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A Simple but Rigorous Micro-Macro Transition

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Abstract

This paper is devoted to a case study of micro-macro transitions. The main objective is the mathematically rigorous description of the macroscopic behavior of highly oscillating microscopic variables. In particular, we show that the theory of YOUNG measures provides an elegant approach to this problem. A nontrivial application of the results is given in [1].

1 Introduction

We consider the following dynamical system

$$\frac{d}{d\tau}Q(\tau) = A\big(\varepsilon\tau,\, Q(\tau)\big), \quad Q = \begin{pmatrix} q \\ p \end{pmatrix}, \quad A\big(t,\, Q\big) = \begin{pmatrix} p \\ -\partial_q G(t,\, q) \end{pmatrix}. \tag{1}$$

From a physical point of view, this system describes the motion of a particle in the potential G, whereas the quantities q and p correspond to the position and to the momentum of the particle, respectively. In the System (1) there appear two time variables τ and t which we call the *micro time* and *macro time*, respectively. Both time scales are coupled by the algebraic equation

$$t \;=\; \varepsilon\tau, \tag{2}$$

where $\varepsilon > 0$ is a small parameter. Since ε is small, t is the slow time, whereas τ is the fast time. At a first glance, the namings *micro time* and *macro time* for the fast and slow time, respectively, may look somehow artificial. Thus we refer to [1] for a more detailed motivation.

We give two typical examples for the systems which we have in mind.

Example 1.1 *We consider a harmonic oscillator with external force f, i.e. we set*

$$G(t,\, q) \;=\; \frac{1}{2}q^2 - qf(t), \quad f \in C^1(\mathbb{R}). \tag{3}$$

Example 1.2 *We consider an anharmonic oscillator with*

$$G(t,\, q) = \frac{1}{2}g\big(d(t) - 2q\big) + \frac{1}{2}g\big(d(t) + 2q\big) \tag{4}$$

and $d,\, g \in C^1(\mathbb{R})$, g convex and $\lim\limits_{q\to\pm\infty} g(q) = \infty$.

We next describe the mathematical problem in detail. Let Q^0 be initial data that do not depend on ε. For any ε there exists a function $Q^\varepsilon = Q^\varepsilon(\tau)$, defined for all $\tau \geq 0$, that gives the solution of (1) with initial data Q^0. In order to describe the macroscopic behavior of (1) we introduce the scaled solutions $Q_\varepsilon = Q_\varepsilon(t)$ by

$$Q_\varepsilon(t) \quad := \quad Q^\varepsilon\big(\frac{t}{\varepsilon}\big), \quad t \geq 0. \tag{5}$$

A characteristic example is depicted in Figure 1. The potential G is given as in Example 1.1 with a slowly varying external force f. The function Q_ε is highly oscillating with a frequency proportional to ε^{-1}.

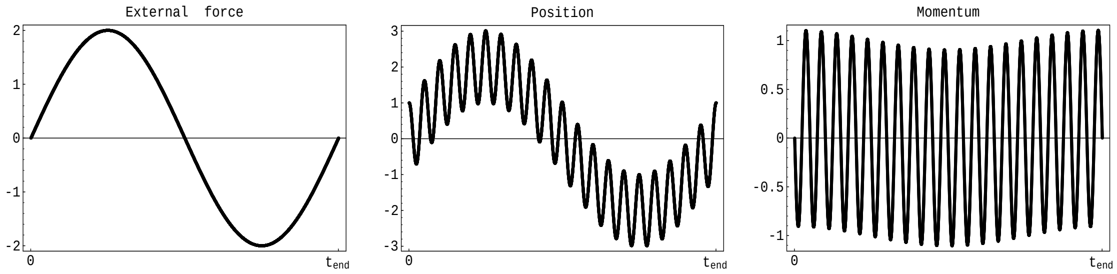

Figure 1: Macroscopic behavior of the scaled solutions

From the physical point of view we are interested not only in the scaled solution but also in the evolution of certain observables. An observable is a continuous function Ψ_u of Q that may additionally depend on the macro time t. The macroscopic evolution of an observable $\Psi_u = \Psi_u(t,\, Q)$ is described by a function u_ε which is defined as follows

$$u_\varepsilon(t) \quad := \quad \Psi_u\big(t,\, Q_\varepsilon(t)\big). \tag{6}$$

The most prominent observable is the energy Ψ_{e} which is defined by

$$\Psi_{\mathrm{e}}(t,\, Q) := \frac{1}{2}p^2 + G(t,\, Q). \tag{7}$$

The function e_ε with

$$e_\varepsilon(t) \quad := \quad \Psi_{\mathrm{e}}\big(t,\, Q_\varepsilon(t)\big) \tag{8}$$

describes the macroscopic evolution of the energy. From (1) we obtain by a straight forward calculation

$$\frac{d}{dt}e_\varepsilon(t) = \partial_t G\big(t,\, Q_\varepsilon(t)\big). \tag{9}$$

The two time scales t and τ in System (1) are coupled by the algebraic equation (2). However, if ε tends to zero we expect a decoupling of micro time and macro time. From the mathematical point of view there arise some interesting questions.

1. Which is the origin of the decoupling of micro time and macro time?

2. Is there any kind of convergence of the scaled solutions if $\varepsilon \to 0$?

3. Which are the governing equations that determine the evolution of observables with respect to the macro time in the limiting case $\varepsilon = 0$?

The main objective of this study is to answer these questions in terms of YOUNG measures. To this end we first summarize some properties of YOUNG measures in Section 2. In Section 3 we state and prove our result concerning the three posed questions.

