Emergence of a nonconstant entropy for a fast-slow Hamiltonian system in its second-order asymptotic expansion

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October 22, 2020

Abstract

A system of ordinary differential equations describing the interaction of a fast and a slow particle is studied, where the interaction potential U_ε depends on a small parameter ε. The parameter ε can be interpreted as the mass ratio of the two particles. For positive ε, the equations of motion are Hamiltonian. It is known [6] that the homogenised limit $\varepsilon \to 0$ results again in a Hamiltonian system with homogenised potential U_{hom}. In this article, we are interested in the situation where ε is small but positive. In the first part of this work, we rigorously derive the second-order correction to the homogenised degrees of freedom, notably for the slow particle $y_\varepsilon = y_0 + \varepsilon^2(\bar{y}_2 + [y_2]^\varepsilon)$. In the second part, we give the resulting asymptotic expansion of the energy associated with the fast particle $E_\varepsilon^\perp = E_0^\perp + \varepsilon[E_1^\perp]^\varepsilon + \varepsilon^2(\bar{E}_2^\perp + [E_2^\perp]^\varepsilon)$, a thermodynamic interpretation. In particular, we note that to leading-order $\varepsilon \to 0$, the dynamics of the fast particle can be identified as an *adiabatic* process with *constant entropy*, $dS_0 = 0$. This limit $\varepsilon \to 0$ is characterised by an energy relation that describes equilibrium thermodynamic processes, $dE_0^\perp = F_0 dy_0 + T_0 dS_0 = F_0 dy_0$, where T_0 and F_0 are the leading-order temperature and external force terms respectively. In contrast, we find that to second-order ε^2, a *non-constant entropy* emerges, $d\bar{S}_2 \neq 0$, effectively describing a non-adiabatic process. Remarkably, this process satisfies on average (in the weak* limit) a similar thermodynamic energy relation, i.e., $d\bar{E}_2^\perp = F_0 d\bar{y}_2 + T_0 d\bar{S}_2$.

1 Introduction

Fast-slow Hamiltonian systems constitute a class of mechanical systems in which the interacting degrees of freedom evolve on different time-scales. As such, they play a fundamental role in the description of molecular processes. A motivational example for such a molecular process is the motion of a molecule in a solvent, where the typical fast evolution of the lightweight solvent molecules is in stark contrast to the slow conformal motion of the heavyweight molecule. To analyse this molecular process, one heavily relies on accurate computer simulations. Typical molecular dynamic simulations update the position of each degree of freedom, according to Newton's law of motion, iteratively for each time-step. In practice, however, these simulations become quickly infeasible because of the large number of solvent molecules that constitute the system, which can easily range in the tens of thousands, and the small time-step that is essential to capture their fast motion accurately. In light of these computational problems, there is a strong need for mathematical formalisms that establish effective and computable approximate models for the given fast-slow Hamiltonian system.

A fundamental strategy in the derivation of such mathematical formalisms is the introduction of a scale-parameter ε into the model (representing, for instance, the mass ratio). One can then approach the fast-slow system by considering the limit $\varepsilon \to 0$ and thus derive a homogenised model that is, in some sense, oblivious to the small-scale motion in the system. Although computationally more favourable, this homogenised model must be understood as an idealised approximation to the originally given system only. To approximate natural phenomena more realistically, however, an analysis away from the limit $\varepsilon \to 0$ is necessary.

In this article, we study a fast-slow Hamiltonian system away from the limit $\varepsilon \to 0$, by expanding it to second-order in ε. For small but positive $\varepsilon > 0$, the most dominant small-scale motions enter again into the finer approximate model. To address the related computational problems, we explore a new approach by considering the fast-slow dynamics as a thermodynamic process in which the fast degrees of freedom are

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described by a notion of temperature and entropy. More precisely, we study a simple fast-slow Hamiltonian system with four degrees of freedom. By keeping a molecular dynamic picture in mind, we can regard it as a system of one fast particle that is coupled to one slow particle. We assume that their interaction is governed by the Lagrangian (1) below, for which the homogenised limit $\varepsilon \to 0$ has been derived by Bornemann [6]. We point out that the corresponding homogenised Lagrangian describes the average dynamics of the slow particle only; yet, the fast particle's effect enters as a computable constant into the homogenised limit. This constant results in a homogenised evolution that can be interpreted, from a thermodynamic perspective (as already pointed out in [12]), as an idealised thermodynamic process, i.e., an adiabatic process with constant entropy which satisfies the thermodynamic relation (3). Remarkably, we show in this work, that a higher-order homogenisation approach leads to a more general thermodynamic description of the system. Specifically, continuing the work of Bornemann, we rigorously derive the second-order expansion in ε of the system's dynamics which can be formulated as a second-order two-scale expansion. It then turns out that a nonconstant entropy appears at second-order which satisfies the thermodynamic relation (4).

Our model problem is a simple fast-slow Hamiltonian system which falls into the class of mechanical systems described by the Lagrangian

$$\mathscr{L}_\varepsilon(x, \dot{x}) = \tfrac{1}{2} \langle \dot{x}, \dot{x} \rangle - W_\varepsilon(x), \qquad \dot{x} \in T_x M, \tag{1}$$

where M is the configuration space, taken to be a smooth Riemannian manifold with metric $\langle \cdot, \cdot \rangle$ and $W_\varepsilon \colon M \to \mathbb{R}$ is a smooth potential function of the form

$$W_\varepsilon(x) = V(x) + \varepsilon^{-2} U(x).$$

Taking the limit $\varepsilon \to 0$, the above system converges to a system with a strong constraining force (see, e.g., [18]). More precisely, if U is non-negative and coercive, the second term in W_ε constrains the motion in the limit $\varepsilon \to 0$ to a critical submanifold $N = U^{-1}(0) \subset M$, which characterises the large-scale evolution of the system. This limit system, i.e., the homogenised limit, can be seen as the lowest order approximation in ε of the original system. To derive a more accurate approximation of the mechanical system, which above all includes the most dominant small-scale interactions into the approximate model, a detailed analysis of the motion in a small neighbourhood around N is necessary. For this reason, we derive in the first part of this work a higher-order approximation of system (1) for small but *non-zero* ε. Since a more accurate approximation of the mechanical system increases the computational complexity, we analyse subsequently the resulting motion in the vicinity of N from a thermodynamic point of view, with the intention of deriving a mathematical formalism that can improve current numerical integration schemes.

We recall existing results for system (1) in the limit $\varepsilon \to 0$, established by Bornemann [6] in a very elegant framework. In short, if the initial data is chosen such that the total energy is uniformly bounded as $\varepsilon \to 0$, then the solutions x_ε of the equations of motion oscillate on a time-scale of order $\mathcal{O}(\varepsilon)$ within a distance of order $\mathcal{O}(\varepsilon)$ to the submanifold N. Moreover, the sequence of solutions x_ε converges uniformly to a function x_0 of time, taking values in N, where x_0 is the unique solution to the Euler-Lagrange equations corresponding to the homogenised Lagrangian

$$\mathscr{L}_{\mathrm{hom}}(x, \dot{x}) = \tfrac{1}{2} \langle \dot{x}, \dot{x} \rangle - V(x) - U_{\mathrm{hom}}(x), \qquad \dot{x} \in T_x N, \tag{2}$$

where U_{hom} can be derived from the Hessian of the constraining potential U. We point out that the limit evolution is in general *not* the original Hamiltonian motion constrained to the submanifold N; instead, for generic initial data the small-scale oscillatory motion in the neighbourhood of N gives rise to information which persists in the limit $\varepsilon \to 0$. In other words, the limit Hamiltonian depends on the structure of U near N.

The interaction of a fast and a slow particle is one of the simplest models falling into the class of Hamiltonian mechanical systems described by (1); here ε can be interpreted as the stiffness of the underlying potential resulting in the two disparate time-scales. To visualise this system in the context of (1), we describe the fast particle by z and the slow particle by y. The interaction can then be pictured in $x = (y, z)$ coordinates as a motion governed by a potential which is flat in direction of y and steep in direction of z, taking without loss of generality the minimum of this potential as 0. A motion starting on the zero level set (the submanifold N) with non-vanishing velocity component in direction y will then oscillate rapidly around N. The homogenised limit (2) then describes the motion in the limit $\varepsilon \to 0$.

The main motivation for studying a simple fast-slow Hamiltonian system of two particles is, that it is the simplest possible system that can potentially exhibit thermodynamic effects. Indeed, one of the core assumptions of thermodynamics is that the system under consideration has a clear separation of scales (such as conformal motion described by elasticity combined with fast oscillations described by temperature). It is not essential that the number of particles is large or infinite. Indeed, the physicist Paul Hertz developed a thermodynamic theory [10] for Hamiltonian systems under a slow external perturbation. Specifically, he introduced an entropy, using a notion of temperature as developed by Boltzmann. The book by Berdichevsky [5] gives an excellent introduction to this theory.

If one applies the theory of Hertz to our prototypical two-dimensional system (5), one can interpret the dynamics associated with z_ε as a fast subsystem that is slowly being perturbed by the motion resulting from the slow subsystem governed by y_ε. On an energy level, this is reflected by the total energy $E_\varepsilon(y_\varepsilon, \dot{y}_\varepsilon, z_\varepsilon, \dot{z}_\varepsilon)$, which can be decomposed into the fast subsystem's energy $E_\varepsilon^\perp(z_\varepsilon, \dot{z}_\varepsilon; y_\varepsilon)$ and the slow subsystem's energy $E_\varepsilon^\parallel = E_\varepsilon - E_\varepsilon^\perp$, respectively. Hertz' theory then allows to describe the fast subsystem from a thermodynamic point of view, using a notion of temperature T_ε, entropy S_ε and external force F_ε (the force that y_ε exerts on z_ε). With ε as a scale-parameter, the model allows for a detailed analysis of the system on different scales in time and space. In the first part of this article, we rigorously derive a higher order asymptotic expansion beyond the limit system (2). For instance, the expansion of the slow particle takes the form $y_\varepsilon = y_0 + \varepsilon^2(\bar{y}_2 + [y_2]^\varepsilon)$, where $\bar{y}_2$ is the (slow) averaged and $[y_2]^\varepsilon$ is the rapidly oscillating component of the second-order expansion. In conjunction with Hertz' theory, we similarly apply, in the second part of this article, the asymptotic expansion to the fast subsystem's energy and the thermodynamic quantities, i.e., $E_\varepsilon^\perp = E_0^\perp + \varepsilon[E_1^\perp]^\varepsilon + \varepsilon^2(\bar{E}_2^\perp + [E_2^\perp]^\varepsilon)$, $T_\varepsilon = T_0 + \mathcal{O}(\varepsilon)$, $S_\varepsilon = S_0 + \varepsilon[S_1]^\varepsilon + \varepsilon^2(\bar{S}_2 + [S_2]^\varepsilon)$ and $F_\varepsilon = F_0 + \mathcal{O}(\varepsilon)$. By analysing the limit $\varepsilon \to 0$ one finds, that the entropy associated with the fast subsystem remains constant during the motion, i.e., $dS_0 = 0$. Hence, in the limit of infinite separation of time-scales, the evolution of the fast subsystem is adiabatic, which is by definition an idealised thermodynamic process with constant entropy [23, Chapter 1.4]. This is above all reflected in the energy relation which resembles the equation that describes equilibrium thermodynamic processes, i.e.,

$$dE_0^\perp = F_0 dy_0 + T_0 dS_0 = F_0 dy_0. \tag{3}$$

Furthermore, the model allows for a detailed thermodynamic analysis away from the limit $\varepsilon \to 0$. We show in this article that on scale ε^2, a non-constant entropy appears, $d\bar{S}_2 \neq 0$, which satisfies on average (in the weak* limit) a similar thermodynamic energy relation, i.e.,

$$d\bar{E}_2^\perp = F_0 d\bar{y}_2 + T_0 d\bar{\bar{S}}_2. \tag{4}$$

Hence in this very simple situation, the system is described to leading-order by an effective energy (which is not the naïve limit, as shown in [6]) with constant entropy, while a non-constant entropy appears to second-order.

We remark that the thermodynamic interpretation uses the formulas developed by Hertz. The derivation of the second-order correction is rigorous, using methods of weak convergence. The method of weak convergence is an effective tool for averaging oscillatory behaviour in partial differential equations. The macro-scale dynamics (effective dynamics for y_ε) can be viewed as the averaged motion of the mechanical system. Various other asymptotic and averaging methods have been developed to describe situations when singular perturbations cause rapid, micro-scale fluctuations in the solution. Often an asymptotic description — involving an explicit *ansatz* for the oscillatory part of the solution — is necessary to analyse the dynamics for $\varepsilon > 0$. Some examples are provided by the perturbation theory of integrable Hamiltonian systems [3], the WBK method [13] or multiple-scale-asymptotics [4]; modern presentations for several of these approaches include [11] and [16].

While we have the simplest model for atomistic interaction in mind, the setting is potentially more broadly applicable; notably in cases where the homogenisation theory outlined above and related work as in [17] finds relevance, such as the problem of deriving the guiding centre motion is plasma physics [7], the elimination of fast molecular vibration in classical molecular dynamics [19] or in the description of quantum-classical models in quantum-chemistry [6]. This homogenisation approach was recently used in [12] to coarse-grain the coupled thermoelastic behaviour of solids from the atomistic scale.

1.1 The model problem

For a small scale-parameter $0 < \varepsilon < \varepsilon_0$, we study a family of mechanical systems described by the Lagrangian

$$\mathscr{L}_\varepsilon(y_\varepsilon, z_\varepsilon, \dot{y}_\varepsilon, \dot{z}_\varepsilon) = \tfrac{1}{2}\dot{y}_\varepsilon^2 + \tfrac{1}{2}\dot{z}_\varepsilon^2 - \tfrac{1}{2}\varepsilon^{-2}\omega^2(y_\varepsilon)z_\varepsilon^2, \tag{5}$$

on the two-dimensional Euclidean configuration space $M = \mathbb{R}^2$. This system is a simplified version of the model problem introduced in [6, §1.2.1]. The corresponding Newtonian equations of motion take the form

$$\ddot{y}_\varepsilon = -\varepsilon^{-2}\omega(y_\varepsilon)\omega'(y_\varepsilon)z_\varepsilon^2, \tag{6a}$$
$$\ddot{z}_\varepsilon = -\varepsilon^{-2}\omega^2(y_\varepsilon)z_\varepsilon. \tag{6b}$$

We assume that $\omega \in C^\infty(\mathbb{R})$ is a uniformly positive function, i.e., there is a constant $\omega_* > 0$ such that

$$\omega(y) \geq \omega_*, \qquad \text{for all } y \in \mathbb{R}, \tag{7}$$

and consider ε-independent initial values,

$$y_\varepsilon(0) = y_*, \qquad \dot{y}_\varepsilon(0) = p_*, \qquad z_\varepsilon(0) = 0, \qquad \dot{z}_\varepsilon(0) = u_*. \tag{8}$$

Notice that the particular choice $z_\varepsilon(0) = 0$ makes the conserved energy E_ε of the system independent of ε,

$$E_\varepsilon = \tfrac{1}{2}\dot{y}_\varepsilon^2 + \tfrac{1}{2}\dot{z}_\varepsilon^2 + \tfrac{1}{2}\varepsilon^{-2}\omega^2(y_\varepsilon)z_\varepsilon^2 = \tfrac{1}{2}p_*^2 + \tfrac{1}{2}u_*^2 = E_*. \tag{9}$$

We are primarily interested in the time evolution of the slow degree of freedom y_ε. The following theorem [6, Theorem 1, Chapter I §2] shows that y_ε converges in the limit $\varepsilon \to 0$ to a function y_0 which is given as the solution to a second-order differential equation. The constant θ_* in the effective potential is of the form $\theta_* = u_*^2/2\omega(y_*)$, with y_* and u_* as in (8). We will later see that θ_* is proportional to the action of the fast subsystem in the limit $\varepsilon \to 0$. As a consequence, some information of the fast subsystem is retained in the slow evolution of y_0.

Theorem 1.1 (Bornemann, [6])**.** *Let y_0 be the solution to the second-order differential equation*

$$\ddot{y}_0 = -\theta_*\omega'(y_0),$$

with initial values $y_0(0) = y_*$, $\dot{y}_0(0) = p_*$. Then, for every finite time interval $[0, T]$, one obtains the strong convergence

$$y_\varepsilon \to y_0 \quad \text{in} \quad C^1([0,T])$$

and the weak convergences $\varepsilon^{-1}z_\varepsilon \overset{*}{\rightharpoonup} 0$ and $\dot{z}_\varepsilon \overset{*}{\rightharpoonup} 0$ in $L^\infty([0,T])$.*

We extend the theory developed in [6] by deriving rigorously the second-order asymptotic expansion for the solution of the equations of motion (6) and interpret the corresponding expansion of the energy (9) from a thermodynamic point of view. A crucial step in the derivation of these expansions is the introduction of action-angle variables for the rapidly oscillating degree of freedom $(z_\varepsilon, \dot{z}_\varepsilon) \mapsto (\theta_\varepsilon, \phi_\varepsilon)$, which also involves a transformation of the generalised momentum $\dot{y}_\varepsilon \mapsto p_\varepsilon$ to preserve the symplectic structure on the phase-space as a whole.

