Asymptotics Problems for Laser-Matter Modeling; Quantum and Classical Models

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Abstract. This paper is devoted to the asymptotic analysis of both quantum and classical models which describe the evolution of electrons subject to the potential of an atomic crystal perturbed by the highly oscillating potential of external electro-magnetic waves. We derive either Einstein rate equations or diffusion equations with respect to the energy variable, depending on whether the initial model is quantum or classical. We point out the analogies and differences in the treatment of the two models, considering successively the cases of (quasi-)periodic perturbations or random ones. We point out the different role of the relaxation effects according to the nature of the perturbation.

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1. Introduction

We are interested in asymptotic problems motivated by the modeling of wave-particles interactions. Precisely, we consider the evolution of the electrons of an atomic crystal subject to electromagnetic solicitations. We consider two different frameworks:
- A classical framework, where electrons are seen as classical particles, and the unknown is their density in phase space $f(t,x,p) \geq 0$, so that $f(t,x,p)\,\mathrm{d}p\,\mathrm{d}x$ gives the number of charged particles at time $t \geq 0$ in the infinitesimal volume $\mathrm{d}p\,\mathrm{d}x$ centered at $(x,p) \in \mathbb{R}^D \times \mathbb{R}^D$, with space dimension $D \in \{1,2,3\}$. This quantity obeys a Vlasov-type equation

$$\partial_t f + \{H_{\mathrm{c}}, f\} = \frac{1}{\tau}\, Q_{\mathrm{c}}(f), \tag{1}$$

where

$$\{H_{\rm c}, f\} = \nabla_p H_{\rm c} \cdot \nabla_x f - \nabla_x H_{\rm c} \cdot \nabla_p f,$$

the Hamiltonian $H_{\rm c}$ being a (smooth enough) function $\mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}$.
- A quantum framework, where the unknown is a density matrix $(\rho(t;n,m))_{n,m\in\mathbb{N}}$ which describes the populations and coherences of the electrons on the various atomic levels. The diagonal elements $\rho(t;n,n)$ describe the probability of finding the system in the state characterized by the index n while off-diagonal elements $\rho(t;n,m)$, $n \neq m$, describe quantum coherences between the contributions of the different states n and m. The evolution of the density matrix is governed by

$$i\hbar\, \partial_t \rho + [H_{\rm q}, \rho] = \frac{1}{\tau}\, Q_{\rm q}(\rho), \tag{2}$$

where

$$[H_{\rm q}, \rho](n,m) = \sum_{k\in\mathbb{N}} \left(H_{\rm q}(n,k)\rho(k,m) - \rho(n,k)H_{\rm q}(k,m) \right),$$

the Hamiltonian $H_{\rm q}$ being a (possibly infinite) matrix. We can restrict to a finite set of energy levels by assuming that the coefficients vanish for $n, m \geq N$, for a fixed $N \in \mathbb{N}$.

In both situations, the dynamics is driven by a Hamiltonian H, and a certain interaction operator Q. We assume that H splits into a leading order contribution, say H_0, which is time independent, and a small perturbation, V, that (time-)oscillates very fast. Precisely, H_0 corresponds to the confining potential of the atomic nucleus, while V corresponds to the potential created by the wave. Let $0 < \varepsilon \ll 1$ be the ratio of the strength of the perturbation compared to the free Hamiltonian and let θ be the characteristic time scale of the evolution of the perturbation. Then, we have

$$H = \begin{cases} H_{0\rm c}(x,p) + \varepsilon V_{\rm c}(t, t/\theta; x, p), \\ H_{0\rm q}(n,m) + \varepsilon V_{\rm q}(t, t/\theta; n, m), \end{cases}$$

depending on the context. These quantities characterize the electro-magnetic interactions that the system is subject to, and the variations of the electro-magnetic waves are embodied into the potential V. Furthermore, the surrounding medium also produces some relaxation effects which are characterized by the operator Q, the detailed expression of which will be discussed later on, and the relaxation time $\tau > 0$. We consider the asymptotic regime that corresponds to the following scaling assumptions. Given time, length and momentum units T, L and P respectively, we suppose that