We proceed with further definitions. In order to simplify some technical arguments we consider a finite macro time interval T with

$$T := \big[0,\, t_{\text{end}}\big], \quad 0 < t_{\text{end}} < \infty. \tag{10}$$

As we shall see in Section 3, the decoupling of micro time and macro time can be best understood by introducing the following dynamical system

$$\frac{d}{d\theta} Q(\theta) = A\big(t,\, Q(\theta)\big). \tag{11}$$

Note that in (11) the macro time t appears only as a parameter. In particular, there is no coupling between θ and t. In the following we call the System (11) the *associated system* to (1). There exists a corresponding stationary LIOUVILLE equation which can be written in the form

$$\operatorname{div}_Q\big[\mu(dQ)\cdot A(t,\, Q)\big] \;=\; 0, \tag{12}$$

where $\mu = \mu(dQ) \in \operatorname{Prob}(\mathbb{R}^2)$ is a measure, cf. Section 2.

In this study we consider exclusively potentials G that satisfy the following assumption.

Assumption 1.3

1. ***(Domain of definition)***
   For any $t \in T$ there exists an open set $\mathcal{O}_t \subset \mathbb{R}$ and a set $\mathcal{E}_t \subset \mathbb{R}$ with

   $$\mathcal{E}_t = \{e \,:\, e \geq e_{\min}(t)\}, \tag{13}$$

   such that the potential $G(t,\,\cdot)$ is well defined on $\mathcal{O}_t$ and maps $\mathcal{O}_t$ into $\mathcal{E}_t$. The function $e_{\min}$ is continuous on T.

2. ***(Regularity of the potential)***
   The potential G is continuously differentiable and $\partial_q G$ is uniformly continuous on sets

   $$\big\{(t,\, Q) \,:\, t \in T,\ \Psi_{\mathrm{e}}(t,\, Q) \leq e_{\max}\big\}, \quad e_{\max} \in \mathbb{R}. \tag{14}$$

3. ***(Boundedness)***
There exist two compact sets $K \subset \mathbb{R}^2$ and $L \subset \mathbb{R}$, such that for all $\varepsilon \leq 1$ and all $t \in T$ there holds

$$Q_\varepsilon(t) \in K \quad \textit{and} \quad e_\varepsilon(t) \in L. \tag{15}$$

Without loss of generality we assume $\Psi_{\mathrm{e}}(t, \cdot) : K \to L$ for all $t \in T$.

4. ***(Closed orbits)***
Let $t \in T$ and $\tilde{Q}^0 \in \mathcal{O} \times \mathbb{R}$ be fixed and let $\tilde{Q} = \tilde{Q}(\theta)$, $\theta \geq 0$ be the solution of System (11) with initial data $\tilde{Q}^0$. We assume that (i) the function $\tilde{Q}$ is periodic in θ, and (ii) the corresponding closed orbit is completely determined by the initial energy $\Psi_{\mathrm{e}}(\tilde{Q}^0)$.

The last two assumptions are crucial, whereas the two first ones simplify some reasonings. The next lemma illustrates the methods which lead to uniform bounds of $Q_\varepsilon(t)$ and $e_\varepsilon(t)$.

Lemma 1.4 *Let G be as in Example 1.1. There exist two compact sets $K \subset \mathbb{R}^2$ and $L \subset \mathbb{R}$ so that the conditions (15) are satisfied.*

Proof: Due to the definition of the energy observable we have

$$|Q| \leq \sqrt{2\Psi_e(t, Q) + f^2(t)} + |f(t)|. \tag{16}$$

From the energy balance (9) and from (16) we conclude that

$$\begin{aligned}
|e_\varepsilon(t)| &\leq e_\varepsilon(0) + \int_0^t |f'(s)||Q_\varepsilon(s)|\, ds \\
&\leq \Psi_e(0, Q^0) + \| f' \|_\infty \int_0^t |Q_\varepsilon(s)|\, ds \\
&\leq \Psi_e(0, Q^0) + \| f' \|_\infty \Big(\int_0^t y\big(e_\varepsilon(s)\big)\, ds + \int_0^t y\big(f(s)^2\big) + |f|(s)\, ds \Big), \\
&\leq C_1 + C_2 \int_0^t y\big(e_\varepsilon(s)\big)\, ds,
\end{aligned} \tag{17}$$

where $y(x) = \max\{1, x\}$. Note that C_1 and C_2 are two constants which depend on f and on the initial energy $e^0 = \Psi_{\mathrm{e}}(t, Q^0)$, but which do not depend on ε. GRONWALL's Lemma provides estimates for $e_\varepsilon(t)$, $0 \leq t \leq T$, that are independent of ε. In particular, we can choose K and L sufficiently large. □

2 YOUNG measures

In this section we summarize the definition and the most important properties of YOUNG measures. For a detailed introduction in the theory of YOUNG measures we refer to the literature, see for instance [4], [5] and [6].

Let Ω be a subset of $\mathbb{R}^d$. As usual we denote by $C_c(\Omega)$ the space of all continuous functions on Ω that have a compact support in Ω. The closure of $C_c(\Omega)$ with respect to the norm $\|\ \|_\infty$ is abbreviated by $C_0(\Omega)$. In the case that Ω is compact, we have $C_c(\Omega) = C_0(\Omega) = C(\Omega)$. A *observable* on Ω is an element of $C_0(\Omega)$.

A measure on Ω in the sense of functional analysis is a linear continuous functional on $C_0(\Omega)$. Within this paper, measure means always measure in the sense of functional analysis. We denote the space of all measures by $M(\Omega) = C_0(\Omega)^*$. According to a famous theorem by RIESZ and RADON, any measure in the sense of functional analysis is also a measure in the sense of measure theory, but not vice versa. A probability measure on Ω is a positive measure whose norm is equal to 1. We write $\mathrm{Prob}\,(\Omega)$ for the space of all probability measures.

Let μ be a measure on Ω. The elements of Ω will be denoted by y. In order to have a clear and suggestive distinction between measures which are defined on different sets, we write sometimes $\mu(dy)$ instead of μ.
Let ψ be a function that is integrable with respect to μ but not necessary continuous. In order to abbreviate the integral of ψ with respect to μ we use the following notation

$$\langle \mu(dy),\, \psi(y)\rangle_{y\,\in\,\Omega} := \int\limits_\Omega \psi\, d\mu = \int\limits_\Omega \psi(y)\mu(dy). \tag{18}$$

The usual dual pair of a measure and an observable reads

$$\langle \mu,\, \psi\rangle_{C_0(\Omega)} = \langle \mu(dy),\, \psi(y)\rangle_{y\,\in\,\Omega} \quad \forall\, \psi \,\in\, C(\Omega). \tag{19}$$

Note that the left hand side makes sense only for continuous ψ whereas the right hand side is well defined for a wider class of functions.