1.2 Main results

The main results in this work can be stated as follows:

1. There is a second-order asymptotic expansion of the variables y_ε, p_ε, θ_ε ϕ_ε introduced in the previous paragraph and defined precisely in Section 3; this expansion is of the form

$$\begin{aligned}
y_\varepsilon &= y_0 + \varepsilon[\bar{y}_1]^\varepsilon + \varepsilon^2[\bar{y}_2]^\varepsilon + \varepsilon^2 y_3^\varepsilon,\\
p_\varepsilon &= p_0 + \varepsilon[\bar{p}_1]^\varepsilon + \varepsilon^2[\bar{p}_2]^\varepsilon + \varepsilon^2 p_3^\varepsilon,\\
\theta_\varepsilon &= \theta_* + \varepsilon[\bar{\theta}_1]^\varepsilon + \varepsilon^2[\bar{\theta}_2]^\varepsilon + \varepsilon^2 \theta_3^\varepsilon,\\
\phi_\varepsilon &= \phi_0 + \varepsilon[\bar{\phi}_1]^\varepsilon + \varepsilon^2[\bar{\phi}_2]^\varepsilon + \varepsilon^2 \phi_3^\varepsilon,
\end{aligned}$$

   where for $i \in \{1, 2\}$,

$$\begin{aligned}
[\bar{y}_i]^\varepsilon &:= \bar{y}_i + [y_i]^\varepsilon \overset{*}{\rightharpoonup} \bar{y}_i \quad \text{in} \quad L^\infty((0,T)), & y_3^\varepsilon &\to 0 \quad \text{in} \quad C([0,T]),\\
[\bar{p}_i]^\varepsilon &:= \bar{p}_i + [p_i]^\varepsilon \overset{*}{\rightharpoonup} \bar{p}_i \quad \text{in} \quad L^\infty((0,T)), & p_3^\varepsilon &\to 0 \quad \text{in} \quad C([0,T]),\\
[\bar{\theta}_i]^\varepsilon &:= \bar{\theta}_i + [\theta_i]^\varepsilon \overset{*}{\rightharpoonup} \bar{\theta}_i \quad \text{in} \quad L^\infty((0,T)), & \theta_3^\varepsilon &\to 0 \quad \text{in} \quad C([0,T]),\\
[\bar{\phi}_i]^\varepsilon &:= \bar{\phi}_i + [\phi_i]^\varepsilon \overset{*}{\rightharpoonup} \bar{\phi}_i \quad \text{in} \quad L^\infty((0,T)), & \phi_3^\varepsilon &\to 0 \quad \text{in} \quad C([0,T]).
\end{aligned}$$

   In other words, for each variable the second-order asymptotic expansion is characterised — to leading-order by the theory developed in [6] (Theorem 1.1) — to i-th order by a decomposition into a slow term, indicated by an overbar, which constitutes the average motion of the i-th order expansion, and a fast term, indicated by square brackets, which oscillate rapidly and converge weakly* to zero — and by a residual term, indicated with a subscript three, that converges uniformly to zero. In particular, we show that

$$[\bar{y}_1]^\varepsilon = 0, \qquad [\bar{p}_1]^\varepsilon = 0, \qquad [\bar{\theta}_1]^\varepsilon = [\theta_1]^\varepsilon, \qquad [\bar{\phi}_1]^\varepsilon = 0, \tag{10}$$

   and that $(\bar{\phi}_2, \bar{\theta}_2, \bar{y}_2, \bar{p}_2)$ is given as the solution to an inhomogeneous linear system of differential equations (Theorem 3.2). Moreover the rapidly oscillating functions $[\theta_1]^\varepsilon$, $[y_2]^\varepsilon$, $[p_2]^\varepsilon$, $[\theta_2]^\varepsilon$ and $[\phi_2]^\varepsilon$, are explicitly given in Definition 3.1.

   Finally, we show that this expansion can be interpreted as a nonlinear version of a two-scale expansion, which we briefly introduce in Appendix A.

2. Using the framework of Hertz [10], we define a temperature T_ε, an entropy S_ε and an external force F_ε for the fast subsystem based on a scaling of space and time of the fast degree of freedom z_ε, such that in the limit $\varepsilon \to 0$, the system is in thermal equilibrium (see Appendix B.4). In combination with the

analytic result discussed under 1, we decompose the total energy E_ε into the energy associated with the fast particle $E_\varepsilon^\perp$ and the residual energy $E_\varepsilon^\parallel = E_\varepsilon - E_\varepsilon^\perp$, and expand, similar as above $E_\varepsilon^\perp$, $E_\varepsilon^\parallel$, T_ε, S_ε and F_ε into the form

$$\begin{aligned} E_\varepsilon^\perp &= E_0^\perp + \varepsilon[\bar{E}_1^\perp]^\varepsilon + \varepsilon^2[\bar{E}_2^\perp]^\varepsilon + \varepsilon^2 E_3^{\perp\varepsilon}, \\ E_\varepsilon^\parallel &= E_0^\parallel + \varepsilon[\bar{E}_1^\parallel]^\varepsilon + \varepsilon^2[\bar{E}_2^\parallel]^\varepsilon + \varepsilon^2 E_3^{\parallel\varepsilon}, \\ S_\varepsilon &= S_0 + \varepsilon[\bar{S}_1]^\varepsilon + \varepsilon^2[\bar{S}_2]^\varepsilon + \varepsilon^2 S_3^\varepsilon, \\ T_\varepsilon &= T_0 + \mathcal{O}(\varepsilon), \\ F_\varepsilon &= F_0 + \mathcal{O}(\varepsilon), \end{aligned}$$

where for $i \in \{1, 2\}$,

$$\begin{aligned} [\bar{E}_i^\perp]^\varepsilon &:= \bar{E}_i^\perp + [E_i^\perp]^\varepsilon \overset{*}{\rightharpoonup} \bar{E}_i^\perp \quad \text{in} \quad L^\infty((0,T)), & E_3^{\perp\varepsilon} &\to 0 \quad \text{in} \quad C([0,T]), \\ [\bar{E}_i^\parallel]^\varepsilon &:= \bar{E}_i^\parallel + [E_i^\parallel]^\varepsilon \overset{*}{\rightharpoonup} \bar{E}_i^\parallel \quad \text{in} \quad L^\infty((0,T)), & E_3^{\parallel\varepsilon} &\to 0 \quad \text{in} \quad C([0,T]), \\ [\bar{S}_i]^\varepsilon &:= \bar{S}_i + [S_i]^\varepsilon \overset{*}{\rightharpoonup} \bar{S}_i \quad \text{in} \quad L^\infty((0,T)), & S_3^\varepsilon &\to 0 \quad \text{in} \quad C([0,T]). \end{aligned}$$

The characterisation of the i-th order expansion is similar as above; moreover, it follows from (9) that

$$E_\varepsilon = E_0^\perp + E_0^\parallel = E_*, \qquad [\bar{E}_1^\perp]^\varepsilon + [\bar{E}_1^\parallel]^\varepsilon = 0, \qquad [\bar{E}_2^\perp]^\varepsilon + [\bar{E}_2^\parallel]^\varepsilon = 0, \qquad E_3^{\perp\varepsilon} + E_3^{\parallel\varepsilon} = 0.$$

In Section 4 we show that

$$[\bar{E}_1^\perp]^\varepsilon = [E_1^\perp]^\varepsilon, \qquad [\bar{E}_1^\parallel]^\varepsilon = [E_1^\parallel]^\varepsilon, \qquad [\bar{S}_1]^\varepsilon = [S_1]^\varepsilon,$$

and interpret the asymptotic expansion from a thermodynamic point of view. In particular, we show that to leading-order the entropy expression remains *constant*, i.e., $dS_0 = 0$, and consequently the dynamics can be interpreted as an adiabatic process characterised by an energy relation that defines processes in thermodynamic equilibrium,

$$dE_0^\perp = F_0 dy_0 + T_0 dS_0 = F_0 dy_0. \tag{11}$$

In contrast, we show that the averaged second-order dynamics, i.e., the dynamics in the weak* limit, indicated by an overbar, represents a non-adiabatic process with an averaged *non-constant entropy*, $d\bar{S}_2 \neq 0$, that similarly as above satisfies relations akin to equilibrium thermodynamics, despite being beyond the limit $\varepsilon \to 0$,

$$d\bar{E}_2^\perp = F_0 d\bar{y}_2 + T_0 d\bar{\bar{S}}_2, \tag{12}$$

where $\bar{\bar{S}}_2$ indicates the averaged second-order entropy expression ignoring interactions with its first-order expansion. Finally, we show in Theorem 4.1 that the evolution of $(\bar{y}_2, \bar{p}_2)$ is governed by equations which resemble Hamilton's canonical equations,

$$\frac{d\bar{y}_2}{dt} = \frac{\partial \bar{E}_2}{\partial p_0}, \qquad \frac{\partial \bar{p}_2}{dt} = -\frac{\partial \bar{E}_2}{\partial y_0},$$

for $\bar{E}_2 = \bar{E}_2^\perp + \bar{E}_2^\parallel$, which are complemented by the ε-independent initial values

$$\bar{y}_2(0) = -[y_2]^\varepsilon(0), \qquad \bar{p}_2(0) = -[p_2]^\varepsilon(0).$$

In summary, Theorem 1.1 shows that the family of mechanical systems (5) converges as $\varepsilon \to 0$ to a mechanical system, which is again Hamiltonian in nature. Based on our asymptotic expansion result we show that the leading-order entropy expression according to Hertz [10] is constant (cf. equation (11)), and that a non-constant entropy appears in the second-order expansion (cf. equation (12)). We refer to the recent study [12], which inspired our analysis. There, a classic thermodynamic description of the elastodynamics of solids is derived by studying thermoelastic coupling for bars of various lengths, thus explicitly controlling the value of ε. The authors then observe that in the limit $\varepsilon \to 0$, the dynamics are Hamiltonian, while dissipation occurs for larger values of ε. The study [12] also combines methods of [6] and [10].

Outline of the paper

Section 2 contains preliminary steps for the analysis of the model problem. We introduce action-angle variables for the rapidly oscillating degree of freedom and prove the existence and uniqueness of a solution to the transformed model problem. Section 3 includes the proof of the second-order asymptotic expansion of $y_\varepsilon, p_\varepsilon, \theta_\varepsilon$ and ϕ_ε. After deriving the leading-order expansion, we introduce some notation that simplifies the subsequent analysis of the first- and second-order expansion. In Section 4 we introduce the thermodynamic quantities and give their detailed interpretation in the context of the model problem. The second-order expansion can be represented as a nonlinear version of a two-scale expansion, which we introduce in Appendix A. Finally, in Appendix B we describe how the thermodynamic quantities can be derived for the model problem using Hertz' original method.

2 The model problem in action-angle variables

To analyse the dynamics of y_ε and z_ε for $0 < \varepsilon < \varepsilon_0$, a detailed asymptotic analysis is required. We build on [6, Appendix A], which introduces action-angle variables and uses tools from the perturbation theory of integrable Hamiltonian systems (as presented, for instance, in [3]), to derive the asymptotic behaviour of y_ε and z_ε to first-order. We will expand the results and determine the explicit form of the second-order correction. As in [6], we start by rephrasing the governing perturbed system of Newtonian equations (6). We denote by $(\eta_\varepsilon, \zeta_\varepsilon)$ the canonical momenta corresponding to the positions $(y_\varepsilon, z_\varepsilon)$. Then the equations of motion (6), together with the velocity relations

$$\dot{y}_\varepsilon = \eta_\varepsilon, \qquad \dot{z}_\varepsilon = \zeta_\varepsilon,$$

are given by the canonical equations of motion belonging to the energy function

$$E_\varepsilon(y_\varepsilon, \eta_\varepsilon, z_\varepsilon, \zeta_\varepsilon) = \tfrac{1}{2}\eta_\varepsilon^2 + \tfrac{1}{2}\zeta_\varepsilon^2 + \tfrac{1}{2}\varepsilon^{-2}\omega^2(y_\varepsilon)z_\varepsilon^2. \tag{13}$$

To take the oscillatory character of z_ε into account, we introduce particular action-angle variables $(\theta_\varepsilon, \phi_\varepsilon)$ for the fast degrees of freedom $(z_\varepsilon, \zeta_\varepsilon)$,

$$z_\varepsilon = \varepsilon\sqrt{\frac{2\theta_\varepsilon}{\omega(y_\varepsilon)}}\sin(\varepsilon^{-1}\phi_\varepsilon), \qquad \zeta_\varepsilon = \sqrt{2\theta_\varepsilon\omega(y_\varepsilon)}\cos(\varepsilon^{-1}\phi_\varepsilon). \tag{14}$$

The transformation $(z_\varepsilon, \zeta_\varepsilon) \mapsto (\theta_\varepsilon, \phi_\varepsilon)$ can be found using the theory of generating functions [2, §48]. For fixed y_ε, the transformation is generated by the function

$$S_0(z_\varepsilon, \phi_\varepsilon; y_\varepsilon) = \tfrac{1}{2}\varepsilon^{-1}\omega(y_\varepsilon)z_\varepsilon^2\cot(\varepsilon^{-1}\phi_\varepsilon),$$

via $\zeta_\varepsilon = \partial S_0/\partial z_\varepsilon$ and $\theta_\varepsilon = -\partial S_0/\partial\phi_\varepsilon$. It turns out, however, that this transformation is symplectic only for fixed y_ε. Therefore, we have to modify the position y_ε or the momentum η_ε. The extended generating function $S(y_\varepsilon, p_\varepsilon, z_\varepsilon, \phi_\varepsilon) = p_\varepsilon y_\varepsilon + S_0(z_\varepsilon, \phi_\varepsilon; y_\varepsilon)$ does not transform the position variable $y_\varepsilon = \partial S/\partial p_\varepsilon$ but changes the momentum η_ε such that the transformation remains symplectic on the phase space as a whole. The missing transformation of the momentum η_ε is thus given by

$$\eta_\varepsilon = \frac{\partial S}{\partial y_\varepsilon} = p_\varepsilon + \varepsilon\frac{\theta_\varepsilon\omega'(y_\varepsilon)}{2\omega(y_\varepsilon)}\sin(2\varepsilon^{-1}\phi_\varepsilon).$$

By construction, the resulting transformation $(y_\varepsilon, \eta_\varepsilon; z_\varepsilon, \zeta_\varepsilon) \mapsto (y_\varepsilon, p_\varepsilon; \phi_\varepsilon, \theta_\varepsilon)$ is symplectic on the whole phase space. The energy function (13) transforms to the expression

$$E_\varepsilon = \frac{1}{2}p_\varepsilon^2 + \theta_\varepsilon\omega(y_\varepsilon) + \varepsilon\frac{\theta_\varepsilon p_\varepsilon\omega'(y_\varepsilon)}{2\omega(y_\varepsilon)}\sin(2\varepsilon^{-1}\phi_\varepsilon) + \frac{\varepsilon^2}{8}\left(\frac{\theta_\varepsilon\omega'(y_\varepsilon)}{\omega(y_\varepsilon)}\sin(2\varepsilon^{-1}\phi_\varepsilon)\right)^2. \tag{15}$$

Thus, by the canonical formalism, the equations of motion take the form

$$\dot{\phi}_\varepsilon = \frac{\partial E_\varepsilon}{\partial\theta_\varepsilon}, \qquad \dot{\theta}_\varepsilon = -\frac{\partial E_\varepsilon}{\partial\phi_\varepsilon}, \qquad \dot{y}_\varepsilon = \frac{\partial E_\varepsilon}{\partial p_\varepsilon}, \qquad \dot{p}_\varepsilon = -\frac{\partial E_\varepsilon}{\partial y_\varepsilon},$$

which gives after some calculations

$$\dot{\phi}_\varepsilon = \omega(y_\varepsilon) + \varepsilon\frac{p_\varepsilon\omega'(y_\varepsilon)}{2\omega(y_\varepsilon)}\sin(2\varepsilon^{-1}\phi_\varepsilon) + \varepsilon^2\frac{\theta_\varepsilon\left(\omega'(y_\varepsilon)\right)^2}{4\omega^2(y_\varepsilon)}\sin^2(2\varepsilon^{-1}\phi_\varepsilon), \tag{16a}$$

$$\dot{\theta}_\varepsilon = -\frac{\theta_\varepsilon p_\varepsilon\omega'(y_\varepsilon)}{\omega(y_\varepsilon)}\cos(2\varepsilon^{-1}\phi_\varepsilon) - \varepsilon\frac{\theta_\varepsilon^2\left(\omega'(y_\varepsilon)\right)^2}{4\omega^2(y_\varepsilon)}\sin(4\varepsilon^{-1}\phi_\varepsilon), \tag{16b}$$

$$\dot{y}_\varepsilon = p_\varepsilon + \varepsilon\frac{\theta_\varepsilon\omega'(y_\varepsilon)}{2\omega(y_\varepsilon)}\sin(2\varepsilon^{-1}\phi_\varepsilon), \tag{16c}$$

$$\begin{aligned}\dot{p}_\varepsilon = {} & -\theta_\varepsilon\omega'(y_\varepsilon) + \varepsilon\frac{\theta_\varepsilon p_\varepsilon\left(\omega'(y_\varepsilon)\right)^2}{2\omega^2(y_\varepsilon)}\sin(2\varepsilon^{-1}\phi_\varepsilon) - \varepsilon\frac{\theta_\varepsilon p_\varepsilon\omega''(y_\varepsilon)}{2\omega(y_\varepsilon)}\sin(2\varepsilon^{-1}\phi_\varepsilon) \\ & + \varepsilon^2\frac{\theta_\varepsilon^2\left(\omega'(y_\varepsilon)\right)^3}{4\omega^3(y_\varepsilon)}\sin^2(2\varepsilon^{-1}\phi_\varepsilon) - \varepsilon^2\frac{\theta_\varepsilon^2\omega'(y_\varepsilon)\omega''(y_\varepsilon)}{4\omega^2(y_\varepsilon)}\sin^2(2\varepsilon^{-1}\phi_\varepsilon).\end{aligned} \tag{16d}$$

