover thermostat transformed to have the thermostatic potential equal to $gkT\nu$.

Some straightforward calculations show that, since $\omega_1 = \sqrt{r_0 c_2/2}$,

$$\omega_2 = \alpha_2 \times |p|^{-2\rho}, \qquad \langle \nabla\omega_1, (G_{0pp})^{-1} \cdot \nabla\omega_1 \rangle = \alpha_1 \times |p|^{2\rho-2} \times \left(gkT/\kappa|p|^2 - 2\right)^{-1}, \tag{32}$$

where α_1, α_2 are constants that depend on the parameters gkT, κ, ρ but are independent of p. Since ω_2 is homogeneous in p and the second term is not homogeneous, it is clear that condition 3 of Proposition 6 nevers holds on an open set.

Note that $\omega_1 = \sqrt{r_0 c_2/2}$ is determined by the 0-jet of r and the 2-jet of c_2. The conclusion of Proposition 5 is that ω_2 is determined by $\mathrm{d}\omega_1$ and hence by the 1-jet of r and the 3-jet of c. On the other hand, equation 26 implies that ω_2 is determined by the 2-jet of r and 4-jet of c. Therefore, the space of C^r maps (r, b) such that the Jellinek–Berry thermostatted Hamiltonian G is totally Kolmogorov-degenerate is of finite co-dimension, i.e. it is nowhere dense. In other words, given the functional parameters (r, b) such that G is totally Kolmogorov-degenerate, there is an arbitrarily small C^r perturbation $(\hat{r}, \hat{c})$ such that the perturbed Hamiltonian $\hat{G}$ is Kolmogorov-nondegenerate on some open set.

4 Non-ideal periodic gas

In the previous section it is assumed that the Hamiltonian H is purely kinetic (see (19)). In this section, that assumption is relaxed: let $V : \mathbf{T}^n \to \mathbf{R}$ be a C^r function, $\tau = gkT$ and

$$G_{\tau,V}(q, p, \nu, \mathrm{N}) = \frac{1}{2} \times \langle c(\nu)p, p \rangle + V(q) + \frac{1}{2} r(\nu)\mathrm{N}^2 + \tau\nu, \tag{33}$$

be the Jellinek-Berry thermostatted Hamiltonian. The rescaling transformation

$$p = P\sqrt{\tau}, \quad q = Q, \quad \mathrm{N} = \Omega\sqrt{\tau}, \quad \nu = \omega$$

is conformally symplectic with the constant conformal factor of $\sqrt{\tau}$. The Hamiltonian $G_{\tau,V}$ is transformed to

$$G_{\tau,V}(q, p, \nu, \mathrm{N}) = \tau \times \left(\frac{1}{2} \times \langle c(\omega)P, P \rangle + \beta V(Q) + \frac{1}{2} r(\omega)\Omega^2 + \omega \right) = \tau \times G_{1,\beta V}(Q, P, \omega, \Omega), \tag{34}$$

which is τ times the original Hamiltonian with temperature $T = 1/gk$ and potential energy βV where $\beta = 1/\tau$.

It follows that, for $T \to \infty$, the orbits of the Hamiltonian G (33) are, up to a temperature-dependent rescaling of time, the orbits of that same Hamiltonian with potential energy βV with $\beta \to 0^+$ and temperature $1/gk$. By Proposition 6, one concludes that

Theorem 7. *There is a $T_0 > 0$ such that if $T > T_0$, then the Hamiltonian (33) has a positive measure set of invariant tori. As $T \to \infty$, the Lebesgue density of that set tends to 1.*

5 Conclusion

This notes studies the Jellinek–Berry thermostat. It shows that, in the typical case, the thermostatted Hamiltonian G, (4), does not admit a reduction similar to the Nosé–Hoover reduction of the Nosé thermostat. Despite this, the thermostatted ideal gas is always completely integrable, the Hamiltonian's frequency map satisfies Rüssmann's non-degeneracy condition and the typical one also satisfies Kolmogorov's non-degeneracy condition. Each of these conditions imply that for suitable perturbations, a majority of invariant tori survive. This includes the case where the ideal-gas Hamiltonian is perturbed by a sufficiently smooth potential energy. Somewhat paradoxically, a sufficiently high temperature of the heat bath increases the measure of the set of invariant tori.

The thermostatted ideal-gas Hamiltonian is the simplest example to consider in this family of thermostatted examples. It is natural to ask what happens when one turns to the thermostatted n-degree of freedom harmonic oscillator:

$$G(x, \nu, \mathrm{N}) = \frac{1}{2}\langle c(\nu)x, x\rangle + \frac{1}{2}r(\nu)\mathrm{N}^2 + gkT\nu. \tag{35}$$

As above, $x = (q, p)$ is the state variable of the harmonic oscillator and $c = b(\nu)^* b(\nu)$ is the symmetric, positive-definite quadratic form induced by the coupling matrix $b(\nu)$.

It is well-known that a perturbation of the harmonic oscillator can destroy all invariant tori via the well-known Anosov–Katok construction [2, 3]. On the other hand, if the Jellinek–Berry coupling form, $c(\nu)$, is sufficiently anisotropic, then one might expect that there are parameter regimes for the Hamiltonian (35) in which it decomposes into a perturbation of a non-degenerate integrable Hamiltonian. This mechanism to frustrate ergodicity would differ significantly from the one observed in [16], which demonstrates non-ergodicity of the Nosé–Hoover thermostatted harmonic oscillator (due to the fact that the Nosé thermostat preserves first integrals of the Hamiltonian H that are homogeneous in the momenta).

Compliance with Ethical Standards

Conflict of Interest: The authors declare that they have no conflict of interest.

Data Availability Statement

The authors declare that the data supporting the findings of this study are available within the paper.

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