Let X be a compact and convex set in $\mathbb{R}^d$ and let T be a closed time interval as in (10). The elements of X and T are denoted by x and t, respectively. In the next section, in which we apply the YOUNG measures, we consider the two cases $X = K$ with $x = Q$ and $X = L$ with $x = e$, respectively.

The space of YOUNG-measures $Y(T;\,K)$ consists of all positive measures μ on $T\times K$ that have the following property

$$\Big\langle \mu\big(d(t,\,x)\big),\, g(t)\Big\rangle_{(t,\,x)\,\in\, T\times X} = \Big\langle \lambda(dt),\, g(t)\Big\rangle_{t\,\in\, T} = \int\limits_T g(t)\, dt \quad \forall\, g \,\in\, C(T), \tag{20}$$

where λ denotes the LEBESGUE measure on T.

A very useful tool in the theory of YOUNG-measures is the disintegration. The disintegration of a YOUNG-measure $\mu \in Y(T;\, X)$ is a family of probability measures

$$\big\{\mu(t)\big\}_{t\in T} \quad \text{with} \quad \mu(t) = \mu(t)(dx) \,\in\, \mathrm{Prob}\,(X), \tag{21}$$

which is defined almost everywhere on T and that satisfies the following property. For any $\Psi = \Psi(t,\, x)$ that is integrable with respect to μ there exists a function

$$\lfloor \mu,\, \Psi \rfloor \,\in\, L^\infty(T;\, X) \tag{22}$$

such that

$$\lfloor \mu,\, \Psi \rfloor(t) \;=\; \big\langle \mu(t)(dx),\, \Psi(t,\, x)\big\rangle_{x\in X}\,, \tag{23}$$

$$\Big\langle \mu\big(d(t,\, x)\big),\, \Psi(t,\, x)\Big\rangle_{(t,\,x)\in T\times X} \;=\; \int_T \lfloor \mu,\, \Psi \rfloor(t)\, dt. \tag{24}$$

The measures $\mu(t)$ is called the disintegration of μ at t. Since there exist disintegrations, we write as usual

$$\mu(t,\, dx) \quad \text{instead of} \quad \mu\big(d(t,\, x)\big). \tag{25}$$

For any function $f \in L^\infty(T;\, X)$ there exists a YOUNG measure δ_f such that

$$\delta_f(t, dx) = \delta_{f(t)}(dx) \tag{26}$$

where $\delta_{f(t)}(dx)$ is the delta-distribution with support $\{f(t)\}$. The measure δ_f is called the YOUNG measure of the function f. There holds

$$\lfloor \delta_f,\, \Psi \rfloor(t) \;=\; \Psi\big(t,\, f(t)\big). \tag{27}$$

Next we discuss convergence of YOUNG measures. Let $(\mu_j)_j$ be a sequence and let μ_∞ be an element of $Y(T;\, X)$. We write

$$\mu_j \;\to\; \mu_\infty \qquad \text{in } Y(T;\, X)$$

provided

$$\mu_j \;\to\; \mu_\infty \qquad \text{weak* in } M(T\times X).$$

This convergence can be characterized as follows.

Lemma 2.1 *A sequence of $(\mu_i)_i$ of* YOUNG*-measures converges to μ_∞ in $Y(T;\, X)$ if and only if*

$$\lim_{i\to\infty} \big\langle \mu_i(t,\, dx),\, \Psi(t,\, x)\big\rangle_{(t,\,x)\in T\times X} \;=\; \big\langle \mu_\infty(t,\, dx),\, \Psi(t,\, x)\big\rangle_{(t,\,x)\in T\times X} \tag{28}$$

holds for all bounded CARATHEODORY *functions $\Psi \in \mathrm{Car}\,(T,\, X)$.*

The next theorem gives another characterization of convergence.

Theorem 2.2 *Let $(\mu_i)_i$ be a sequence of* YOUNG*-measures so that*

$$\mu_i \to \mu_\infty \quad \textit{in} \quad Y(T;\, X). \tag{29}$$

Then there holds

$$\lfloor \mu_i,\, \Psi \rfloor \to \lfloor \mu_\infty,\, \Psi \rfloor \quad \textit{weak}{*} \textit{ in } L^\infty(T;\, X) \tag{30}$$

for all $\Psi \in \operatorname{Car}(T,\, X)$.

The main theorem in the theory of YOUNG measures is the following compactness result.

Theorem 2.3 *For any sequence $(\mu_n)_n$ in $Y(T;\, X)$ there exist a subsequence $(\mu_i)_i$ and a measure $\mu_\infty \in Y(T;\, X)$ such that*

$$\mu_i \to \mu_\infty \quad \textit{in} \quad Y(T;\, X). \tag{31}$$

Let $(\mu_i)_i$ be a sequence which converges to μ_∞. A very important problem is the determination of the disintegration of μ_∞. Unfortunately, $\mu_i(t)$ does not converge weakly* in $\operatorname{Prob}(X)$ to $\mu_\infty(t)$ for almost every $t \in T$. In the following we thus derive a useful description of disintegrations of YOUNG measure limits.