The initial values, as given in (8), transform to

$$\phi_\varepsilon(0) = 0, \qquad \theta_\varepsilon(0) = \theta_* = \frac{u_*^2}{2\omega(y_*)}, \qquad y_\varepsilon(0) = y_*, \qquad p_\varepsilon(0) = p_*. \tag{17}$$

2.1 Existence and uniqueness of a solution to the model problem

Let us denote the right hand side of (16) as $\mathcal{F}_\varepsilon\colon \mathbb{R}^4 \to \mathbb{R}^4$. By assumption, $\omega \in C^\infty(\mathbb{R})$ and therefore $\mathcal{F}_\varepsilon \in C^\infty(\mathbb{R}^4, \mathbb{R}^4)$ for $0 < \varepsilon < \varepsilon_0 < \infty$. In particular, $\mathcal{F}_\varepsilon$ is locally Lipschitz continuous. Hence, by the standard existence and uniqueness theory for ordinary differential equation (see, for example, [20]), there exists a $0 < T < \infty$ such that the initial value problem (16)–(17) has a unique solution

$$(\phi_\varepsilon, \theta_\varepsilon, y_\varepsilon, p_\varepsilon) \in C^\infty([0,T], \mathbb{R}^4), \tag{18}$$

for fixed $0 < \varepsilon < \varepsilon_0$.

3 Second-order asymptotic expansion

In this section, we rigorously derive the second-order asymptotic expansion for ϕ_ε, θ_ε, y_ε and p_ε. The equations in (16) are used to derive the leading-order expansions in 3.1, before we reformulate them in 3.2 to derive jointly the first- and second order expansion in 3.3 and 3.4.

3.1 Leading-order expansion

Let us analyse the sequence of solutions (18) for $\varepsilon \to 0$. The right-hand side of (16) is oscillatory and has in particular a highly oscillatory leading-order term. As a consequence, the sequences $\{d\phi_\varepsilon/dt\}$, $\{\theta_\varepsilon\}$, $\{dy_\varepsilon/dt\}$, $\{dp_\varepsilon/dt\}$ are bounded in the space $C^{0,1}([0,T])$ of uniformly Lipschitz continuous functions, while sequences of higher-order derivatives (in particular $\{d^2\theta_\varepsilon/dt^2\}$, which will require special attention in the later part of this work) become unbounded as $\varepsilon \to 0$. It follows from the extended Arzelà-Ascoli Theorem [6, Principle 4, Chapter I §1] that we can extract a subsequence, not relabelled, and functions $\theta_0 \in C^{0,1}([0,T])$ and $\phi_0, y_0, p_0 \in C^{1,1}([0,T])$, such that

$$\phi_\varepsilon \to \phi_0 \quad \text{in} \quad C^1([0,T]), \qquad \ddot{\phi}_\varepsilon \overset{*}{\rightharpoonup} \ddot{\phi}_0 \quad \text{in} \quad L^\infty((0,T)), \tag{19a}$$

$$\theta_\varepsilon \to \theta_0 \quad \text{in} \quad C([0,T]), \qquad \dot{\theta}_\varepsilon \overset{*}{\rightharpoonup} \dot{\theta}_0 \quad \text{in} \quad L^\infty((0,T)), \tag{19b}$$

$$y_\varepsilon \to y_0 \quad \text{in} \quad C^1([0,T]), \qquad \ddot{y}_\varepsilon \overset{*}{\rightharpoonup} \ddot{y}_0 \quad \text{in} \quad L^\infty((0,T)), \tag{19c}$$

$$p_\varepsilon \to p_0 \quad \text{in} \quad C^1([0,T]), \qquad \ddot{p}_\varepsilon \overset{*}{\rightharpoonup} \ddot{p}_0 \quad \text{in} \quad L^\infty((0,T)). \tag{19d}$$

By taking the limit $\varepsilon \to 0$ in equation (16a), (16c) and (16d) and the weak* limit in (16b) we deduce that

$$\dot{\phi}_0 = \omega(y_0), \qquad \dot{\theta}_0 = 0, \qquad \dot{y}_0 = p_0, \qquad \dot{p}_0 = -\theta_* \omega'(y_0), \tag{20}$$

and in particular $\theta_0 \equiv \theta_*$ (compare with (17)). Moreover, since the right-hand side of the limit equation, $\ddot{y}_0 = -\theta_* \omega'(y_0)$, does not depend on a chosen subsequence, we can discard the extraction of subsequences altogether [6, Principle 5, Chapter I §1].

3.2 Reformulation of the governing equations

For the subsequent part of this work, it is convenient to introduce a notation that simplifies the system of differential equations (16); namely, for $L_\varepsilon \coloneqq \log(\omega(y_\varepsilon))$ and $k, l \in \mathbb{N}_0$, we define

$$D_t^k D_y^l L_\varepsilon \coloneqq \frac{d^k}{dt^k} \frac{\partial^l L_\varepsilon}{\partial y_\varepsilon^l}.$$

Then (16) reads in the new notation

$$\dot{\phi}_\varepsilon = \omega(y_\varepsilon) + \frac{\varepsilon}{2} p_\varepsilon D_y L_\varepsilon \sin(2\varepsilon^{-1}\phi_\varepsilon) + \frac{\varepsilon^2}{4} \theta_\varepsilon (D_y L_\varepsilon)^2 \sin^2(2\varepsilon^{-1}\phi_\varepsilon), \tag{21a}$$

$$\dot{\theta}_\varepsilon = -\theta_\varepsilon p_\varepsilon D_y L_\varepsilon \cos(2\varepsilon^{-1}\phi_\varepsilon) - \frac{\varepsilon}{4} \theta_\varepsilon^2 (D_y L_\varepsilon)^2 \sin(4\varepsilon^{-1}\phi_\varepsilon), \tag{21b}$$

$$\dot{y}_\varepsilon = p_\varepsilon + \frac{\varepsilon}{2} \theta_\varepsilon D_y L_\varepsilon \sin(2\varepsilon^{-1}\phi_\varepsilon), \tag{21c}$$

$$\dot{p}_\varepsilon = -\theta_\varepsilon \omega'(y_\varepsilon) - \frac{\varepsilon}{2} \theta_\varepsilon p_\varepsilon D_y^2 L_\varepsilon \sin(2\varepsilon^{-1}\phi_\varepsilon) - \frac{\varepsilon^2}{4} \theta_\varepsilon^2 D_y L_\varepsilon D_y^2 L_\varepsilon \sin^2(2\varepsilon^{-1}\phi_\varepsilon). \tag{21d}$$

Furthermore, by solving equation (21c) for p_ε and insert the resulting expression into (21a), (21b) and (21d), the equations of motion take the final form

$$\dot{\phi}_\varepsilon = \omega(y_\varepsilon) + \frac{\varepsilon}{2} D_t L_\varepsilon \sin\left(2\varepsilon^{-1}\phi_\varepsilon\right), \tag{22a}$$

$$\dot{\theta}_\varepsilon = -\theta_\varepsilon D_t L_\varepsilon \cos(2\varepsilon^{-1}\phi_\varepsilon), \tag{22b}$$

$$\dot{y}_\varepsilon = p_\varepsilon + \frac{\varepsilon}{2}\theta_\varepsilon D_y L_\varepsilon \sin(2\varepsilon^{-1}\phi_\varepsilon), \tag{22c}$$

$$\dot{p}_\varepsilon = -\theta_\varepsilon \omega'(y_\varepsilon) - \frac{\varepsilon}{2}\theta_\varepsilon D_t D_y L_\varepsilon \sin(2\varepsilon^{-1}\phi_\varepsilon). \tag{22d}$$

3.3 First- and second-order expansion

To analyse the dynamics of the model problem away from the limit $\varepsilon \to 0$, a higher-order asymptotic expansion in ε is required. As already pointed out in 10, the first-order expansion is only non-zero for θ_ε and hence of limited use. For this reason, we expand y_ε, p_ε, θ_ε and ϕ_ε up to second-order in ε.

We first define particular functions that appear in the first- and second-order expansion before we state the theorem that embodies the first main result 1.

Definition 3.1. Let $(\phi_\varepsilon, \theta_\varepsilon, y_\varepsilon, p_\varepsilon)$ be the solution to (16)–(17) and $(\phi_0, \theta_0, y_0, p_0)$ be as in (19). With the notation introduced in Section 3.2, we define the functions

$$\theta_1^\varepsilon := \frac{\theta_\varepsilon - \theta_*}{\varepsilon}, \qquad \phi_2^\varepsilon := \frac{\phi_\varepsilon - \phi_0}{\varepsilon^2}, \qquad y_2^\varepsilon := \frac{y_\varepsilon - y_0}{\varepsilon^2}, \qquad p_2^\varepsilon := \frac{p_\varepsilon - p_0}{\varepsilon^2}, \qquad \theta_2^\varepsilon := \frac{\theta_1^\varepsilon - [\theta_1]^\varepsilon}{\varepsilon}, \tag{23}$$

$$[\theta_1]^\varepsilon := -\frac{\theta_* D_t L_0}{2\omega(y_0)} \sin(2\varepsilon^{-1}\phi_0), \qquad [\phi_2]^\varepsilon := -\frac{D_t L_0}{4\omega(y_0)} \cos(2\varepsilon^{-1}\phi_0),$$

$$[y_2]^\varepsilon := -\frac{\theta_* D_y L_0}{4\omega(y_0)} \cos(2\varepsilon^{-1}\phi_0), \qquad [p_2]^\varepsilon := \frac{d}{dt}\left(\frac{\theta_* D_y L_0}{4\omega(y_0)}\right) \cos(2\varepsilon^{-1}\phi_0)$$

and

$$[\theta_2]^\varepsilon := -\theta_* D_y L_0 [y_2]^\varepsilon - \frac{p_0}{\omega(y_0)}[p_2]^\varepsilon + \frac{\theta_*^2 (D_y L_0)^2}{16\omega(y_0)} \cos(4\varepsilon^{-1}\phi_0) - \frac{\theta_* D_t L_0}{\omega(y_0)} \bar{\phi}_2 \cos(2\varepsilon^{-1}\phi_0).$$

The functions θ_1^ε, ϕ_2^ε, y_2^ε and p_2^ε as defined in (23) describe scaled versions of the residual motion of the originally given degrees of freedom and their homogenised versions. The scaling order is indicated by the corresponding subscript and marks their relevancy in the first- and second-order expansion. To determine the relevant term in the second-order expansion for θ_ε, we similarly define by θ_2^ε the scaled residual motion of θ_ε and its first-order expansion, which is derived in a two-step procedure via θ_1^ε. As hinted before in 1, the second-order expansions comprise of oscillating and non-oscillating terms. The oscillating terms are denoted by expressions in square brackets, as in the remainder of the definition. The non-oscillatory terms are characterised in the following theorem, which is the main analytic result of this article. One key result is that the non-oscillatory terms of the second-order expansion, marked by an overbar and subscript 2, satisfy a system of ordinary differential equations.

Theorem 3.2. *The functions specified in Definition 3.1 satisfy*

$$\theta_1^\varepsilon - [\theta_1]^\varepsilon \to 0 \quad \text{in} \quad C([0,T]), \qquad \frac{d}{dt}\left(\theta_1^\varepsilon - [\theta_1]^\varepsilon\right) \overset{*}{\rightharpoonup} 0 \quad \text{in} \quad L^\infty((0,T)), \tag{24}$$

$$\phi_2^\varepsilon - [\phi_2]^\varepsilon \to \bar{\phi}_2 \quad \text{in} \quad C([0,T]), \qquad \frac{d}{dt}\left(\phi_2^\varepsilon - [\phi_2]^\varepsilon\right) \overset{*}{\rightharpoonup} \frac{d\bar{\phi}_2}{dt} \quad \text{in} \quad L^\infty((0,T)), \tag{25}$$

$$y_2^\varepsilon - [y_2]^\varepsilon \to \bar{y}_2 \quad \text{in} \quad C([0,T]), \qquad \frac{d}{dt}\left(y_2^\varepsilon - [y_2]^\varepsilon\right) \overset{*}{\rightharpoonup} \frac{d\bar{y}_2}{dt} \quad \text{in} \quad L^\infty((0,T)), \tag{26}$$

$$p_2^\varepsilon - [p_2]^\varepsilon \to \bar{p}_2 \quad \text{in} \quad C([0,T]), \qquad \frac{d}{dt}\left(p_2^\varepsilon - [p_2]^\varepsilon\right) \overset{*}{\rightharpoonup} \frac{d\bar{p}_2}{dt} \quad \text{in} \quad L^\infty((0,T)) \tag{27}$$

and

$$\theta_2^\varepsilon - [\theta_2]^\varepsilon \to \bar{\theta}_2 \quad \text{in} \quad C([0,T]), \tag{28}$$

where $(\bar{\phi}_2, \bar{\theta}_2, \bar{y}_2, \bar{p}_2)$ *is the unique solution to the inhomogeneous linear system of differential equations*

$$\frac{d\bar{\phi}_2}{dt} = \omega'(y_0)\bar{y}_2 + \frac{\theta_*(D_yL_0)^2}{8} - \frac{(D_tL_0)^2}{8\omega(y_0)}, \tag{29a}$$

$$\frac{d\bar{\theta}_2}{dt} = \frac{d}{dt}\frac{\theta_*(D_tL_0)^2}{8\omega^2(y_0)}, \tag{29b}$$

$$\frac{d\bar{y}_2}{dt} = \bar{p}_2 - \frac{\theta_* D_yL_0 D_tL_0}{4\omega(y_0)}, \tag{29c}$$

$$\frac{d\bar{p}_2}{dt} = -\omega'(y_0)\bar{\theta}_2 - \theta_*\omega''(y_0)\bar{y}_2 - \frac{\theta_*^2 D_yL_0 D_y^2L_0}{8} + \frac{\theta_* D_tL_0 D_t D_yL_0}{4\omega(y_0)}, \tag{29d}$$

with ε*-independent initial values*

$$\bar{\phi}_2(0) = -[\phi_2]^\varepsilon(0), \qquad \bar{\theta}_2(0) = -[\theta_2]^\varepsilon(0), \qquad \bar{y}_2(0) = -[y_2]^\varepsilon(0), \qquad \bar{p}_2(0) = -[p_2]^\varepsilon(0). \tag{30}$$

The results in Theorem 3.2 are central in two different ways. Firstly, it will be crucial for the thermodynamic interpretation we develop in the second part of this article. Secondly, it is interesting for computational purposes. That is, in simulating a natural evolution of a light particle coupled to a heavy particle, their mass ratio ε will be small but finite and enters into the underlying model through potentials of different strengths. The result above says that rather than solving the coupled system directly, which is restricted to a small step size to ensure numerical stability, the approximation to second-order can be computed by combining explicitly known oscillatory functions (as given in Definition 3.1) with the solution of a linear inhomogeneous system of differential equations, as given in Theorem 3.2.

The proof of Theorem 3.2 is given in the next section. We remark that we will give a thermodynamic interpretation for the equations (29c) and (29d) governing the evolution of the slow particle, in terms of a constraining second-order energy expression. This formulation is given in (53) in Theorem 4.1 below.

At last, we want to give an alternative formulation of the uniform convergence results in Theorem 3.2 in terms of a nonlinear version of two-scale convergence. Appendix A gives a brief introduction to two-scale convergence, including the definition of two-scale convergence with respect to the nonlinear transformation $\phi_0^{-1} \circ \pi$.