$$\frac{\mathrm{T} H_{0\rm c}}{\mathrm{LP}} \simeq \frac{1}{\varepsilon^2} \gg 1, \qquad \frac{\mathrm{T} H_{0\rm q}}{\hbar} \simeq \frac{1}{\varepsilon^2} \gg 1,$$

respectively, and

$$\frac{\mathrm{T}}{\theta} \simeq \frac{1}{\varepsilon^2}, \qquad \frac{\mathrm{T}}{\tau} = \frac{1}{\varepsilon^2}.$$

Therefore, we are concerned with the behavior of the following dimensionless versions of either (1) or (2), namely

$$\partial_t f + \frac{1}{\varepsilon^2}\{H_{0\rm c}, f\} + \frac{1}{\varepsilon}\{V_{\rm c}^{\varepsilon}, f\} = \frac{1}{\varepsilon^2}\, Q_{\rm c}(f), \tag{3}$$

or

$$i\partial_t \rho + \frac{1}{\varepsilon^2}[H_{0\mathrm{q}}, \rho] + \frac{1}{\varepsilon}[V_{\mathrm{q}}^{\varepsilon}, \rho] = \frac{1}{\varepsilon^2}\ Q_{\mathrm{q}}(\rho), \tag{4}$$

respectively, as $\varepsilon \to 0$, where from now on we adopt the notation $V_{\mathrm{c,q}}^{\varepsilon}(t) = V_{\mathrm{c,q}}(t, t/\varepsilon^2)$.

In the limit $\varepsilon \to 0$, we wish to describe the dynamics through a diffusion equation with respect to the "energy variable" in the classical case or to recover Einstein rate equations for quantum populations in the quantum case. Of course, the effective coefficients of the limit equations highly depend on the perturbation V^{ε}. We justify these asymptotic regimes when considering two kinds of fast oscillating perturbations:
- either the oscillations are random, and we obtain the limit equation for the expectations of the unknowns,
- or the oscillations are (quasi-)periodic oscillations.
However, the role of the relaxation effects are very different in the analysis of these situations: in the deterministic (quasi-periodic) framework, it is crucial to consider a non vanishing interaction operator Q, while we can remove it when dealing with random potentials. At first look, this can be compared with the analysis of the behavior of the solutions of

$$\partial_t u + \frac{1}{\varepsilon}\mathrm{div}_x(a^{\varepsilon}(t,x)u) = \eta\Delta_x u, \tag{5}$$

as $\varepsilon \to 0$, where a^{ε} is some oscillating velocity field. For $\eta > 0$ and under periodicity assumptions, the question is well understood, see [29], and the limit is indeed described by a diffusion equation (with a positive effective diffusivity that can be smaller than η, depending on the properties of a^{ε}, see [5], [29]). But, for $\eta = 0$, the behavior is much more involved and cannot be reduced to a so simple equation, as discussed under various approaches in [32, 23, 4, 1, 2]... When the variations of the velocity field are random, we can get rid of the diffusivity η and the limit remains described by a diffusion equation. This is reminiscent of the Kubo analysis [39]. There exists a huge literature on this topics, see e.g. [35, 34, 37]... or [38] for recent breakthrough concerning Hamiltonian systems and for a simple PDE approach [31]. A similar comparison can be made with kinetic equations subject to large oscillating potentials: see [28, 46] for deterministic examples or [24, 25, 6, 47] for random cases. A rough way to explain these different behaviors is to say that damping terms are necessary in the deterministic framework since they introduce irreversibility in the equation. In the random framework, irreversibility comes from the stochastic properties of the oscillations. Another picture of these phenomena can be found in the derivation of the Boltzmann equation from many particles systems [40]. In (3) and (4), the role of the operator Q, beyond its physical meaning, is to introduce some source of irreversibility into the $\varepsilon-$dependent equation. This operator provides some dissipation mechanism which turns out to be crucial for our analysis. The difficulty with dealing with completely reversible equations in the (quasi-)periodic framework can be illustrated by very simple examples: the quantum two-level system in Section 2.2, or classical particles subject to the harmonic potential $H_0(x,p) = (x^2+p^2)/2$ supplemented with the fast oscillating perturbation $\varepsilon\ x\ \cos(\omega t/\varepsilon^2)$ in Section 3.2. These examples are amenable to fully explicit computations that clarify the role of the damping terms.