We denote by χ the indicator function of the interval $[-1,\, 0]$. Furthermore, for $\gamma > 0$ we set

$$\chi^\gamma(t) := \frac{1}{\gamma}\,\chi\Big(\frac{t}{\gamma}\Big), \quad \text{i.e.} \quad \chi^\gamma = \frac{1}{\gamma}\mathbf{1}_{[-\gamma,\,0]}. \tag{32}$$

Let $\mu \in Y(T;\, X)$ be a given YOUNG measure. For any $t \in T$ and $\gamma > 0$ we define a measure

$$\mu^\gamma(t) \;=\; \mu^\gamma(t,\, dx) \;\in\; \operatorname{Prob}(X) \tag{33}$$

by

$$\big\langle \mu^\gamma(t,\, dx),\, \psi(x) \big\rangle_{x\,\in X} \;\;:=\;\; \frac{1}{\gamma}\int_t^{t+\gamma} \big\langle \mu(s,\, dx),\, \psi(x) \big\rangle_{x\,\in X}\, ds \quad \forall\, \psi \in C(X). \tag{34}$$

Lemma 2.4 *For $\mu \in Y(T;\, X)$, $\psi \in C(X)$, $\gamma > 0$ and $t \in T$ there holds*

$$\begin{aligned} \big\langle \mu^\gamma(t,\, dx),\, \psi(x) \big\rangle_{x\,\in X} \;&=\; \Big\langle \mu(s,\, dx),\, \frac{1}{\gamma}\mathbf{1}_{[t;\,t+\gamma]}(s)\, \psi(x) \Big\rangle_{(s,\,x)\,\in T\times X} \\ &=\; \Big(\lfloor \mu,\, \psi \rfloor * \chi^\gamma \Big)(t). \end{aligned} \tag{35}$$

Proof: The identities (35) follow by a straight forward calculation. □

Corollary 2.5

1. *Let $\mu \in Y(T;\, X)$ and $\psi \in C(X)$. If $\gamma \to 0$, the L^∞-functions*

$$t \;\rightsquigarrow\; \big\langle \mu^\gamma(t,\, dx),\, \psi(x)\big\rangle_{x\,\in X} \tag{36}$$

converge to $\lfloor \mu,\, \psi \rfloor$ in $L^r(T)$ for all $1 \le r < \infty$. In particular, if $(\gamma_j)_j$ is a sequence with $\gamma_j \to 0$, there exists a subsequence $(\gamma_k)_k$ and a set $S \subset T$, such that $|S| = 0$ and

$$\lim_{k\to\infty} \big\langle \mu^{\gamma_k}(t,\, dx),\, \psi(x)\big\rangle_{x\,\in X} = \big\langle \mu(t,\, dx),\, \psi(x)\big\rangle_{x\,\in X} \quad \forall\, t \in S. \tag{37}$$

2. *Let $\mu_i \to \mu_\infty$ in $Y(T;\, X)$. For all $\psi \in C(X)$, $\gamma > 0$ and all $t \in T$ there holds*

$$\lim_{i\to\infty} \big\langle \mu_i^\gamma(t,\, dx),\, \psi(x)\big\rangle_{x\,\in X} \;=\; \big\langle \mu_\infty^\gamma(t,\, dx),\, \psi(x)\big\rangle_{x\,\in X}\,. \tag{38}$$

3. *Let $\mu_i \to \mu_\infty$ in $Y(T;\, X)$, let $\psi \in C(X)$ be fixed and let $(\gamma_j)_j$ be a sequence with $\gamma_j \to \infty$. Then there exists a subsequence $(\gamma_k)_k$ and a set $S \subset T$, such that $|S| = 0$ and*

$$\lim_{k\to\infty}\lim_{i\to\infty} \big\langle \mu_i^{\gamma_k}(t,\, dx),\, \psi(x)\big\rangle_{x\,\in X} = \big\langle \mu_\infty(t,\, dx),\, \psi(x)\big\rangle_{x\,\in X} \quad \forall\, t \in S. \tag{39}$$

Proof: 1. is a direct consequence of (35) and the properties of convolution operators, *2.* follows imediately from (35) and Lemma 2.1. Finally, *1.* and *2.* imply *3.* □

The last statement of Corollary 2.5 provides a very useful characterization of YOUNG measure limits. In particular, it relates YOUNG measure limits to averages of observables. To explain this in more detail, let $(f_i)_i$ be a sequence of functions in $L^\infty(T;\, X)$, so that the corresponding YOUNG measures $(\delta_{f_i})_i$ converge to a YOUNG measure μ_∞. Furthermore, let $\psi \in C(X)$ be a fixed observable. Then we can choose a sequence $(\gamma_k)_k$ such that the identity

$$\big\langle \mu_\infty(t,\, dx),\, \psi(x)\big\rangle_{x\,\in X} = \lim_{k\to\infty}\lim_{i\to\infty} \frac{1}{\gamma_k} \int\limits_t^{t+\gamma_k} \psi\big(f_i(s)\big)\, ds \tag{40}$$

holds almost everywhere on T.

Finally we mention that the measures $\mu^\gamma(t,\, dx)$, cf. (32), may be defined by other averaging kernels. In particular, all results remain valid as long as the averaging kernel χ is as usual, i.e. χ is nonnegative and bounded, has compact support and satisfies $\int \chi = 1$.

3 The limit $\varepsilon \to 0$

In this section we study the behavior of Q_ε if ε tends to zero. We choose two compact subsets $K \subset \mathbb{R}^2$ and $L \subset \mathbb{R}$ as in Assumption 1.3. According to Theorem 2.3, the set $\{\delta_{Q_\varepsilon}\}_{\varepsilon \le 1}$ is precompact in $Y(T;\, K)$. Thus, there exist sequences $(\varepsilon_j)_j$ with $\varepsilon_j \to \infty$ such that $\delta_{Q_{\varepsilon_j}}$ converges to a limit measure. In this section we prove the uniqueness of such a limit measure.

Assumption 3.1 *Let $(\varepsilon_j)_j$ be a subsequence with $\varepsilon_j \to 0$ such that*

$$\mu_j := \delta_{Q_{\varepsilon_j}} \to \mu_\infty \quad in \quad Y(T;\, \mathbb{R}^2) \tag{41}$$

Our main result can be formulated as follows

Theorem 3.2 *Let μ_∞ be given as in Assumption 3.1. Then, μ_∞ is uniquely determined by the initial data Q_0. In other words, μ_∞ does not depend on the sequence $(\varepsilon_j)_j$.*

This theorem implies immediately the following Corollary.