Corollary 3.3. *With the notation introduced in Appendix A, the uniform convergences in Theorem 3.2 are equivalent to the following strong two-scale convergences with respect to* $\phi_0^{-1} \circ \pi$*:*

$$\phi_2^\varepsilon \xrightarrow[2]{\phi_0^{-1}\circ\pi} \bar{\phi}_2 + [\phi_2] \quad in \quad C([0,T]\times\mathcal{S}), \qquad \theta_2^\varepsilon \xrightarrow[2]{\phi_0^{-1}\circ\pi} \bar{\theta}_2 + [\theta_2] \quad in \quad C([0,T]\times\mathcal{S}),$$

$$y_2^\varepsilon \xrightarrow[2]{\phi_0^{-1}\circ\pi} \bar{y}_2 + [y_2] \quad in \quad C([0,T]\times\mathcal{S}), \qquad p_2^\varepsilon \xrightarrow[2]{\phi_0^{-1}\circ\pi} \bar{p}_2 + [p_2] \quad in \quad C([0,T]\times\mathcal{S}),$$

$$\theta_1^\varepsilon \xrightarrow[2]{\phi_0^{-1}\circ\pi} [\theta_1] \quad in \quad C([0,T]\times\mathcal{S}),$$

where $(\bar{\phi}_2, \bar{\theta}_2, \bar{y}_2, \bar{p}_2)$ *is the unique solution to the initial value problem* (29)–(30) *and where for* $t \in [0,T]$ *and* $s \in \mathcal{S}$ *we define*

$$[\theta_1](t,s) \coloneqq -\frac{\theta_* D_tL_0(t)}{2\omega(y_0(t))}\sin(2\pi s), \qquad [\phi_2](t,s) \coloneqq -\frac{D_tL_0(t)}{4\omega(y_0(t))}\cos(2\pi s),$$

$$[y_2](t,s) \coloneqq -\frac{\theta_* D_yL_0(t)}{4\omega(y_0(t))}\cos(2\pi s), \qquad [p_2](t,s) \coloneqq \frac{d}{dt}\left(\frac{\theta_* D_yL_0(t)}{4\omega(y_0(t))}\right)\cos(2\pi s)$$

and

$$[\theta_2](t,s) \coloneqq -\theta_* D_yL_0(t)[y_2](t,s) - \frac{p_0(t)}{\omega(y_0(t))}[p_2](t,s) + \frac{\theta_*^2(D_yL_0(t))^2}{16\omega(y_0(t))}\cos(4\pi s) - \frac{\theta_* D_tL_0(t)}{\omega(y_0(t))}\bar{\phi}_2(t)\cos(2\pi s).$$

Proof. The equivalence follows from Theorem 3.2 and [21, Proposition 2.4]. □

3.4 Proof of Theorem 3.2

This section comprises lemmas that collectively prove Theorem 3.2. They are stated separately but should be understood in the context of Theorem 3.2 above.

Lemma 3.4. *There exists* $0 < C < \infty$ *and* $0 < \varepsilon_0 < \infty$*, where* $\varepsilon_0 = \varepsilon_0(\phi_*, \theta_*, y_*, p_*, \omega, C)$*, such that* $0 < C \leq \dot{\phi}_\varepsilon$ *for all* $0 < \varepsilon < \varepsilon_0$ *small enough.*

Proof. The claim follows directly from (7) and (22a). □

Remark. Henceforth we assume that $0 < \varepsilon < \varepsilon_0$ is small enough, so that the conclusion of Lemma 3.4 applies.

Lemma 3.5. *Let $\{u_\varepsilon\}$ and $\{\psi_\varepsilon\}$ be bounded sequences in $C^{0,1}([0,T])$ and $C^{1,1}([0,T])$ respectively and $0 < C \leq \dot{\psi}_\varepsilon$. Then, for all $a, b \in [0,T]$*

$$\int_a^b u_\varepsilon \sin(\varepsilon^{-1}\psi_\varepsilon)\,\mathrm{d}t = \mathcal{O}(\varepsilon), \qquad \int_a^b u_\varepsilon \cos(\varepsilon^{-1}\psi_\varepsilon)\,\mathrm{d}t = \mathcal{O}(\varepsilon).$$

Proof. Integration by parts gives for $0 < \varepsilon < \varepsilon_0$ small enough

$$\left|\int_a^b u_\varepsilon \exp\left(\frac{i\psi_\varepsilon}{\varepsilon}\right)\,\mathrm{d}t\right| \leq \varepsilon\left|\frac{u_\varepsilon(a)}{\dot{\psi}_\varepsilon(a)}\right| + \varepsilon\left|\frac{u_\varepsilon(b)}{\dot{\psi}_\varepsilon(b)}\right| + \varepsilon\left|\int_a^b \frac{d}{dt}\left(\frac{u_\varepsilon}{\dot{\psi}_\varepsilon}\right)\exp\left(\frac{i\psi_\varepsilon}{\varepsilon}\right)\,\mathrm{d}t\right| = \mathcal{O}(\varepsilon).$$

The claim follows by considering real and imaginary part separately and the isometric isomorphism [8, p. 154]

$$C^{k-1,1}([0,T]) \cong W^{k,\infty}((0,T)).$$

□

Lemma 3.6. *Let $u \in C^2(\mathbb{R}_{>0} \times \mathbb{R}^3)$ and $(\phi_\varepsilon, \theta_\varepsilon, y_\varepsilon, p_\varepsilon)$ be the solution to (16)–(17). Then, the sequence of functions $\{u_\varepsilon\}$, where $u_\varepsilon \coloneqq u(\dot{\phi}_\varepsilon, \theta_\varepsilon, \dot{y}_\varepsilon, y_\varepsilon)$, satisfies for all $a, b \in [0,T]$*

$$\int_a^b \dot{u}_\varepsilon \cos(2\varepsilon^{-1}\phi_\varepsilon)\,\mathrm{d}t \to \frac{1}{2}\int_a^b \left[D_t L_0\left(\omega(y_0)\partial_1 u_0 - \theta_* \partial_2 u_0\right) + \theta_* \omega'(y_0)\partial_3 u_0\right]\,\mathrm{d}t$$

and

$$\int_a^b \dot{u}_\varepsilon \sin(2\varepsilon^{-1}\phi_\varepsilon)\,\mathrm{d}t = \mathcal{O}(\varepsilon).$$

Proof. The equations in (22) imply after some calculations that

$$\begin{aligned}\dot{u}_\varepsilon = {} & \partial_1 u_\varepsilon\left(\dot{y}_\varepsilon \omega'(y_\varepsilon) + \frac{\varepsilon}{2} D_t^2 L_\varepsilon \sin(2\varepsilon^{-1}\phi_\varepsilon) + D_t L_\varepsilon \dot{\phi}_\varepsilon \cos(2\varepsilon^{-1}\phi_\varepsilon)\right) - \partial_2 u_\varepsilon \theta_\varepsilon D_t L_\varepsilon \cos(2\varepsilon^{-1}\phi_\varepsilon) \\ & - \partial_3 u_\varepsilon\left(\theta_\varepsilon \omega'(y_\varepsilon) - \theta_\varepsilon \omega'(y_\varepsilon)\cos(2\varepsilon^{-1}\phi_\varepsilon)\right) + \partial_4 u_\varepsilon \dot{y}_\varepsilon.\end{aligned}$$

The claim follows from the uniform convergence results in (19), Lemma 3.5 and the trigonometric identities

$$2\cos(x)\cos(y) = \cos(x+y) + \cos(x-y), \qquad 2\cos(x)\sin(y) = \sin(x+y) - \sin(x-y).$$

□

Lemma 3.7. *The sequences $\{\theta_1^\varepsilon\}$, $\{\phi_2^\varepsilon\}$, $\{y_2^\varepsilon\}$ and $\{p_2^\varepsilon\}$ are uniformly bounded in $L^\infty((0,T))$.*

Proof. In the following proof, the constant $0 \leq C < \infty$ is dependent on T but independent of ε and can take on different values from line to line. Let $t \in [0,T]$ and $0 < \varepsilon < \varepsilon_0$ small enough and let

$$M_1 \coloneqq \sup_{0<\varepsilon<\varepsilon_0}\sup_{h\in[0,1]} \|\omega'((1-h)y_\varepsilon + hy_0)\|_{L^\infty((0,T))}, \qquad M_2 \coloneqq \sup_{0<\varepsilon<\varepsilon_0}\sup_{h\in[0,1]} \|\omega''((1-h)y_\varepsilon + hy_0)\|_{L^\infty((0,T))}.$$

We apply Lemma 3.5 to equation (22a),

$$|\phi_2^\varepsilon(t)| = \left|\int_0^t \dot{\phi}_2^\varepsilon\,\mathrm{d}s\right| \leq \frac{1}{\varepsilon^2}\left|\int_0^t \omega(y_\varepsilon) - \omega(y_0)\,\mathrm{d}s\right| + \frac{1}{2\varepsilon}\left|\int_0^t D_s L_\varepsilon \sin(2\varepsilon^{-1}\phi_\varepsilon)\,\mathrm{d}s\right| \leq M_1 \int_0^t |y_2^\varepsilon|\,\mathrm{d}s + C, \tag{31}$$

then to equation (22b),

$$|\theta_1^\varepsilon(t)| = \left|\int_0^t \dot{\theta}_1^\varepsilon\,\mathrm{d}s\right| = \frac{1}{\varepsilon}\left|\int_0^t \theta_\varepsilon D_s L_\varepsilon \cos(2\varepsilon^{-1}\phi_\varepsilon)\,\mathrm{d}s\right| \leq C, \tag{32}$$

to equation (22c),

$$|y_2^\varepsilon(t)| = \left|\int_0^t \dot{y}_2^\varepsilon\,\mathrm{d}s\right| \leq \int_0^t |p_2^\varepsilon|\,\mathrm{d}s + \frac{1}{2\varepsilon}\left|\int_0^t \theta_\varepsilon D_y L_\varepsilon \sin(2\varepsilon^{-1}\phi_\varepsilon)\,\mathrm{d}s\right| \leq \int_0^t |p_2^\varepsilon|\,\mathrm{d}s + C, \tag{33}$$

and finally to equation (22d),

$$|p_2^\varepsilon(t)| = \left|\int_0^t \dot{p}_2^\varepsilon \,\mathrm{d}s\right| \le \frac{1}{\varepsilon^2}\left|\int_0^t \theta_\varepsilon \omega'(y_\varepsilon) - \theta_* \omega'(y_0)\,\mathrm{d}s\right| + \frac{1}{2\varepsilon}\left|\int_0^t \theta_\varepsilon D_s D_y L_\varepsilon \sin(2\varepsilon^{-1}\phi_\varepsilon)\,\mathrm{d}s\right|$$
$$\le \frac{1}{\varepsilon}\left|\int_0^t \omega'(y_\varepsilon)\theta_1^\varepsilon \,\mathrm{d}s\right| + \frac{\theta_*}{\varepsilon^2}\left|\int_0^t \omega'(y_\varepsilon) - \omega'(y_0)\,\mathrm{d}s\right| + C$$
$$\le \frac{1}{\varepsilon}\left|\int_0^t \omega'(y_\varepsilon)\theta_1^\varepsilon \,\mathrm{d}s\right| + \theta_* M_2 \int_0^t |y_2^\varepsilon| \,\mathrm{d}s + C. \tag{34}$$

Furthermore, integration by parts in combination with equation (22b) and Lemma 3.5 and 3.6 imply

$$\frac{1}{\varepsilon}\left|\int_0^t \omega'(y_\varepsilon)\theta_1^\varepsilon \,\mathrm{d}s\right| = \frac{1}{\varepsilon}\left|\int_0^t \omega'(y_\varepsilon)\int_0^s \dot{\theta}_1^\varepsilon \,\mathrm{d}r\,\mathrm{d}s\right| = \frac{1}{\varepsilon^2}\left|\int_0^t \omega'(y_\varepsilon)\int_0^s \theta_\varepsilon D_r L_\varepsilon \cos(2\varepsilon^{-1}\phi_\varepsilon)\,\mathrm{d}r\,\mathrm{d}s\right|$$
$$\le \frac{1}{2\varepsilon}\left|\int_0^t \frac{\theta_\varepsilon D_s L_\varepsilon}{\dot{\phi}_\varepsilon}\omega'(y_\varepsilon)\sin(2\varepsilon^{-1}\phi_\varepsilon)\,\mathrm{d}s\right| + \frac{1}{2\varepsilon}\left|\int_0^t \omega'(y_\varepsilon)\int_0^s \frac{d}{dr}\left(\frac{\theta_\varepsilon D_r L_\varepsilon}{\dot{\phi}_\varepsilon}\right)\sin(2\varepsilon^{-1}\phi_\varepsilon)\,\mathrm{d}r\,\mathrm{d}s\right| \le C. \tag{35}$$

By combining the inequalities (33)–(35) we obtain

$$|y_2^\varepsilon(t)| \le C + \theta_* M_2 \int_0^T \int_0^T |y_2^\varepsilon| \,\mathrm{d}r\,\mathrm{d}s.$$

Finally, a variation of the classical Grönwall inequality (see [14, p. 383]) implies that

$$|y_2^\varepsilon(t)| \le C\exp\left(\theta_* M_2 T^2\right),$$

for $t \in [0,T]$, which together with (31)–(35) yields the uniform bound for $\{\theta_1^\varepsilon\}$, $\{\phi_2^\varepsilon\}$, $\{y_2^\varepsilon\}$ and $\{p_2^\varepsilon\}$. □

Lemma 3.8. *The sequence $\{\theta_2^\varepsilon\}$ is uniformly bounded in $L^\infty((0,T))$.*

Proof. According to Lemma 3.7, the sequences $\{\theta_1^\varepsilon\}$, $\{\phi_2^\varepsilon\}$, $\{y_2^\varepsilon\}$ and $\{p_2^\varepsilon\}$ are uniformly bounded in $L^\infty((0,T))$. Therefore, writing

$$\theta_\varepsilon = \theta_* + \varepsilon\theta_1^\varepsilon, \qquad \phi_\varepsilon = \phi_0 + \varepsilon^2\phi_2^\varepsilon, \qquad y_\varepsilon = y_0 + \varepsilon^2 y_2^\varepsilon, \qquad p_\varepsilon = p_0 + \varepsilon^2 p_2^\varepsilon$$

and expanding the energy function (15) up to second-order in ε gives $E_\varepsilon = E_0 + \varepsilon E_1^\varepsilon + \mathcal{O}(\varepsilon^2)$ with

$$E_0 \coloneqq \frac{1}{2}p_0^2 + \theta_*\omega(y_0), \qquad E_1^\varepsilon \coloneqq \omega(y_0)\theta_1^\varepsilon + \frac{\theta_* D_t L_0}{2}\sin(2\varepsilon^{-1}\phi_0),$$

for $0 < \varepsilon < \varepsilon_0$ small enough. According to (20), the energy E_0 is constant. It follows from (9) that $E_\varepsilon = E_0 = E_*$ and thus $E_1^\varepsilon = \mathcal{O}(\varepsilon)$. This yields the claim as

$$\theta_1^\varepsilon - [\theta_1]^\varepsilon = \mathcal{O}(\varepsilon).$$

□

Due to the oscillatory character of the problem, Lemma 3.8 shows that the first-order asymptotic expansion in θ_ε is expressed by a high-frequency term which represents small-scale oscillations of order ε. Averaging over these oscillations, that is, taking the weak* limit shows that on average θ_1^ε has zero effect on the first-order macro-scale dynamics. In the following, Lemma 3.9, 3.10 and 3.11 provide information about the decomposition of the second-order asymptotic expansion of $\phi_\varepsilon, \theta_\varepsilon, y_\varepsilon$ and p_ε into high-frequency terms with zero average contribution and terms with non-zero average contribution, specifying the macro-scale dynamics to second-order.

Lemma 3.9. *Let $u_0, \psi_0 \in C^1([0,T])$ and let $\{u_\varepsilon\}, \{\psi_\varepsilon\}$ be sequences in $C^1([0,T])$ such that the sequences $\{\dot{u}_\varepsilon\}$, $\{\varepsilon^{-1}(u_\varepsilon - u_0)\}$, $\{\varepsilon^{-2}(\psi_\varepsilon - \psi_0)\}$ and $\{\varepsilon^{-1}(\dot{\psi}_\varepsilon - \dot{\psi}_0)\}$ are bounded in $L^\infty((0,T))$. Then for v_ε such that*

$$v_\varepsilon \coloneqq u_\varepsilon\cos(\varepsilon^{-1}\psi_\varepsilon) - u_0\cos(\varepsilon^{-1}\psi_0),$$

the sequence $\{\varepsilon^{-1}v_\varepsilon\}$ is bounded in $L^\infty((0,T))$ and in particular

$$v_\varepsilon \to 0 \quad \text{in} \quad C([0,T]), \qquad \dot{v}_\varepsilon \overset{*}{\rightharpoonup} 0 \quad \text{in} \quad L^\infty((0,T)).$$

Proof. By writing

$$w_\varepsilon \coloneqq (u_\varepsilon - u_0)\exp(i\varepsilon^{-1}\psi_\varepsilon) - u_0\exp(i\varepsilon^{-1}\psi_0)(1-\exp(i\varepsilon^{-1}(\psi_\varepsilon-\psi_0)))$$

and

$$\begin{aligned}\dot{w}_\varepsilon = &\Big((\dot{u}_\varepsilon - \dot{u}_0) + i\varepsilon^{-1}\dot{\psi}_\varepsilon(u_\varepsilon-u_0) + i\varepsilon^{-1}u_0(\dot{\psi}_\varepsilon-\dot{\psi}_0)\Big)\exp(i\varepsilon^{-1}\psi_\varepsilon)\\ &-(\dot{u}_0 + i\varepsilon^{-1}u_0\dot{\psi}_0)(1-\exp(i\varepsilon^{-1}(\psi_\varepsilon-\psi_0)))\exp(i\varepsilon^{-1}\psi_0),\end{aligned}$$

the assumptions imply that the sequences $\{\varepsilon^{-1}w_\varepsilon\}$ and $\{\dot{w}_\varepsilon\}$ are bounded in $L^\infty((0,T),\mathbb{C})$, which yields directly the uniform convergence of $v_\varepsilon = \Re(w_\varepsilon)$ to zero. The weak* convergence of $\dot{v}_\varepsilon = \Re(\dot{w}_\varepsilon)$ follows from [6, Principle 1, Chapter I §1]. □

Remark. Lemma 3.8 and Lemma 3.9 imply the convergence (24).