Corollary 3.3 *The* YOUNG *measures corresponding to the functions Q_ε converge for $\varepsilon \to 0$ to a unique limit measure μ_∞.*

In the following we consider a fixed sequence $(\varepsilon_j)_j$ that satisfies the Assumptions 3.1.

We prove Theorem 3.2 in several steps. In Subsection 3.1 we introduce some further notations. In particular, we define an energy measure ν_∞ corresponding to μ_∞. In Subsection 3.2 we prove, that the measure μ_∞ is completely determined by ν_∞. Finally, in Subsection 3.3 we derive a deterministic evolution equation for ν_∞.

3.1 Further notations

For shortness we write

$$Q^j := Q^{\varepsilon_j}, \quad Q_j = Q_{\varepsilon_j} \quad \text{and} \quad e_j := e_{\varepsilon_j} \tag{42}$$

for all $j \in \mathbb{N}$. According to (5) we have

$$Q_j(t) \;=\; Q^j\big(\frac{t}{\varepsilon_j}\big). \tag{43}$$

Let $\overline{\mathbb{N}} = \mathbb{N} \cup \{\infty\}$. We consider the probability measures $\mu_j^\gamma(t)$ which are defined in Section 2, cf. (34). We find

$$\big\langle \mu_j^\gamma(t,\, dQ),\, \psi(Q)\big\rangle_{Q \in K} = \frac{1}{\gamma}\int_t^{t+\gamma} \big\langle \mu_j(s,\, dQ),\, \psi(Q)\big\rangle_{Q \in K}\, ds \quad \forall\, \psi \in C(K). \tag{44}$$

Recall that (44) is well defined for all $j \in \overline{\mathbb{N}}$, $\gamma > 0$ and all $t \in T$. According to Corollary 2.5, the measures $\mu_j^\gamma(t)$ can be regarded as good approximations of $\mu_\infty(t)$. In particular, for any observable $\psi \in C(K)$ there exists a sequence $(\gamma_k)_k$, $\gamma_k \to 0$, such that for almost every $t \in T$ there holds

$$\begin{aligned}\big\langle \mu_\infty(t, dQ), \psi(Q)\big\rangle_{Q\in K} &= \lim_{k\to\infty} \big\langle \mu_\infty^{\gamma_k}(t, dQ), \psi(Q)\big\rangle_{Q\in K} \\ &= \lim_{k\to\infty}\lim_{j\to\infty} \big\langle \mu_j^{\gamma_k}(t, dQ), \psi(Q)\big\rangle_{Q\in K}. \end{aligned} \tag{45}$$

Moreover, for $j \in \overline{\mathbb{N}}$ we define the energy measure $\nu_j \in Y(T; L)$ corresponding to μ_j by

$$\langle \nu_j, \Phi\rangle_{C(T\times L)} := \langle \mu_j, \Phi\circ\Psi_e\rangle_{C(T\times L)} \quad \forall\, \Phi \in C(T\times L) \tag{46}$$

where

$$(\Phi\circ\Psi_e)(t, Q) := \Phi\Big(t, \Psi_e(t, Q)\Big). \tag{47}$$

Obviously we have

1. $\nu_j = \delta_{e_j}$ if $j \neq \infty$, and
2. $\nu_j \to \nu_\infty$ for $j \to \infty$ in $Y(T; L)$.

3.2 Nontrivial relation between μ_∞ and ν_∞

As mentioned in Section 1 we expect a decoupling of micro time and macro time if $\varepsilon \to 0$. The next theorem describes the mechanism of this decoupling.

Theorem 3.4 *The measure $\mu_\infty(t) = \mu_\infty(t, dQ)$ satisfies for almost every $t \in T$ the following equation*

$$\mathrm{div}_Q\big[\mu_\infty(t, dQ)\cdot A(t, Q)\big] = 0. \tag{48}$$

In other words, $\mu_\infty(t)$ is a solution of the stationary LIOUVILLE *equation* (12) *that corresponds to the associated system* (11).

Proof:

1. Let $j \in \mathbb{N}$, $t \in T$, $\gamma > 0$ be fixed. We find

$$\begin{aligned}&\mathrm{div}_Q\big[\mu_j^\gamma(t, dQ)\cdot A(t, Q)\big] = \\ &\quad= \frac{1}{\gamma}\int_t^{t+\gamma} \mathrm{div}_Q\big[\mu_j(s, dQ)\cdot A(t, Q)\big]\,ds \\ &\quad= \frac{1}{\gamma}\int_t^{t+\gamma} \mathrm{div}_Q\big[\mu_j(s, dQ)\cdot A(s, Q)\big]\,ds\, + \\ &\qquad \frac{1}{\gamma}\int_t^{t+\gamma} \mathrm{div}_Q\big[\mu_j(s, dQ)\cdot \{A(t, Q) - A(s, Q)\}\big]\,ds. \end{aligned} \tag{49}$$

Let $\varphi = \varphi(Q) \in C_c^1(\mathbb{R}^2)$ be a smooth test function. For any $s \in T$ we set $\sigma := \varepsilon_j^{-1} s$. There holds

$$\begin{aligned} X_1(s) &:= \Big\langle \mathrm{div}_Q\big[\mu_j(s,\,dQ)\cdot A(s,\,Q)\big],\,\varphi\Big\rangle_{C_c^1(\mathbb{R}^2)} \\ &= \Big\langle \mu_j(s,\,dQ),\,(\mathrm{grad}_Q\varphi)(Q)\cdot A(s,\,Q)\Big\rangle_{Q\in K} \\ &= -\mathrm{grad}_Q\varphi\big(Q_j(s)\big)\cdot A\big(s,\,Q_j(s)\big) \\ &= -\mathrm{grad}_Q\varphi\big(Q^j(\sigma)\big)\cdot A\big(s,\,Q^j(\sigma)\big). \end{aligned} \tag{50}$$