Lemma 3.10. *There exists a subsequence $\{\varepsilon'\}$ and functions $\bar{\phi}_2$, $\bar{y}_2$, $\bar{p}_2 \in C^{0,1}([0,T])$ such that the convergences* (25)–(27) *hold.*

Proof. By taking the time derivative of the functions $\phi_2^\varepsilon - [\phi_2]^\varepsilon$, $y_2^\varepsilon - [y_2]^\varepsilon$ and $p_2^\varepsilon - [p_2]^\varepsilon$, we obtain

$$\frac{d}{dt}\left(\phi_2^\varepsilon - [\phi_2]^\varepsilon\right) = \frac{\omega(y_\varepsilon)-\omega(y_0)}{\varepsilon^2} + \frac{d}{dt}\left(\frac{D_tL_\varepsilon}{4\dot{\phi}_\varepsilon}\right)\cos(2\varepsilon^{-1}\phi_\varepsilon) - \frac{d}{dt}\left([\phi_2]^\varepsilon + \frac{D_tL_\varepsilon}{4\dot{\phi}_\varepsilon}\cos(2\varepsilon^{-1}\phi_\varepsilon)\right), \tag{36}$$

$$\frac{d}{dt}\left(y_2^\varepsilon - [y_2]^\varepsilon\right) = \frac{p_\varepsilon - p_0}{\varepsilon^2} + \frac{d}{dt}\left(\frac{\theta_\varepsilon D_yL_\varepsilon}{4\dot{\phi}_\varepsilon}\right)\cos(2\varepsilon^{-1}\phi_\varepsilon) - \frac{d}{dt}\left([y_2]^\varepsilon + \frac{\theta_\varepsilon D_yL_\varepsilon}{4\dot{\phi}_\varepsilon}\cos(2\varepsilon^{-1}\phi_\varepsilon)\right), \tag{37}$$

$$\begin{aligned}\frac{d}{dt}\left(p_2^\varepsilon - [p_2]^\varepsilon\right) = &-\theta_*\frac{\omega'(y_\varepsilon)-\omega'(y_0)}{\varepsilon^2} - \frac{\theta_1^\varepsilon - [\theta_1]^\varepsilon}{\varepsilon}\omega'(y_\varepsilon)\\ &-\frac{d}{dt}\left(\frac{\theta_\varepsilon D_tD_yL_\varepsilon}{4\dot{\phi}_\varepsilon}\right)\cos(2\varepsilon^{-1}\phi_\varepsilon) - \frac{d}{dt}\left([p_2]_1^\varepsilon - \frac{\theta_\varepsilon D_tD_yL_\varepsilon}{4\dot{\phi}_\varepsilon}\cos(2\varepsilon^{-1}\phi_\varepsilon)\right)\\ &+\frac{d}{dt}\left(\frac{\theta_*D_tL_0}{4\omega^2(y_0)}\omega'(y_\varepsilon)\right)\cos(2\varepsilon^{-1}\phi_0) - \frac{d}{dt}\left([p_2]_2^\varepsilon + \frac{\theta_*D_tL_0}{4\omega^2(y_0)}\omega'(y_\varepsilon)\cos(2\varepsilon^{-1}\phi_0)\right),\end{aligned} \tag{38}$$

where we write $[p_2]^\varepsilon = [p_2]_1^\varepsilon + [p_2]_2^\varepsilon$ with

$$[p_2]_1^\varepsilon \coloneqq \frac{\theta_*D_tD_yL_0}{4\omega(y_0)}\cos(2\varepsilon^{-1}\phi_0), \qquad [p_2]_2^\varepsilon \coloneqq -\frac{\theta_*D_tL_0D_yL_0}{4\omega(y_0)}\cos(2\varepsilon^{-1}\phi_0).$$

For the derivation of equation (38), we note that in

$$\frac{dp_2^\varepsilon}{dt} = -\theta_*\frac{\omega'(y_\varepsilon)-\omega'(y_0)}{\varepsilon^2} - \frac{\theta_\varepsilon-\theta_*}{\varepsilon^2}\omega'(y_\varepsilon) - \frac{d}{dt}\left(\frac{\theta_\varepsilon D_tD_yL_\varepsilon}{4\dot{\phi}_\varepsilon}\right)\cos(2\varepsilon^{-1}\phi_\varepsilon) + \frac{d}{dt}\left(\frac{\theta_\varepsilon D_tD_yL_\varepsilon}{4\dot{\phi}_\varepsilon}\cos(2\varepsilon^{-1}\phi_\varepsilon)\right),$$

we can rewrite the second term on the right hand side by introducing $[\theta_1]^\varepsilon$, i.e.,

$$\frac{\theta_\varepsilon-\theta_*}{\varepsilon^2}\omega'(y_\varepsilon) = \frac{\theta_1^\varepsilon - [\theta_1]^\varepsilon}{\varepsilon}\omega'(y_\varepsilon) - \frac{d}{dt}\left(\frac{\theta_*D_tL_0}{4\omega^2(y_0)}\omega'(y_\varepsilon)\right)\cos(2\varepsilon^{-1}\phi_0) + \frac{d}{dt}\left(\frac{\theta_*D_tL_0}{4\omega^2(y_0)}\omega'(y_\varepsilon)\cos(2\varepsilon^{-1}\phi_0)\right).$$

By Lemma 3.7, 3.8 and 3.9, the sequences $\{\phi_2^\varepsilon - [\phi_2]^\varepsilon\}, \{y_2^\varepsilon - [y_2]^\varepsilon\}$ and $\{p_2^\varepsilon - [p_2]^\varepsilon\}$ are bounded in the space $C^{0,1}([0,T])$ of uniformly Lipschitz continuous functions. The claim follows after successive applications of [6, Principle 4, Chapter I §1]. □

Lemma 3.11. *Under the subsequence extracted in Lemma 3.10, we obtain the convergence* (28)*, where $\bar{\theta}_2$ is of the form*

$$\bar{\theta}_2 = -\frac{p_0}{\omega(y_0)}\bar{p}_2 - \theta_*D_yL_0\bar{y}_2 - \frac{\theta_*^2(D_yL_0)^2}{16\omega(y_0)} + \frac{\theta_*(D_tL_0)^2}{4\omega^2(y_0)}. \tag{39}$$

Proof. By Lemma 3.10 we can write

$$\begin{aligned}\phi_\varepsilon &= \phi_0 + \varepsilon^2\left(\bar{\phi}_2 + [\phi_2]^\varepsilon\right) + \varepsilon^2\phi_3^\varepsilon, & y_\varepsilon &= y_0 + \varepsilon^2\left(\bar{y}_2 + [y_2]^\varepsilon\right) + \varepsilon^2 y_3^\varepsilon,\\ \theta_\varepsilon &= \theta_* + \varepsilon[\theta_1]^\varepsilon + \varepsilon^2\theta_2^\varepsilon, & p_\varepsilon &= p_0 + \varepsilon^2\left(\bar{p}_2 + [p_2]^\varepsilon\right) + \varepsilon^2 p_3^\varepsilon,\end{aligned}$$

where $\phi_3^\varepsilon, y_3^\varepsilon, p_3^\varepsilon \to 0$ in $C([0,T])$. An expansion of the energy function (15) up to second-order in ε gives $E_\varepsilon = E_0 + \varepsilon E_1^\varepsilon + \varepsilon^2 E_2^\varepsilon + \varepsilon^2 E_3^\varepsilon$, where $E_3^\varepsilon \to 0$ in $C([0,T])$ and

$$\begin{aligned}
E_0 &\coloneqq \frac{1}{2}p_0^2 + \theta_* \omega(y_0),\\
E_1^\varepsilon &\coloneqq \omega(y_0)[\theta_1]^\varepsilon + \frac{\theta_* p_0 \omega'(y_0)}{2\omega(y_0)} \sin(2\varepsilon^{-1}\phi_0),\\
E_2^\varepsilon &\coloneqq p_0\left(\bar{p}_2 + [p_2]^\varepsilon\right) + \theta_* \omega'(y_0)\left(\bar{y}_2 + [y_2]^\varepsilon\right) + \omega(y_0)\theta_2^\varepsilon + \frac{\theta_*^2 (D_y L_0)^2}{8}\sin^2(2\varepsilon^{-1}\phi_0)\\
&\quad + \theta_* D_t L_0\left(\bar{\phi}_2 + [\phi_2]^\varepsilon\right)\cos(2\varepsilon^{-1}\phi_0) + \frac{[\theta_1]^\varepsilon D_t L_0}{2}\sin(2\varepsilon^{-1}\phi_0)\\
&= \omega(y_0)\left(\theta_2^\varepsilon - [\theta_2]^\varepsilon - \bar{\theta}_2\right).
\end{aligned}$$

It follows from (9) that $E_\varepsilon = E_0 = E_*$ and by Lemma 3.8 that $E_1^\varepsilon = 0$. This implies that $E_2^\varepsilon + E_3^\varepsilon = 0$ and hence $E_2^\varepsilon = -E_3^\varepsilon \to 0$ in $C([0,T])$. The claim follows with the identity

$$\theta_* D_t L_0 [\phi_2]^\varepsilon \cos(2\varepsilon^{-1}\phi_0) + \frac{[\theta_1]^\varepsilon D_t L_0}{2}\sin(2\varepsilon^{-1}\phi_0) = -\frac{\theta_*(D_t L_0)^2}{4\omega(y_0)}.$$

□

Lemma 3.12. *The extraction of a subsequence in Lemma 3.10 can be discarded altogether and* $(\bar{\phi}_2, \bar{\theta}_2, \bar{y}_2, \bar{p}_2)$ *is the unique solution to the initial value problem* (29)–(30).

Proof. The differential equations (29a), (29c) and (29d) follow from (25)–(27) by taking the weak* limit in combination with Lemma 3.6 and Lemma 3.9 and [6, Lemma 1, Chapter I §1]. To prove formula (29b), we differentiate equation (39) with respect to time and use equation (29c) and (29d) together with

$$D_t^2 L_0 = -\theta_* \omega'(y_0) D_y L_0 + \dot{y}_0^2 D_y^2 L_0.$$

The initial values (30) can be derived from the uniform convergence in (25)–(28). Furthermore, since the right-hand side of (29) — and therefore the solution $(\bar{\phi}_2, \bar{\theta}_2, \bar{y}_2, \bar{p}_2) \in C^\infty([0,T], \mathbb{R}^4)$ — does not depend on the chosen subsequence, [6, Principle 5, Chapter I §1] allows us to discard the extraction of subsequences altogether. □

4 Thermodynamic expansion and interpretation

We now give a thermodynamic interpretation of the analytic result presented in Theorem 3.2. Thermodynamic effects can in principle occur when a separation of scales exist; Hertz [10] developed a thermodynamic theory for Hamiltonian systems with slowly varying external parameter [10]. The model considered in this article is an example of this kind if we restrict the analysis to the fast particle (variable z_ε) and consider the slow particle (variable y_ε) as an external parameter. The question we want to address in this section is "Can we replace the dynamics of the fast particle by a thermodynamic description in terms of temperature and entropy?" An answer to this question could potentially lead to new algorithms that reduce the computational complexity of large-scale molecular dynamics simulations either by allowing for a larger step size or a reduction of the system's dimensions. Although a larger step size can be used to integrate the system of differential equations (29), which decreases the computational complexity, a reduction in the dimension of the model problem is not expected because a new algorithm would only involve a substitution of two degrees of freedom, i.e., the generalised position and momentum of one particle, by two thermodynamic state variables. Nonetheless, we study this problem to develop a first thermodynamic understanding. As it turns out, even in this simple model problem, an interesting adiabatic/non-adiabatic characteristic emerges through a higher-order asymptotic expansion.

For a thermodynamic interpretation of the system, we will regard the fast particle z_ε as a heat bath acting on the slow particle y_ε. As such, we will mainly focus our thermodynamic analysis on the energy associated with the fast particle, which we call in the following the *heat bath energy* $E_\varepsilon^\perp$, in contrast to the residual energy, which we call the *environmental energy* $E_\varepsilon^\parallel$. Both energies can be read of from the total energy (9), i.e.,

$$E_\varepsilon^\perp = \tfrac{1}{2}\dot{z}_\varepsilon^2 + \tfrac{1}{2}\varepsilon^{-2}\omega^2(y_\varepsilon) z_\varepsilon^2, \qquad E_\varepsilon^\parallel = E_\varepsilon - E_\varepsilon^\perp. \tag{40}$$

Note that the evolution of the fast degree of freedom z_ε is governed by the energy $E_\varepsilon^\perp = E_\varepsilon^\perp(z_\varepsilon, \dot{z}_\varepsilon; y_\varepsilon)$, which is subject to a dynamically varying external parameter given by the evolution of the slow degree of freedom y_ε. This framework allows us to apply the theory developed by Hertz [5]. From a lengthy analysis, which we describe in the Appendix B, we derive for $\varepsilon > 0$ the following expressions for the *temperature* T_ε, the *entropy* S_ε and the *external force* F_ε in the fast subsystem:

$$T_\varepsilon = \theta_\varepsilon \omega(y_\varepsilon), \qquad S_\varepsilon = \log(\theta_\varepsilon) + C, \qquad F_\varepsilon = \theta_\varepsilon \omega'(y_\varepsilon). \tag{41}$$

In combination with the second-order expansion derived in Theorem 3.2 we will analyse the asymptotic properties of the thermodynamic expressions (41) above, by expanding $T_\varepsilon = T_0 + \mathcal{O}(\varepsilon)$, $F_\varepsilon = F_0 + \mathcal{O}(\varepsilon)$ and $S_\varepsilon = S_0 + \varepsilon[\bar{S}_1]^\varepsilon + \varepsilon^2[\bar{S}_2]^\varepsilon + \varepsilon^2 S_3^\varepsilon$ with $S_3^\varepsilon \to 0$ in $C([0,T])$, where

$$T_0 \coloneqq \theta_* \omega(y_0), \qquad F_0 \coloneqq \theta_* \omega'(y_0) \tag{42}$$

and

$$S_0 \coloneqq \log(\theta_*) + C, \qquad [\bar{S}_1]^\varepsilon \coloneqq \frac{[\theta_1]^\varepsilon}{\theta_*}, \qquad [\bar{S}_2]^\varepsilon \coloneqq \frac{\bar{\theta}_2 + [\theta_2]^\varepsilon}{\theta_*} - \frac{1}{2}\left(\frac{[\theta_1]^\varepsilon}{\theta_*}\right)^2. \tag{43}$$

Analogously, we expand the energy of the fast subsystem $E_\varepsilon^\perp = \theta_\varepsilon \omega(y_\varepsilon) = E_0^\perp + \varepsilon[\bar{E}_1^\perp]^\varepsilon + \varepsilon^2[\bar{E}_2^\perp]^\varepsilon + \varepsilon^2 E_3^{\perp\varepsilon}$ where $E_3^{\perp\varepsilon} \to 0$ in $C([0,T])$ and

$$E_0^\perp \coloneqq \theta_* \omega(y_0), \qquad [\bar{E}_1^\perp]^\varepsilon \coloneqq \omega(y_0)\,[\theta_1]^\varepsilon, \qquad [\bar{E}_2^\perp]^\varepsilon \coloneqq \theta_* \omega'(y_0)\,(\bar{y}_2 + [y_2]^\varepsilon) + \omega(y_0)\left(\bar{\theta}_2 + [\theta_2]^\varepsilon\right). \tag{44}$$

4.1 Leading-order thermodynamics: constant entropy

We show in this section, following Bornemann [6], that to leading-order (limit $\varepsilon \to 0$), the resulting thermodynamic process is adiabatic or in other words a thermodynamic process with constant entropy.

4.1.1 Thermodynamics of the limit process

As an aside, we briefly sketch how the thermodynamic nature of the problem considered in this article materialises in the thermodynamic principles that underpin the proof of Theorem 1.1. This observation is independent of the conclusions we will draw about the adiabatic nature of the limit process.

Firstly, the proof in [6] uses the equi-partitioning of the heat bath energy $E_\varepsilon^\perp$ in the weak* limit. To illustrate this, we consider the quantity $\Xi_\varepsilon \coloneqq \dot{z}_\varepsilon z_\varepsilon$, which is of order ε and hence converges uniformly to zero. Its time derivative is given by

$$\dot{\Xi}_\varepsilon = \ddot{z}_\varepsilon z_\varepsilon + \dot{z}_\varepsilon^2 = -\varepsilon^{-2}\omega^2(y_\varepsilon) z_\varepsilon^2 + \dot{z}_\varepsilon^2 = -2U_\varepsilon^\perp + 2K_\varepsilon^\perp, \tag{45}$$

where $U_\varepsilon^\perp$ is the potential and $K_\varepsilon^\perp$ kinetic energy of the fast degree of freedom. It follows from [6, Principle 1, Chapter I §1] that (45) converges weakly* to $0 = -U_0^\perp + K_0^\perp$, which implies the equipartition of the energy $E_0^\perp$ into kinetic and potential energy, i.e., $U_0^\perp = \frac{1}{2}E_0^\perp$ and $K_0^\perp = \frac{1}{2}E_0^\perp$.

Secondly, the proof in [6] utilises the adiabatic invariance of the action $\theta_\varepsilon \to \theta_*$ in the limit $\varepsilon \to 0$, see (19b). The action, which was used in the transformation into action-angle variables (14), takes the form of the energy-frequency ratio $\theta_\varepsilon = E_\varepsilon^\perp/\omega(y_\varepsilon)$. Since the time evolution of the energy $E_\varepsilon^\perp$ and the external variable y_ε are in general independent, the adiabatic invariance of the action reveals their dependence in the limit $\varepsilon \to 0$, as $\theta_* = E_0^\perp/\omega(y_0)$.

4.1.2 Leading-order thermodynamics: Adiabatic invariance

The concept of adiabatic invariance finds applications in the analysis of slowly perturbed dynamical systems, where one is primarily interested in the derivation of the effective evolution of the system. It emerged in celestial mechanics in form of the perturbation theory of Hamiltonian dynamical systems [2, Chapter 10], and can be found in many other fields. In particular, adiabatic invariance plays a key role in thermodynamics. There, *adiabatic processes* are idealised models in the limit of an infinite separation of time-scales and are, by definition, processes with constant entropy. Thus, for adiabatic processes the entropy reveals, similar to above, a dependence of the internal energy E and the external parameter y, as $S(E,y) = \text{const}$. An introduction to the thermodynamic theory as developed by Hertz can be found in Appendix B.

Let us now have a closer look at $\theta_* = \text{const}$. Naturally, every function of $\theta_* = E_0^\perp/\omega(y_0)$ is a constant of motion. On the other hand, every differentiable invariant of motion must be a function of θ_*. This follows from a contradiction argument [5, Chapter 1.5], which we sketch for the reader's convenience. Assume that there is another invariant $S(E_0^\perp, y_0)$ with $\dot{S} = 0$. Then with $E_0^\perp = E_0^\perp(\theta_*, y_0)$ we can write, with slight abuse of the notation, $S(E_0^\perp(\theta_*, y_0), y_0) = S(\theta_*, y_0)$. Taking the time derivative we get

$$0 = \frac{dS}{dt} = \frac{\partial S}{\partial \theta_*}\dot{\theta}_* + \frac{\partial S}{\partial y_0}\dot{y_0} = \frac{\partial S}{\partial y_0}\dot{y_0}.$$

Since in general $\dot{y_0} \neq 0$, it follows that $\partial S/\partial y_0 = 0$ and hence $S = S(\theta_*)$. Therefore, since the entropy is a constant of motion for an adiabatic thermodynamic process, we can conclude that in the limit $\varepsilon \to 0$ the entropy is a function of θ_*, i.e., $S = S(\theta_*)$.

In fact, by comparing this result with the leading-order expansion of the temperature, entropy and external force in the model problem as derived in (42) and (43), i.e.

$$T_0 = \theta_* \omega(y_0), \qquad S_0 = \log(\theta_*) + C, \qquad F_0 = \theta_* \omega'(y_0), \tag{46}$$

we observe, that $S_0 = S_0(\theta_*) = \text{const.}$ and hence reason that the *limit process is adiabatic*. This is in particular a result of the external parameter y_0, which affects the fast system to leading-order only slowly. The energy in the limit $\varepsilon \to 0$ (see equation (44)) is given by $E_0^\perp(y_0) = \theta_* \omega(y_0)$, and therefore (cf. equation (57))

$$dE_0^\perp = F_0 dy_0 + T_0 dS_0 = F_0 dy_0, \tag{47}$$

which coincides with the qualitative intuition presented in Section B.1. Note that by action and reaction, the force exerted on the fast subsystem F_0 is equal but of opposite sign to the force acting on the environment $\ddot{y}_0 = -F_0$ (see also (20)).

4.2 Second-order thermodynamics

4.2.1 Rescaling of the process

Recall that our main goal is the derivation of a higher-order effective evolution of the slow degree of freedom y_ε. With a thermodynamic description, we aim to supplement the most dominant motion of y_ε, i.e. y_0, by an effective description of the interacting fast particle z_ε, which can be thought of as a heat bath acting on y_ε. For the slow degree of freedom, the typical time-scale is of order $\mathcal{O}(1)$, whereas for the fast degree of freedom z_ε it is of order $\mathcal{O}(1/\varepsilon)$. We remark that for the thermodynamic analysis, it is important to shift the viewpoint — while the overarching aim is to derive thermodynamic corrections to the slow sub-system, from a thermodynamic point of view the analysis itself has to focus on the fast system with its exposure to the slow external agent.

To derive this dualistic viewpoint, we introduce a scaling of z_ε in space and time such that its typical time- and length-scale is of order $\mathcal{O}(1)$ and consequently $\dot{y}_\varepsilon = \mathcal{O}(\varepsilon)$. We show in Appendix B that the dynamics of z_ε is then described by a prototypical thermodynamic model, namely a slowly perturbed harmonic oscillator, which is in the limit of an infinite separation of time-scale in thermal equilibrium. Here, in the limit $\varepsilon \to 0$, the change of the external agent y_0 is regarded as infinitely small and the constant value θ_* is geometrically given as the phase space volume enclosed by the energy surface for a fixed value of y_0 (see [5] or [10]). In this context, a thermodynamic process can be defined as a sequence of thermodynamic equilibrium states in which y_0 is static for every instance in time but dynamically changing in the course of the sequence. Such processes are called *quasi-static adiabatic processes* in classical thermodynamics [23, Chapter 1.4]. These processes are characterised by a constant entropy. In contrast, processes with non-constant entropy involve a fast change of the external parameter, as noted in [5, Chapter 1.2].

4.2.2 Higher-order thermodynamic properties

Using this scaling of space and time of z_ε as worked out in Appendix B, we are able to derive the temperature T_0 and external force F_0 based on the time average of certain quantities for fixed energy $E_0^\perp$ and external parameter y_0. To analyse the thermodynamic properties for dynamically changing $E_0^\perp$ and y_0, we will focus on the original scaling as in (40) and regard the evolution as a quasi-static thermodynamic process. Inspired by the equipartitioning of the energy $E_0^\perp$ (see (45)), we take the weak* limit as the corresponding averaging operator in the original scaling to derive thermodynamic quantities.

Therefore, we calculate the average contribution of the higher-order micro-scale oscillations in $E_\varepsilon^\perp$ and S_ε by taking the weak* limit of the asymptotic expansion terms $[\bar{E}_1^\perp]^\varepsilon$, $[\bar{E}_2^\perp]^\varepsilon$, $[\bar{S}_1]^\varepsilon$ and $[\bar{S}_2]^\varepsilon$. This yields

$$[\bar{E}_1^\perp]^\varepsilon \overset{*}{\rightharpoonup} 0 \quad \text{in} \quad L^\infty((0,T)), \qquad [\bar{E}_2^\perp]^\varepsilon \overset{*}{\rightharpoonup} \bar{E}_2^\perp \coloneqq \theta_* \omega'(y_0)\bar{y}_2 + \omega(y_0)\bar{\theta}_2 \quad \text{in} \quad L^\infty((0,T)), \tag{48}$$

$$[\bar{S}_1]^\varepsilon \overset{*}{\rightharpoonup} 0 \quad \text{in} \quad L^\infty((0,T)), \qquad [\bar{S}_2]^\varepsilon \overset{*}{\rightharpoonup} \bar{S}_2 \coloneqq \frac{\bar{\theta}_2}{\theta_*} - \left(\frac{D_t L_0}{4\omega(y_0)}\right)^2 \quad \text{in} \quad L^\infty((0,T)). \tag{49}$$

We can now define the *second-order average heat bath energy* and *entropy* as

$$\bar{E}_\varepsilon^\perp \coloneqq E_0^\perp + \varepsilon^2 \bar{E}_2^\perp, \qquad \bar{S}_\varepsilon \coloneqq S_0 + \varepsilon^2 \bar{\bar{S}}_2, \tag{50}$$

where $\bar{\bar{S}}_2 \coloneqq \bar{\theta}_2/\theta_*$. Note that we do not include the second term of the weak* limit of $[\bar{S}_2]^\varepsilon$ in (49) in the definition of $\bar{\bar{S}}_2$, since this term does not appear in the energy expansion. It describes the effects of the first-order fast dynamics on the second-order dynamics, which does not affect the average second-order energy correction $\bar{E}_2^\perp$.

To analyse the thermodynamic properties of $\bar{E}_\varepsilon^\perp$ for $\varepsilon > 0$, we focus now on the second-order expansion term $\bar{E}_2^\perp$. The appropriate temperature, entropy and external force can be read off from (48) and (49),

$$T_0 = \theta_* \omega(y_0), \qquad \bar{\bar{S}}_2 = \bar{\theta}_2/\theta_*, \qquad F_0 = \theta_* \omega'(y_0). \tag{51}$$

Note that the entropy in this case is *not* constant. This can be explained by the second-order correction of the external parameter y_ε, which exhibits according to Theorem 3.2 a decomposition into a slowly varying component

$\bar{y}_2$ and a rapidly varying component $[y_2]^\varepsilon$. By considering $\bar{E}_2^\perp = \bar{E}_2^\perp(\bar{\bar{S}}_2, \bar{y}_2)$ we obtain (cf. equation (55))

$$d\bar{E}_2^\perp = F_0 d\bar{y}_2 + T_0 d\bar{\bar{S}}_2, \tag{52}$$

which agrees with the qualitative discussion of Section B.1 below.

Finally, let us inspect how the thermodynamic energy balance is realised in the total second-order energy correction of E_ε. Analogous to the decomposition above (40), we split the total energy E_ε in (15) into the heat bath energy $E_\varepsilon^\perp$ and the environmental energy $E_\varepsilon^\parallel$, i.e., $E_\varepsilon = E_\varepsilon^\parallel + E_\varepsilon^\perp$, where

$$E_\varepsilon^\parallel = \frac{1}{2}p_\varepsilon^2 + \frac{\varepsilon}{2}\theta_\varepsilon p_\varepsilon D_y L_\varepsilon \sin(2\varepsilon^{-1}\phi_\varepsilon) + \frac{\varepsilon^2}{8}\theta_\varepsilon^2 (D_y L_\varepsilon)^2 \sin^2(2\varepsilon^{-1}\phi_\varepsilon).$$

We then use the expressions derived in Theorem 3.2 to expand $E_\varepsilon^\parallel = E_0^\parallel + \varepsilon[\bar{E}_1^\parallel]^\varepsilon + \varepsilon^2[\bar{E}_2^\parallel]^\varepsilon + \varepsilon^2 E_3^{\parallel\varepsilon}$, where $E_3^{\parallel\varepsilon} \to 0$ in $C([0,T])$ with

$$E_0^\parallel \coloneqq \frac{1}{2}p_0^2, \qquad [\bar{E}_1^\parallel]^\varepsilon \coloneqq \frac{\theta_*}{2} D_t L_0 \sin(2\varepsilon^{-1}\phi_0)$$

and

$$[\bar{E}_2^\parallel]^\varepsilon \coloneqq p_0\left(\bar{p}_2 + [p_2]^\varepsilon\right) + \frac{\theta_*^2 (D_y L_0)^2}{8}\sin^2(2\varepsilon^{-1}\phi_0) + \theta_* D_t L_0 \left(\bar{\phi}_2 + [\phi_2]^\varepsilon\right)\cos(2\varepsilon^{-1}\phi_0) + \frac{[\theta_1]^\varepsilon D_t L_0}{2}\sin(2\varepsilon^{-1}\phi_0).$$

As before, we take the weak* limit to determine the average energy correction at first- and second-order, and find

$$[\bar{E}_1^\parallel]^\varepsilon \overset{*}{\rightharpoonup} 0 \quad \text{in} \quad L^\infty((0,T)), \qquad [\bar{E}_2^\parallel]^\varepsilon \overset{*}{\rightharpoonup} \bar{E}_2^\parallel \coloneqq p_0\bar{p}_2 + \left(\frac{\theta_* D_y L_0}{4}\right)^2 - \frac{\theta_*(D_t L_0)^2}{4\omega(y_0)} \quad \text{in} \quad L^\infty((0,T))$$

and define the averaged environmental energy $\bar{E}_\varepsilon^\parallel \coloneqq E_0^\parallel + \varepsilon^2 \bar{E}_2^\parallel$. The following theorem shows how the Hamiltonian character of the model problem and the thermodynamic interpretation materialise for the averaged total second-order energy correction $\bar{E}_2 = \bar{E}_2^\parallel + \bar{E}_2^\perp$.

Theorem 4.1. *Let (y_0, p_0) be as in (19) and $(\bar{y}_2, \bar{p}_2)$ be as in Theorem 3.2. Let $\bar{E}_2$ be the averaged total second-order energy correction*

$$\bar{E}_2\left(\bar{y}_2, \bar{p}_2, \bar{\bar{S}}_2; y_0, p_0\right) = \bar{A}(\bar{p}_2; y_0, p_0) + F_0(y_0)\bar{y}_2 + T_0(y_0)\bar{\bar{S}}_2,$$

with

$$\bar{A}(\bar{p}_2; y_0, p_0) = p_0\bar{p}_2 + \left(\frac{\theta_*\omega'(y_0)}{4\omega(y_0)}\right)^2 - T_0(y_0)\left(\frac{p_0\omega'(y_0)}{2\omega^2(y_0)}\right)^2,$$

and

$$T_0(y_0) = \theta_*\omega(y_0), \qquad F_0(y_0) = \theta_*\omega'(y_0), \qquad \bar{\bar{S}}_2 = \bar{\bar{S}}_2(y_0, p_0) = \frac{1}{2}\left(\frac{p_0\omega'(y_0)}{2\omega^2(y_0)}\right)^2 + C_{\bar{\bar{S}}_2},$$

where

$$C_{\bar{\bar{S}}_2} = -\frac{1}{2}\left(\frac{p_*\omega'(y_*)}{2\omega^2(y_*)}\right)^2 - \frac{5\theta_*\omega'(y_*)^2}{16\omega^3(y_*)} + \frac{p_*^2\omega''(y_*)}{4\omega^3(y_*)} - \frac{p_*^2\omega'(y_*)^2}{4\omega^4(y_*)}.$$

Then, the differential equations (29c) and (29d) and the constituent equations (59) take the form

$$\frac{d\bar{y}_2}{dt} = \frac{\partial \bar{E}_2}{\partial p_0}, \qquad \frac{\partial \bar{p}_2}{dt} = -\frac{\partial \bar{E}_2}{\partial y_0} \qquad \textit{and} \qquad F_0 = \frac{\partial \bar{E}_2}{\partial \bar{y}_2}, \qquad T_0 = \frac{\partial \bar{E}_2}{\partial \bar{\bar{S}}_2}. \tag{53}$$

Proof. The claim follows directly from (29c) and (29d). □

Remark. We point out that (53) gives a thermodynamic interpretation of the slow second-order evolution derived in Theorem 3.2. Moreover, with the special initial values as in (30), one finds that $\bar{E}_2 \equiv 0$, in accordance with equation (9). In this special case, the second-order energy correction $\bar{E}_2\left(\bar{y}_2, \bar{p}_2, \bar{\bar{S}}_2; y_0, p_0\right) \equiv 0$ acts as a constraint on the system and ε^2 in the expansion can be regarded as a Lagrange multiplier. Additionally, note that the expression for $\bar{\bar{S}}_2$ was chosen as the part of the averaged second-order energy correction that does not include the self-interaction with the averaged first-order correction and that corresponds to the appropriate expression found in $\bar{E}_2^\perp$. Finally, note that the term

$$T_0(y_0)\left(\frac{p_0\omega'(y_0)}{2\omega^2(y_0)}\right)^2$$

can be found both in $\bar{A}$ and in $\bar{\bar{S}}_2$, which indicates an energy exchange of heat and work in the averaged total second-order energy correction $\bar{E}_2$.