Since $Q^j = Q^j(\tau)$ is a solution of the dynamical system (1) with parameter ε_j we end up with

$$\begin{aligned} X_1(s) &= \mathrm{grad}_Q\varphi\big(Q^j(\sigma)\big)\cdot\frac{d}{d\tau}Q^j(\sigma) \\ &= \mathrm{grad}_Q\varphi\big(Q_j(s)\big)\cdot\varepsilon_j\frac{d}{dt}Q_j(s) \\ &= \varepsilon_j\frac{d}{dt}(\varphi\circ Q_j)(s). \end{aligned} \tag{51}$$

Finally we find

$$\begin{aligned} \Big|\frac{1}{\gamma}\int_t^{t+\gamma} X_1(s)\,ds\Big| &= \Big|\frac{\varepsilon_j}{\gamma}\int_t^{t+\gamma}\frac{d}{dt}(\varphi\circ Q_j)(s)\Big)\,ds\Big| \\ &= \frac{\varepsilon_j}{\gamma}\big|(\varphi\circ Q_j)(t+\gamma)-(\varphi\circ Q_j)(t)\big| \\ &\le \frac{2*\varepsilon_j}{\gamma}\,\|\varphi\|_\infty\,. \end{aligned} \tag{52}$$

Furthermore there holds

$$\begin{aligned} X_2(s) &:= \Big\langle \mathrm{div}_Q\big[\mu_j(s,\,dQ)\cdot\big\{A(t,\,Q)-A(s,\,Q)\big\}\big],\,\varphi\Big\rangle_{C_c^1(\mathbb{R}^2)} \\ &= \Big\langle \mu_j(s,\,dQ),\,\mathrm{grad}_Q\varphi(Q)\cdot\big\{A(t,\,Q)-A(s,\,Q)\big\}\Big\rangle_{Q\in K} \\ &= \Big\langle \mu_j(s,\,dQ),\,\partial_p\varphi(Q)\big\{\partial_qG(s,\,Q)-\partial_qG(t,\,Q)\big\}\Big\rangle_{Q\in K}. \\ &= \partial_p\varphi\big(Q_j(s)\big)\Big(\partial_qG\big(s,\,Q_j(s)\big)-\partial_qG\big(t,\,Q_j(s)\big)\Big). \end{aligned} \tag{53}$$

According to Assumption (1.3), the function ∂_qG is uniformly continuous on sets with finite energy. We find

$$\big|X_2(s)\big| \;\le\; \|\mathrm{grad}_Q\varphi\|_\infty\,m(t-s), \tag{54}$$

where m denotes the modulus of continuity of ∂_qG. The inequalities (52) and

(54) imply

$$
\begin{aligned}
\Big| \langle \operatorname{div}_Q \big[\mu_j^\gamma(t,\, dQ) \cdot A(t,\, Q) \big],\, \varphi \rangle_{C_c^1(\mathbb{R}^2)} \Big| =& \\
=& \ \frac{1}{\gamma} \int_t^{t+\gamma} X_1(s) + X_2(s)\, ds \\
\leq& \ \frac{2\varepsilon_j}{\gamma} \, \|\varphi\|_\infty + \frac{1}{\gamma} \, \|\operatorname{grad}_Q \varphi\|_\infty \int_t^{t+\gamma} m(t-s)\, ds \\
\leq& \ \frac{2\varepsilon_j}{\gamma} \, \|\varphi\|_\infty + m(\gamma) \, \|\operatorname{grad}_Q \varphi\|_\infty \, .
\end{aligned}
\tag{55}
$$

2. Let $\varphi = \varphi(Q) \in C_c^1(\mathbb{R}^2)$ be fixed and let

$$
\psi(Q) \ := \ A(t,\, Q) \cdot \operatorname{grad}_Q \varphi(Q). \tag{56}
$$

Corollary 2.5 provides a sequence $(\gamma_k)_k$ with $\gamma_k \to 0$, such that

$$
\big\langle \mu_\infty(t,\, dQ),\, \psi(Q) \big\rangle_{Q \in K} \ = \ \lim_{k \to \infty} \lim_{j \to \infty} \big\langle \mu_j^{\gamma_k}(t,\, dQ),\, \psi(Q) \big\rangle_{Q \in K} \, .
$$

almost everywhere on T. From (55) we obtain

$$
\big\langle \mu_\infty(t,\, dQ),\, \psi(Q) \big\rangle_{Q \in K} \ = \ 0 \tag{57}
$$

for almost every $t \in T$, and therefore

$$
\lfloor \mu_\infty,\, A \cdot \operatorname{grad}_Q \varphi \rfloor \ = \ 0. \tag{58}
$$

3. Let $(\varphi_n)_n$ be a dense sequence in $C_c^1(\mathbb{R}^2)$. For any n there exists a set $S_n \subset T$ such that $|S_n| = 0$ and

$$
\lfloor \mu_\infty,\, A \cdot \operatorname{grad}_Q \varphi_n \rfloor(t) \ = \ 0 \quad \forall\, t \in T \setminus S_n. \tag{59}
$$

We set $S = \bigcup_{n \in \mathbb{N}} S_n$. For any $t \in T \setminus S$ we find

$$
\langle \operatorname{div}_Q \big[\mu_\infty(t,\, dQ) \cdot A(t,\, Q) \big],\, \varphi_n \rangle_{C_c^1(\mathbb{R}^2)} \ = \ 0 \quad \forall\, n \in \mathbb{N}, \tag{60}
$$

and finally (48).

$\square$

This theorem has an important consequence. As we will see below, it provides that the measure $\mu_\infty(t)$ is completely determined by the energy measure $\nu_\infty(t)$. This fact will be explained in the following.