5 Conclusion

In this paper, we analysed a simple fast-slow Hamiltonian system with energy function of the form

$$E_\varepsilon(y_\varepsilon, \dot{y}_\varepsilon, z_\varepsilon, \dot{z}_\varepsilon) = \tfrac{1}{2}\dot{y}_\varepsilon^2 + \tfrac{1}{2}\dot{z}_\varepsilon^2 + \tfrac{1}{2}\varepsilon^{-2}\omega^2(y_\varepsilon)z_\varepsilon^2,$$

where y_ε is the slow and z_ε is the fast degree of freedom and $0 < \varepsilon < \varepsilon_0$ is a parameter determining the scale separation. This fast-slow Hamiltonian system was introduced and studied in [6], where a theory is established to describe the dynamics of y_ε in the limit $\varepsilon \to 0$, i.e., the coarse-grained dynamics of the system.

In the first part of this paper, we gave a finer description of the dynamics, for a small but non-zero ε, by deriving the second-order correction of the system's dynamical evolution. The second-order expansion can be decomposed into a highly oscillatory term with zero mean and a remainder; remarkably, the remainder can be characterised explicitly in form of a linear inhomogeneous system of differential equations as shown in Theorem 3.2. This gives in principle a computationally tractable way to simulate the dynamics efficiently to accuracy ε^2. Moreover, the expansion can be interpreted in a two-scale sense (see Appendix A). Furthermore, in Theorem 4.1 we provided a thermodynamic interpretation of the slow second-order evolution derived in Theorem 3.2.

In the second part of this paper, we investigated the fast subsystem with energy function

$$E_\varepsilon^\perp(z_\varepsilon, \dot{z}_\varepsilon; y_\varepsilon) = \tfrac{1}{2}\dot{z}_\varepsilon^2 + \tfrac{1}{2}\varepsilon^{-2}\omega^2(y_\varepsilon)z_\varepsilon^2,$$

which we interpret as the system of a harmonic oscillator in which the frequency is slowly perturbed by y_ε. After appropriate scaling, the perturbation disappears in the limit $\varepsilon \to 0$, and the resulting system is a standard harmonic oscillator with one degree of freedom, which is a simple example of an ergodic Hamiltonian system. Hence, in the limit, we can regard the system studied here as a thermodynamic system evolving in a sequence of thermodynamic equilibrium states. (Here we use a setting developed by Hertz [10] which, despite being described beautifully in [5], seems little known, and is thus sketched in Appendix B.) Based on this observation, we defined for $\varepsilon > 0$ a temperature T_ε, an external force F_ε and an entropy S_ε of the fast subsystem $E_\varepsilon^\perp$.

Using the results from the first part of this paper, we expanded $E_\varepsilon^\perp$, T_ε, F_ε and S_ε and showed that the first and second law of thermodynamics (according to Carathéodory) are satisfied in the expansion of $E_\varepsilon^\perp$. In particular, we found that the leading-order expansion of $E_\varepsilon^\perp$ exhibits a constant entropy, $dS_0 = 0$, and hence describes an adiabatic thermodynamic process, as shown in (47),

$$dE_0^\perp = F_0 dy_0 + T_0 dS_0 = F_0 dy_0.$$

The form of the entropy in this adiabatic limit is given in (46) by

$$S_0 = \log(\theta_*) + C.$$

Moreover, we showed that the averaged second-order expansion of the fast subsystem $E_2^\perp$ defines a non-adiabatic process, characterised by a non-constant entropy, $d\bar{S}_2 \neq 0$, see (52). Remarkably, this entropy satisfies the equation

$$d\bar{E}_2^\perp = F_0 d\bar{y}_2 + T_0 d\bar{\bar{S}}_2,$$

which is only expected in thermal equilibrium $\varepsilon \to 0$, though it is shown here to hold true beyond that limit.

The non-constant entropy to second-order is given in (51) by

$$\bar{\bar{S}}_2 = \bar{\theta}_2/\theta_*.$$

In summary, the limit process is described by an energy which is not the naïve energy that one obtains by setting $z_\varepsilon \equiv 0$, as shown by Bornemann [6], and is characterised by a constant entropy, while a nonconstant entropy appears only at second-order.

Acknowledgements

MK is supported by a scholarship from the EPSRC Centre for Doctoral Training in Statistical Applied Mathematics at Bath (SAMBa), under the project EP/L015684/1. JZ gratefully acknowledges funding by a Royal Society Wolfson Research Merit Award. All authors thank Celia Reina for stimulating discussions and helpful suggestions over the duration of this project.

A Interpretation of the analytic expansion as two-scale convergence

The converge results in Theorem 3.2 exhibit scale separations that are characteristic of the theory of two-scale convergence. In this appendix, we give a summary of the theory and introduce a nonlinear version of two-scale convergence which is used in Corollary 3.3.

A.1 Two-scale convergence

The theory of two-scale convergence was first introduced by Nguetseng [15]. We follow here the presentation in [1] and [21], though restricted to the one-dimensional case. We denote by $\mathcal{S}$ the set $S \coloneqq [0,1)$ equipped with the topology of the 1-dimensional torus, and identify any function on $\mathcal{S}$ with its S-periodic extension on $\mathbb{R}$.

In general a bounded sequence $\{u_\varepsilon\}$ of functions in $L^2(\Omega)$ is said to *weakly two-scale converge* to $u \in L^2(\Omega \times \mathcal{S})$, symbolically indicated by $u_\varepsilon \overset{2}{\rightharpoonup} u$, if and only if

$$\lim_{\varepsilon \to 0} \int_\Omega u_\varepsilon(t) \psi\left(t, \varepsilon^{-1} t\right) \,\mathrm{d}t = \iint_{\Omega \times S} u(t,s) \psi(t,s) \,\mathrm{d}t \,\mathrm{d}s,$$

for any smooth function $\psi \colon \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ which is S-periodic with respect to the second argument.

A.2 Two-scale decomposition

For any $\varepsilon > 0$, one can decomposes a real number $t \in \mathbb{R}$ as $t = \varepsilon[\mathcal{N}(t/\varepsilon) + \mathcal{R}(t/\varepsilon)]$, where

$$\mathcal{N}(t) \coloneqq \max\{n \in \mathbb{Z} \colon n \le t\}, \quad \mathcal{R}(t) \coloneqq t - \mathcal{N}(t) \in \mathcal{S}.$$

If ε is the ratio between two disparate scales, $\mathcal{N}(t/\varepsilon)$ and $\mathcal{R}(t/\varepsilon)$ may then be regarded as a coarse-scale and a fine-scale variable, respectively. Besides this two-scale decomposition, one defines a *two-scale composition function*:

$$h_\varepsilon(t,s) \coloneqq \varepsilon \mathcal{N}(t/\varepsilon) + \varepsilon s \qquad \forall (t,s) \in \mathbb{R} \times \mathcal{S}, \qquad \forall \varepsilon > 0.$$

The two-scale composition function can be written as $h_\varepsilon(t,s) = t + \varepsilon[s - \mathcal{R}(t/\varepsilon)]$, and thus

$$h_\varepsilon(t,s) \to t \quad \text{uniformly in } \mathbb{R} \times \mathcal{S}, \text{ as } \varepsilon \to 0.$$

Definition A.1 (Two-scale convergence, [21])**.** Let $\mathcal{S}$ and h_ε be defined as above. A sequence of functions $\{u_\varepsilon\}$ in $L^p(\mathbb{R})$ with $1 \le p \le \infty$ *two-scale converges* strongly respectively weakly (weakly star for $p = \infty$), denoted by $u_\varepsilon \underset{2}{\to} u, u_\varepsilon \underset{2}{\rightharpoonup} u, u_\varepsilon \overset{*}{\underset{2}{\rightharpoonup}} u$, respectively, to a limit $u_0(t,s)$ in $L^p(\mathbb{R} \times \mathcal{S})$ if it satisfies the following corresponding relation:

$$\begin{aligned}
u_\varepsilon \underset{2}{\to} u \quad &\text{in} \quad L^p(\mathbb{R} \times \mathcal{S}) \quad \Leftrightarrow \quad u_\varepsilon \circ h_\varepsilon \to u \quad \text{in} \quad L^p(\mathbb{R} \times \mathcal{S}), \quad \forall p \in [1, \infty]; \\
u_\varepsilon \underset{2}{\rightharpoonup} u \quad &\text{in} \quad L^p(\mathbb{R} \times \mathcal{S}) \quad \Leftrightarrow \quad u_\varepsilon \circ h_\varepsilon \rightharpoonup u \quad \text{in} \quad L^p(\mathbb{R} \times \mathcal{S}), \quad \forall p \in [1, \infty); \\
u_\varepsilon \overset{*}{\underset{2}{\rightharpoonup}} u \quad &\text{in} \quad L^\infty(\mathbb{R} \times \mathcal{S}) \quad \Leftrightarrow \quad u_\varepsilon \circ h_\varepsilon \overset{*}{\rightharpoonup} u \quad \text{in} \quad L^\infty(\mathbb{R} \times \mathcal{S}).
\end{aligned}$$

For any domain $\Omega \subset \mathbb{R}$, two-scale convergence in $L^p(\Omega \times \mathcal{S})$ is then defined by extending functions to $\mathbb{R} \setminus \Omega$ with vanishing value.

It is shown in [21] that this definition of two-scale convergence is equivalent to the definition first introduced in [15]. However, it is more versatile. In particular, it allows defining two-scale convergence in C^0.

A.3 Two-scale convergence in C^0

Some modifications are needed to extend the definition of two-scale convergence in [21] to C^0, for in general the function $u_\varepsilon \circ h_\varepsilon$ is discontinuous with respect to $t \in \mathbb{R}$ and $s \in \mathcal{S}$, even if u_ε is continuous. One therefore replaces $u_\varepsilon \circ h_\varepsilon$ by a continuous function, $L_\varepsilon u_\varepsilon$, constructed via linear interpolation with respect to each argument. More precisely, for $(t,s) \in \mathbb{R} \times \mathcal{S}$ and $w \colon \mathbb{R} \times \mathcal{S} \to \mathbb{R}$, we define

$$\begin{aligned}
(I_\varepsilon w)(t,s) &\coloneqq w(\varepsilon \mathcal{N}(t/\varepsilon), s) + \mathcal{R}(t/\varepsilon)[w(\varepsilon \mathcal{N}(t/\varepsilon) + \varepsilon, s) - w(\varepsilon \mathcal{N}(t/\varepsilon), s)], \\
(Jw)(t,s) &\coloneqq w(t,s) - s \left(\lim_{r \to 1^-} w(t,r) - w(t,0) \right).
\end{aligned}$$

Then, for $v \colon \mathbb{R} \to \mathbb{R}$, the linear interpolation is defined as

$$L_\varepsilon v \coloneqq (J \circ I_\varepsilon)(v \circ h_\varepsilon).$$

Thus $v \circ h_\varepsilon$ is piecewise constant with respect to t, whereas $L_\varepsilon v$ is piecewise linear and continuous with respect to t and periodic in s, i.e.,

$$\lim_{r \to 1^-} (L_\varepsilon v)(t,r) = (L_\varepsilon v)(t,0) \qquad \forall t \in \mathbb{R}.$$

Note that if $v \in C^0(\mathbb{R})$, then $L_\varepsilon v \in C^0(\mathbb{R} \times \mathcal{S})$.

We say that u_ε *strongly two-scale converges* to u in $C^0([0,T] \times \mathcal{S})$ if and only if

$$L_\varepsilon u_\varepsilon \to u \quad \text{in} \quad C^0([0,T] \times \mathcal{S}).$$

A.4 Nonlinear two-scale convergence

The two-scale convergence theory is a generalisation of the weak* convergence theory which retains information about the oscillatory character of u_ε in the limit $\varepsilon \to 0$. For instance, we have $\sin(2\pi\varepsilon^{-1}t) \overset{2}{\rightharpoonup} \sin(2\pi s)$. Notice, however, that $\sin\left(2\pi\varepsilon^{-1}\phi(t)\right) \overset{2}{\rightharpoonup} 0$ for any nonlinear function ϕ. To derive a non-zero two-scale limit in such a case we introduce a nonlinear change of coordinates that temporarily annihilates the nonlinearity so that the standard two-scale limit can be taken before it is reintroduced into the two-scale limit. This procedure is expressed in the following definition. Note that the constant π was chosen to normalise the period of the rapidly oscillating functions in Corollary 3.3.

Definition A.2 (Two-scale convergence with respect to $\phi_0^{-1} \circ \pi$)**.** Let $\{u_\varepsilon\} \subset C([0,T])$ and $u \in C([0,T] \times \mathcal{S})$. We say that u_ε *two-scale convergences* with respect to $\phi_0^{-1} \circ \pi$ to u in $C([0,T] \times \mathcal{S})$ if $u_\varepsilon \circ \phi_0^{-1} \circ \pi$ two-scale converges to $u \circ (\phi_0^{-1} \circ \pi, \mathrm{Id})$ in $C([0, \pi^{-1}\phi_0(T)] \times \mathcal{S})$, i.e.,

$$u_\varepsilon \xrightarrow[2]{\phi_0^{-1}\circ\pi} u \quad \text{in} \quad C([0,T] \times \mathcal{S}) \qquad \Longleftrightarrow \qquad u_\varepsilon(\phi_0^{-1}(\pi r)) \overset{2}{\to} u(\phi_0^{-1}(\pi r), s) \quad \text{in} \quad C([0, \pi^{-1}\phi_0(T)] \times \mathcal{S}).$$

With this definition at hand, we can express the uniform convergence results of Theorem 3.2 using the notation of two-scale convergence. Rephrasing the weak* convergence results in Theorem 3.2 in a similar way requires more notation. It is for this reason that we do not pursue the analysis any further.

B Hertz' approach to thermodynamics

As the theory of Hertz does not seem to be very well known, we recall the thermodynamic setting and the theory here, following the presentation in [5].

B.1 The first and second law of thermodynamics

Hertz considers a thermodynamic system under a slowly changing external parameter y. A classical example is a vessel filled with gas, where y indicates the height of a piston which compresses the gas. In line with Hertz' analysis, we considered for the problem studied in this article the *fast subsystem* with energy $E_\varepsilon^\perp$ as a thermodynamic system under a slowly changing external parameter represented by y_ε. We point out that Hertz' theory is based on dynamical systems which are inherently reversible in time and are thus regarded as idealised thermodynamic systems. As such, on a macro-scale level, the dynamics is described by the first and second law of thermodynamics, where the second law is given in Carathéodory's form.

The first law states that for every infinitesimal thermodynamical process dy, one can introduce the work of an external force $dA = F dy$ and the heat supply dQ such that the sum $dA + dQ$ is the differential of some energy function E,

$$dE = dA + dQ. \tag{54}$$

The second law of thermodynamics states that, for reversible processes, there are two functions of state, namely the absolute *temperature* T and the *entropy* S such that

$$dQ = T dS.$$

Hence, the first and second law of thermodynamics combined read

$$dE = F dy + T dS. \tag{55}$$

Equation (55) can be reduced to the statement that there exists an entropy $S = S(E, y)$ such that the *constitutive equations*

$$\frac{1}{T} = \frac{\partial S(E,y)}{\partial E} \qquad \text{and} \qquad F = -T\frac{\partial S(E,y)}{\partial y} \tag{56}$$

are satisfied.

The special case of a process without heat exchange, $dQ = 0$, is called an *adiabatic process*. In this case, all work dA is converted into a change of energy,

$$dE = dA, \tag{57}$$

or, equivalently, the entropy of the system stays constant,

$$S(E, y) = \text{const.} \tag{58}$$

Remark. With $E = E(S, y)$ the constitutive equations (56) read equivalently

$$T = \frac{\partial E(S,y)}{\partial S} \qquad \text{and} \qquad F = \frac{\partial E(S,y)}{\partial y}. \tag{59}$$

B.2 Derivation of thermodynamics from mechanics

We will give a first intuitive and informal explanation of the macroscopic thermodynamic behaviour for microscopic mechanical systems of Hamiltonian nature. Let $H(z, \zeta; y)$ be a Hamiltonian, where z and ζ denote the generalised coordinate and generalised momentum respectively, and where y is an external parameter. If we divide the external parameter into a slowly varying component s and a rapidly varying component r, then the time derivative of the Hamiltonian can be written as

$$\frac{dH}{dt} = \frac{\partial H}{\partial s}\frac{ds}{dt} + \frac{\partial H}{\partial r}\frac{dr}{dt}. \tag{60}$$

This equation expresses the balance of the energy on the micro-scale in the same way as the first law of thermodynamics (54) does on the macro-scale. By comparing these two equations, one can reason that the first term on the right of (60) represents the work of an external force $dA = Fdy$ for an adiabatic process. It corresponds to the case of a slowly varying external parameter y which conserves the entropy, $dQ = TdS = 0$. On the other hand, if y has a rapidly varying component, then the entropy changes. Hence, we can identify the last term in (60) with the heat supply of the system averaged over time to obtain the macro-scale effect of the micro-scale motion.

This informal and qualitative derivation of thermodynamic properties in Hamiltonian systems can be developed into a quantitative theory for ergodic Hamiltonian systems, as discussed in the following section.

B.3 Thermodynamic description of a slowly perturbed harmonic oscillator

We now sketch how Hertz' theory makes the previous informal arguments precise in the case of an harmonic oscillator with slowly perturbed frequency. There, the dynamics of the generalised position z_ε and momentum ζ_ε are governed by a Hamiltonian of the form

$$H_\varepsilon^\perp(z_\varepsilon, \zeta_\varepsilon; y_\varepsilon) = \tfrac{1}{2}\zeta_\varepsilon^2 + \tfrac{1}{2}\omega^2(y_\varepsilon)z_\varepsilon^2, \tag{61}$$

where $y_\varepsilon(t) = y(\varepsilon t)$ is a slow external parameter with $\dot{y}_\varepsilon = \mathcal{O}(\varepsilon)$. For $\varepsilon = 0$, the unperturbed Hamiltonian is given by

$$H_0^\perp(z_0, \zeta_0; y_*) = \tfrac{1}{2}\zeta_0^2 + \tfrac{1}{2}\omega^2(y_*)z_0^2, \tag{62}$$

where $y_0(t) = y(0) = y_*$ is constant. Let the corresponding canonical equations be complemented by the initial values $z_0(0) = 0$ and $\zeta_0(0) = \sqrt{2E_*^\perp}$, where $E_*^\perp$ is a constant energy level such that $H_0^\perp(z_0(t), \zeta_0(t), y_*) \equiv E_*^\perp$. The solution of the unperturbed system is thus given by

$$z_0(t) = \frac{\sqrt{2E_*^\perp}}{\omega(y_*)}\sin\left(\omega(y_*)t\right), \qquad \zeta_0(t) = \sqrt{2E_*^\perp}\cos\left(\omega(y_*)t\right). \tag{63}$$

We note that the unperturbed Hamiltonian $H_0^\perp$ is ergodic, as trajectories in phase-space coincide with the whole energy surface.

B.3.1 Derivation of T and S via time-averaging

For an ergodic Hamiltonian system, the temperature in thermal equilibrium is defined via the time average, indicated by angle brackets $\langle\cdot\rangle$, of twice the kinetic energy,

$$\left\langle \zeta_0 \frac{\partial H_0^\perp}{\partial \zeta_0} \right\rangle,$$

relating the temperature to the "speed" of the system's degrees of freedom. The *temperature* T for the system (62) is hence of the form

$$T(E_*^\perp, y_*) \coloneqq \left\langle \zeta_0 \frac{\partial H_0^\perp(z_0, \zeta_0; y_*)}{\partial \zeta_0} \right\rangle \coloneqq \lim_{\theta\to\infty} \frac{1}{2\theta}\int_{-\theta}^{+\theta} 2E_*^\perp \cos^2\left(\omega(y_*)t\right)\,\mathrm{d}t = E_*^\perp. \tag{64}$$

The system's *entropy* can then be derived from the first constitutive equation in (56), namely

$$S(E_*^\perp, y_*) = \log\left(E_*^\perp\right) + f(y_*),$$

where $f(y_*)$ is a constant of integration with respect to $E_*^\perp$. To find the function f, we use the second equation in (56), with the macro-scale *external force* F defined as the time average of the micro-scale force:

$$F(E_*^\perp, y_*) \coloneqq \left\langle \frac{\partial H_0^\perp(z_0, \zeta_0; y_*)}{\partial y_*} \right\rangle = E_*^\perp \frac{\omega'(y_*)}{\omega(y_*)}.$$

Therefore

$$S(E_*^\perp, y_*) = \log\left(\frac{E_*^\perp}{\omega(y_*)}\right) + C, \tag{65}$$

where C is an integration constant. Note that there are various definitions of entropy in the classical thermodynamic literature and (65) coincides with a definition for infinitely large systems [5, Chapter 1.5].

B.3.2 Derivation of T and S via ensemble-averaging

In this subsection, we sketch the derivation of an equivalent expression for the entropy, (74) below, as given by Hertz, still for the perturbed harmonic oscillator. Since this section is largely a modern reformulation of [10] applied to a special case, we only sketch the argument and dispense with rigour.

As the harmonic oscillator is ergodic, it admits a unique invariant measure, given by

$$\mu(A) = \frac{\displaystyle\int_A \frac{\mathrm{d}\sigma}{|\nabla H_0^\perp|}}{\displaystyle\int_\Sigma \frac{\mathrm{d}\sigma}{|\nabla H_0^\perp|}}, \tag{66}$$

where $A \subseteq \Sigma$ is a region on the level set $\Sigma = \{(z_0, \zeta_0) \in \mathbb{R}^2 \colon H_0^\perp(z_0, \zeta_0; y_*) = E_*^\perp\}$, $\mathrm{d}\sigma$ is an area element on the energy surface and

$$|\nabla H_0^\perp| = \left[\left(\frac{\partial H_0^\perp}{\partial z_0}\right)^2 + \left(\frac{\partial H_0^\perp}{\partial \zeta_0}\right)^2\right]^{1/2}.$$

By the ergodic theorem of Birkhoff and Khinchin, see, e.g., [22], the invariant measure μ can be used to find the time average in (64) simply by integration, without knowing the trajectory, since all the quantities on the right-hand side of equation (66) are known,

$$T(E_*^\perp, y_*) = \left\langle \zeta_0 \frac{\partial H_0^\perp(z_0, \zeta_0; y_*)}{\partial \zeta_0} \right\rangle = \frac{\displaystyle\int_\Sigma \zeta_0 \frac{\partial H_0^\perp}{\partial \zeta_0} \frac{\mathrm{d}\sigma}{|\nabla H_0^\perp|}}{\displaystyle\int_\Sigma \frac{\mathrm{d}\sigma}{|\nabla H_0^\perp|}}. \tag{67}$$

The numerator can be evaluated by noting that $\partial H_0^\perp/\partial \zeta_0$ is the second component of the vector $\nabla H_0^\perp$ and hence

$$n_\zeta \coloneqq \frac{\partial H_0^\perp/\partial \zeta_0}{|\nabla H_0^\perp|}, \tag{68}$$

is the second component of the outer unit vector $n = \nabla H_0^\perp/|\nabla H_0^\perp|$ on the energy surface. Therefore, we can write the numerator in the form

$$\int_\Sigma \zeta_0 \frac{\partial H_0^\perp}{\partial \zeta_0} \frac{\mathrm{d}\sigma}{|\nabla H_0^\perp|} = \int_\Sigma \zeta_0 n_\zeta \,\mathrm{d}\sigma = \int_{H_0^\perp(z_0,\zeta_0;y_*) \le E_*^\perp} \mathrm{d}(z_0, \zeta_0) =: \Gamma(E_*^\perp, y_*), \tag{69}$$

which follows from Gauss' theorem, where $\Gamma(E_*^\perp, y_*)$ is the phase-space volume enclosed by the trajectory of (63) and is also known as the action of the orbit in Hamiltonian dynamics [9]. To derive the denominator in (68), we calculate the derivative of $\Gamma(E_*^\perp, y_*)$ with respect to $E_*^\perp$. We find

$$\Gamma(E_*^\perp + \Delta E_*^\perp, y_*) - \Gamma(E_*^\perp, y_*) = \int_{E_*^\perp \le H_0^\perp(z_0,\zeta_0;y_*) \le E_*^\perp + \Delta E_*^\perp} \mathrm{d}(z_0, \zeta_0) \approx \int_{H_0^\perp(z_0,\zeta_0;y_*) = E_*^\perp} \Delta n \,\mathrm{d}\sigma,$$

where Δn is the distance between the energy surface $H_0^\perp(z_0, \zeta_0; y_*) = E_*^\perp$ and $H_0^\perp(z_0 + n_z\Delta n, \zeta_0 + n_\zeta \Delta n; y_*) = E_*^\perp + \Delta E_*^\perp$. A Taylor expansion gives $\Delta n = \Delta E_*^\perp/|\nabla H_0^\perp|$, and hence

$$\frac{\partial \Gamma(E_*^\perp, y_*)}{\partial E_*^\perp} = \int_{H_0^\perp(z_0,\zeta_0;y_*) = E_*^\perp} \frac{\mathrm{d}\sigma}{|\nabla H_0^\perp|}. \tag{70}$$

Combining equations (67)–(70), the temperature T can thus be expressed in terms of the phase-space volume $\Gamma(E_*^\perp, y_*)$,

$$T(E_*^\perp, y_*) = \frac{\Gamma(E_*^\perp, y_*)}{\partial \Gamma(E_*^\perp, y_*)/\partial E_*^\perp}. \tag{71}$$

According to equation (56) we integrate (71) with respect to $E_*^\perp$ and obtain as formula for the entropy,

$$S(E_*^\perp, y_*) = \log\big(\Gamma(E_*^\perp, y_*)\big) + f(y_*).$$

It remains to show that the function f is constant. To see this, we investigate the dependence of S on y_* and will, similar as above, use equation (56). Employing again the Birkhoff–Kinchin Theorem, we calculate

$$F(E_*^\perp, y_*) = \left\langle \frac{\partial H_0^\perp(z_0, \zeta_0; y_*)}{\partial y_*} \right\rangle = \frac{\displaystyle\int_\Sigma \frac{\partial H_0^\perp}{\partial y_*} \frac{\mathrm{d}\sigma}{|\nabla H_0^\perp|}}{\displaystyle\int_\Sigma \frac{\mathrm{d}\sigma}{|\nabla H_0^\perp|}}. \tag{72}$$

For the numerator, we calculate the derivative of $\Gamma(E_*^\perp, y_*)$ with respect to y_*. Similarly as before, we have

$$\begin{aligned}\Gamma(E_*^\perp, y_* + \Delta y_*) - \Gamma(E_*^\perp, y_*) &= \int_{H_0^\perp(z_0,\zeta_0;y_*+\Delta y_*)\le E_*^\perp} \mathrm{d}(z_0,\zeta_0) - \int_{H_0^\perp(z_0,\zeta_0;y_*)\le E_*^\perp} \mathrm{d}(z_0,\zeta_0) \\ &\approx \int_{H_0^\perp(z_0,\zeta_0;y_*)=E_*^\perp} \Delta n \,\mathrm{d}\sigma,\end{aligned}$$

where Δn is the distance between the energy surface $H_0^\perp(z_0, \zeta_0; y_*) = E_*^\perp$ and $H_0^\perp(z_0 + n_z\Delta n, \zeta_0 + n_\zeta \Delta n; y_* + \Delta y_*) = E_*^\perp$. A Taylor expansion gives

$$\Delta n = -\frac{1}{|\nabla H_0^\perp|} \frac{\partial H_0^\perp}{\partial y_*} \Delta y_*$$

and we obtain

$$\frac{\partial \Gamma(E_*^\perp, y_*)}{\partial y_*} = -\int_{H_0^\perp(z_0,\zeta_0;y_*)=E_*^\perp} \frac{\partial H_0^\perp}{\partial y_*} \frac{\mathrm{d}\sigma}{|\nabla H_0^\perp|}. \tag{73}$$

Combining equations (70), (72) and (73) we obtain

$$F(E_*^\perp, y_*) = \left\langle \frac{\partial H_0^\perp}{\partial y_*} \right\rangle = -\frac{\partial \Gamma(E_*^\perp, y_*)/\partial y_*}{\partial \Gamma(E_*^\perp, y_*)/\partial E_*^\perp}.$$

We thus find the desired formula for the entropy,

$$S(E_*^\perp, y_*) = \log\big(\Gamma(E_*^\perp, y_*)\big) + C, \tag{74}$$

where C is an arbitrary constant. This is a key result of Hertz: the entropy of a Hamiltonian system under the influence of a slowly varying parameter is, up to a constant, the logarithm of the phase space volume.

B.4 Thermodynamic description of the model problem

In Section B.3, we derived thermodynamic properties of a perturbed harmonic oscillator in the limit of infinitesimal small perturbations. This case corresponds to a situation where the motion of the external parameter is infinitely slow and can thus be regarded as constant.

For the model problem (5), we expect to see thermodynamic effects as a description of the fast subsystem. Now, however, the slow parameter is not constant. We nevertheless derive a description, using a suitable mapping to the harmonic oscillator studied in Section B.3. To this behalf, let us now introduce a scaling that focuses on the dynamics of the slow parameter. Here, the external parameter will affect the system dynamically of order one, while the frequency of the harmonic oscillator becomes infinitely high.

The energy of the slowly perturbed harmonic oscillator in (61) is given by

$$E_\varepsilon^\perp(z_\varepsilon(t), \zeta_\varepsilon(t); y_\varepsilon(t)) = \tfrac{1}{2}\zeta_\varepsilon^2(t) + \tfrac{1}{2}\omega^2(y(\varepsilon t))z_\varepsilon^2(t). \tag{75}$$

We introduce a scaling in space and time of the form

$$z_\varepsilon(t) = \varepsilon^{-1}\tilde{z}_\varepsilon(\varepsilon t), \quad \zeta_\varepsilon(t) = \tilde{\zeta}_\varepsilon(\varepsilon t) \quad \text{and} \quad \tau = \varepsilon t. \tag{76}$$

With this scaling, the new energy takes the form

$$\tilde{E}_\varepsilon^\perp(\tilde{z}_\varepsilon(\tau), \tilde{\zeta}_\varepsilon(\tau); \tilde{y}_\varepsilon(\tau)) = \tfrac{1}{2}\tilde{\zeta}_\varepsilon^2(\tau) + \tfrac{1}{2}\varepsilon^{-2}\omega^2(\tilde{y}_\varepsilon(\tau))\tilde{z}_\varepsilon^2(\tau), \tag{77}$$

which corresponds to the energy of the fast subsystem in our model problem (13). This establishes the mapping between perturbed harmonic oscillator and the problem under consideration.

For (75), Section B.3 describes how to derive the temperature, entropy and external force in the limit $\varepsilon \to 0$. They are given by

$$T(E_*^\perp, y_*) = \frac{\Gamma(E_*^\perp, y_*)}{\partial \Gamma(E_*^\perp, y_*)/\partial E_*^\perp}, \quad S(E_*^\perp, y_*) = \log\big(\Gamma(E_*^\perp, y_*)\big) + C, \quad F(E_*^\perp, y_*) = -\frac{\partial \Gamma(E_*^\perp, y_*)/\partial y_*}{\partial \Gamma(E_*^\perp, y_*)/\partial E_*^\perp},$$

where the phase space volume is

$$\Gamma(E_*^\perp, y_*) = 2\pi \frac{E_*^\perp}{\omega(y_*)}.$$

In analogy, we define in the case of (77) with a time-dependent external parameter y_ε and energy $E_\varepsilon^\perp$ the *temperature*, *entropy* and *external force* as

$$T_\varepsilon(E_\varepsilon^\perp, y_\varepsilon) := \frac{\Gamma_\varepsilon(E_\varepsilon^\perp, y_\varepsilon)}{\partial\Gamma_\varepsilon(E_\varepsilon^\perp, y_\varepsilon)/\partial E_\varepsilon^\perp}, \quad S_\varepsilon(E_\varepsilon^\perp, y_\varepsilon) := \log\left(\Gamma_\varepsilon(E_\varepsilon^\perp, y_\varepsilon)\right) + C_\varepsilon, \quad F_\varepsilon(E_\varepsilon^\perp, y_\varepsilon) := -\frac{\partial\Gamma_\varepsilon(E_\varepsilon^\perp, y_\varepsilon)/\partial y_\varepsilon}{\partial\Gamma_\varepsilon(E_\varepsilon^\perp, y_\varepsilon)/\partial E_\varepsilon^\perp},$$

where C_ε is an arbitrary constant and Γ_ε is the time dependent phase-space volume derived from (14),

$$\Gamma_\varepsilon(E_\varepsilon^\perp, y_\varepsilon) = 2\pi\varepsilon \frac{E_\varepsilon^\perp}{\omega(y_\varepsilon)}.$$

Since entropy is a extensive property, it scales with the size, according to (76). To compare it with intensive quantities and to avoid a divergent entropy in the limit $\varepsilon \to 0$, the constant in the entropy has to be chosen accordingly, for example $C_\varepsilon = -\log(\Gamma_\varepsilon(E_*^\perp, y_*))$. With (14), the phase-space volume Γ_ε can be written as

$$\Gamma_\varepsilon(t) = 2\pi\varepsilon\theta_\varepsilon(t)$$

and consequently with $E_\varepsilon^\perp = \theta_\varepsilon\omega(y_\varepsilon)$ we obtain the desired final thermodynamic formulas in (41):

$$T_\varepsilon = \theta_\varepsilon\omega(y_\varepsilon), \qquad S_\varepsilon = \log(\theta_\varepsilon) + C_\varepsilon, \qquad F_\varepsilon = \theta_\varepsilon\omega'(y_\varepsilon). \tag{78}$$

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