For a fixed energy value $e \in \mathcal{E}_t$ and fixed macro time $t \in T$ we consider the solution

$$\theta \quad \rightsquigarrow \quad \tilde{Q}_{t,e}(\theta), \quad 0 \leq \theta \leq \infty, \tag{61}$$

of the associated system at time t (cf. (11)) with initial data $\tilde{Q}^0_{t,e}$. The initial data $\tilde{Q}^0_{t,e}$ are choosen such that

$$\Psi_{\mathrm{e}}(t,\, \tilde{Q}^0_{t,e}) = e. \tag{62}$$

The function $\tilde{Q}_{t,e}$ describes an orbit Γ in the $(q,\, p)$ plane. Obviously, Γ depends on t because the associated system depends on t. The Assumption 1.3 provides, that Γ is closed. Furthermore, Γ depends on the initial data $\tilde{Q}^0_{t,e}$ only via the energy, i.e. $\Gamma = \Gamma_{t,e}$. We define a probability measure

$$\Delta_{t,e} = \Delta_{t,e}(dQ) \,\in\, \mathrm{Prob}\,(\mathbb{R}^2) \tag{63}$$

by

1. The support of $\Delta_{t,e}$ is $\Gamma_{t,e}$.
2. $\Delta_{t,e}$ is uniformly distributed along $\Gamma_{t,e}$.

These two properties imply

$$\big\langle \Delta_{t,e},\, \psi \big\rangle_{C(\mathbb{R}^2)} = \big|\Gamma_{t,e}\big|^{-1} \int\limits_{\Gamma_{t,e}} \psi\, d\sigma, \quad \forall\, \psi \,\in\, C(\mathbb{R}^2), \tag{64}$$

where σ denotes the measure on $\Gamma_{t,e}$.

It can be shown that any measure $\Delta_{t,e}$ solves the stationary LIOUVILLE equation (12) corresponding to the associated system (11), i.e. there holds

$$\mathrm{div}_Q \big[\Delta_{t,e}(dQ) \cdot A(t,\, Q)\big] \;=\; 0. \tag{65}$$

Another, but equivalent characterization of the measure $\Delta_{t,e}$ relates the measure to temporal averages of observables. In particular, for fixed t and e and for any observable $\psi \in C(K)$ there holds

$$\begin{aligned} \langle \Delta_{t,e},\, \psi \rangle_{C(K)} \;&=\; \big\langle \Delta_{t,e}(dQ),\, \psi(Q) \big\rangle_{Q \in K} \\ &=\; \lim_{\theta_{\mathrm{end}} \to \infty} \frac{1}{\theta_{\mathrm{end}}} \int\limits_0^{\theta_{\mathrm{end}}} \psi\big(\tilde{Q}_{t,e}(\theta)\big)\, d\theta. \end{aligned} \tag{66}$$

This formula reveals that the probability measure $\Delta_{t,e}$ describes an infinite number of oscillation of the associated system (11).

The measures $\Delta_{t,e}$ are in a certain sense fundamental solutions of (12), because any solution of (12) is a linear superposition of such measures $\Delta_{t,e}$ with fixed t. Regarding the case which is studied here, we summarize this result in the next theorem.

Theorem 3.5 *For almost every $t \in T$ and all $\psi \in C(K)$ there holds*

$$\big\langle \mu_\infty(t,\, dQ),\, \psi(Q) \big\rangle_{Q \in K} \;\; = \;\; \big\langle \nu_\infty(t,\, e),\, \phi_\psi(e) \big\rangle_{e \in L} \,. \tag{67}$$

where ϕ_ψ is a continuous function with respect to e with

$$\phi_\psi(e) := \big\langle \Delta_{t,\, e}(dQ),\, \psi(Q) \big\rangle_{Q \in \mathbb{R}} \,. \tag{68}$$

For shortness we omit the proof of Theorem 3.5.

There remains the determination of the energy measure $\nu_\infty(t)$ for all times t. This will be done in the next subsection. In particular we will prove, that for any macro time t we have a well defined energy value $e_\infty(t)$, i.e.

$$\nu_\infty(t) = \delta_{e_\infty(t)}, \tag{69}$$

and henceforth

$$\mu_\infty(t) = \Delta_{t,\, e_\infty(t)}. \tag{70}$$

We mention that

1. The existence of a well defined energy value $e_\infty(t)$ has to be proved. The YOUNG measure approach yields a priorily only the existence of an energy measure $\nu_\infty(t)$.
2. $e_\infty(t)$ generally varies with the macro time t.

The existence of a well defined energy value $e_\infty(t)$ allows the following interpretation of the decoupling of micro time and macro time. In the limiting case $\varepsilon = 0$ we have for any macro time t another microscopic oscillator. This oscillator is described by the associated system (11) and performs an infinite number of oscillations. The ergodic behavior of the microscopic oscillator is given by the measure $\mu_\infty(t)$ that describes temporal averages of observables, see Equation (66).

3.3 The evolution of $\nu_\infty(t)$

As mentioned at the end of the last subsection, we now will determine the energy measure ν_∞.

Theorem 3.6 *The energy measure ν_∞ satisfies the transport equation*

$$\partial_t \nu_\infty + \partial_e \big(h \nu_\infty \big) \;\; = \;\; 0, \tag{71}$$

where

$$h(t,\, e) \;\; = \;\; \big\langle \Delta_{t,\, e}(dQ),\, \partial_t G(t,\, Q) \big\rangle_{Q \in K} \,. \tag{72}$$

Proof: Let $t \in T$ and $\varphi \in C_0^1(L)$ with compact support be fixed. For any $j \in \mathbb{N}$ Equation (9) implies

$$
\begin{aligned}
\frac{d}{dt}\langle \nu_j(t,\,de),\,\varphi(e)\rangle_{e\in L} &= \frac{d}{dt}\varphi\big(e_j(t)\big) \\
&= \varphi'\big(e_j(t)\big)\frac{d}{dt}e_j(t) \\
&= \varphi'\big(e_j(t)\big)\partial_t G\big(t,\,Q_j(t)\big) \\
&= \Psi_1\big(t,\,Q_j(t)\big) \\
&= \big\langle \mu_j(t,\,dQ),\,\Psi_1(t,\,Q)\big\rangle_{Q\in K}. \qquad (73)
\end{aligned}
$$

where $\Psi_1(t,\,Q) = \partial_t G(t,\,Q)\varphi'\big(\Psi_e(t,\,Q)\big)$. We conclude

$$
\frac{d}{dt}\lfloor \nu_j,\,\varphi\rfloor = \lfloor \mu_j,\,\Psi_1\rfloor. \qquad (74)
$$

Now we can pass to the limit in the sense of YOUNG measures. We end up with

$$
\frac{d}{dt}\lfloor \nu_\infty,\,\varphi\rfloor = \lfloor \mu_\infty,\,\Psi_1\rfloor, \qquad (75)
$$

which is an equality of distributions. From Theorem (3.4) and the identity

$$
\begin{aligned}
\big\langle \Delta_{t,\,e}(dQ),\,\Psi_1(t,\,Q)\big\rangle_{Q\in K} &= \varphi'(e)\big\langle \Delta_{t,\,e}(dQ),\,\partial_t G(t,\,Q)\big\rangle_{Q\in K} \\
&= \varphi'(e)h(t,\,e) \qquad (76)
\end{aligned}
$$

we find

$$
\begin{aligned}
\lfloor \mu_\infty,\,\Psi_1\rfloor(t) &= \big\langle \mu_\infty(t,\,dQ),\,\Psi_1(Q,\,t)\big\rangle_{Q\in K} \\
&= \Big\langle \nu_\infty(t,\,de),\,\big\langle \Delta_{t,\,e}(dQ),\,\Psi_1(Q,\,t)\big\rangle_{Q\in K}\Big\rangle_{e\in L} \\
&= \Big\langle \nu_\infty(t,\,de),\,\varphi'(e)h(t,\,e)\Big\rangle_{e\in L} \\
&= \Big\langle h(t,\,e)\nu_\infty(t,\,de),\,\varphi'(e)\Big\rangle_{e\in L} \\
&= -\Big\langle \partial_e\big(h(t,\,e)\nu_\infty(t,\,de)\big),\,\varphi(e)\Big\rangle_{e\in L}. \qquad (77)
\end{aligned}
$$

Finally we conclude

$$
\begin{aligned}
\Big\langle \partial_t\nu_\infty(t,\,de),\,\varphi(e)\Big\rangle_{e\in L} &= \frac{d}{dt}\lfloor \nu_\infty,\,\varphi\rfloor(t) = \lfloor \mu_\infty,\,\Psi_1\rfloor(t) \\
&= -\Big\langle \partial_e\big(h(t,\,e)\nu_\infty(t,\,de)\big),\,\varphi(e)\Big\rangle_{e\in L}. \qquad (78)
\end{aligned}
$$

□

This Theorem implies the following

Corollary 3.7

1. *The energy measure $\nu_\infty(t)$ at time $t \in T$ is a delta distribution in $e_\infty(t)$, i.e.*

$$\nu_\infty(t) = \delta_{e_\infty(t)}. \tag{79}$$

2. *The function e_∞ is completely determined by the initial energy measure δ_{e^0}. In particular there holds*

$$\frac{d}{dt} e_\infty(t) = h\big(t,\, e_\infty(t)\big) \quad \textit{and} \quad e_\infty(0) = e^0. \tag{80}$$

Obviously, we obtain this nice result because we have assumed, that the initial data Q^0 do not depend on ε. However, Theorem 3.6 can be generalized to initial data that depend on ε.

For the Examples 1.1 and 1.2 the explicit form of Equation (80) is given by

$$\frac{d}{dt} e_\infty(t) = f(t) f'(t) \tag{81}$$

and

$$\frac{d}{dt} e_\infty(t) = d'(t) \Big\langle \Delta_{t,\, e_\infty(t)}(dQ),\; g'\big(d(t) + 2q\big) + g'\big(d(t) - 2q\big) \Big\rangle_{Q \in K}, \tag{82}$$

respectively.

Theorem 3.2 and Corollary 3.3 are immediate consequences of Corollary 3.7.

4 Summary

We have studied a simple dynamical equation (1) which describes the high frequent motion of a single particle under the influence of slowly varying external perturbations. Consequently, there are two different time scales, which are coupled by a small scaling parameter ε.

The theory of YOUNG measures provides an elegant description of the limiting case $\varepsilon \to 0$, where the time scales decouple. The main results can be summarized as follows.

1. The highly oscillating solutions of (1) converge to a unique limit measure μ_∞ whose disintegration is given by a family of probability measures $\{\mu_\infty(t)\}_t$.
2. For any macro time t there holds: The measure $\mu_\infty(t)$ is completely determined by the energy $e_\infty(t)$. In particular, $\mu_\infty(t)$ corresponds to an microscopic oscillator performing an infinite number of oscillations.

3. There exists a macroscopic evolution equation for the energy function $e_\infty(t)$.

Finally, we refer to [1], where these results are used in order to describe micro-macro transitions of atomic chains.

References

[1] W. Dreyer, M. Herrmann, *Towards rigorous micro-macro transitions: The microscopic oscillator motion.*, WIAS-Preprint No. 724 (2002).

[2] W. Dreyer, M. Kunik, *Cold, thermal and oscillator closure of the atomic chain*, J. Physics. A: Math. Gen **33**, pp. 2097-2129 (2000).

[3] A. Mielke, *Flow properties for Young-measure solutions of semilinear hyperbolic problems*, Proc. Roy. Soc. Edinburgh Sect. A **129(1)**, pp. 85-123, (1999).

[4] M. Taylor, *Partial Differential Equations, 3. Nonlinear Equations*, Springer, New York (1996).

[5] M. Valadier, *A course on Young measures*, Rend. Istit. Mat. Univ. Trieste **28** pp. 349-394 (1994).

[6] G. Warnecke, *Analytische Methoden in der Theorie der Erhaltungsgleichungen*, Teubner, Stuttgart (1999).