Besides, the analysis of (3) and (4) is slightly more involved than those of (5) since, in the limit $\varepsilon \to 0$, we expect a coupling of the homogenization process to relaxation effects implying that the limit unknown (which we could call the local equilibrium) depends on a smaller set of variables

than the original unknown: in the classical case, the limit only depends on the energy $H_0(x,p)$; in the quantum case it only involves the level populations. Therefore, the leading order terms in the asymptotic expansion of the equations should provide some relaxation mechanism towards this manifold of equilibria, which leads to imposing some non-degeneracy assumptions on H_0. Since, from a physical viewpoint, these assumptions could be seen as somewhat unsatisfactory, they are replaced by the explicit introduction of the collision operator Q. Summarizing, we shall provide a mathematically rigorous theory of the asymptotic limits which lead from (3) to a diffusion equation in the energy variable and from (4) to Einstein rates equations in the following situations:
- either when V^ε oscillates in a (quasi-)periodic fashion, and with the introduction of an O(1) operator Q at the right hand side (Theorems 1 and 4);
- or when V^ε oscillates randomly, in which case we can either completely remove relaxations at the price of additional non degeneracy assumptions on H_0 (Theorems 2 and 5), or we can at least consider relaxation operators Q that vanish at a rate slower than ε^2 (Theorems 3 and 6).

This work completes the analysis of the quantum model in [11], [12] and those of the classical model in [19], [20] for periodic, quasi-periodic or, more generally "KBM" oscillations. In particular, we emphasize the numerous analogies between the two models (3) and (4) and we treat their asymptotic analysis in a unified way. Our approach is based on energy estimates and standard homogenization techniques for (quasi-)periodic PDEs: double-scale convergence [3, 44] and the use of suitable oscillating test functions, in the spirit of the seminal works [50, 51, 26, 27]. Hence, in the deterministic framework, the present proofs are based on somewhat different functional analytical tools than those of [11], [12] (possibly at the price of less precise results). In the random framework (which, for the present problem and to our knowledge, has not been treated in the literature so far), we follow the strategy introduced in the reference paper [47] which relies on short-time decorrelation properties. These techniques have been successfully used in various physical contexts [13, 41, 30, 31, 8]. The remainder of the paper is organized as follows. Section 2 is devoted to the quantum model, and Section 3 deals with the classical one. In both cases, we first introduce more details on the model, then we treat (quasi-)periodic oscillations and we end with the study of the random framework.

2. Quantum Model

2.1. Modeling Issues and Mathematical Preliminaries

Considering the quantum model (4), the relaxation operator is intended to describe the loss of coherence due to the interaction of the electrons with the surrounding medium [21, 42]. Precisely, for a given sequence $\{\rho(n,m),\ n\in\mathbb{N},\ m\in\mathbb{N}\}$, we set

$$P\rho(n,m)=\begin{cases}\rho(n,m) & \text{if } n=m,\\ 0 & \text{if } n\neq m,\end{cases}\qquad Q\rho(n,m)=i\gamma(n,m)(P-I)\rho(n,m),$$

with $\gamma(n,m)\geq 0$. The action of the free Hamiltonian $H_{0,\mathrm{q}}$ through the commutator $[H_{0,\mathrm{q}},\rho]$ only affects on the coherences; its action is essentially defined by the difference of energy levels. Namely, we suppose that

$$H_{0,\mathrm{q}}(n,m)=0 \qquad \text{if } n\neq m$$

which amounts to looking at the quantum system in the eigenbasis of the unperturbed Hamiltonian, and we set $\omega(n,m) = H_{0,\mathrm{q}}(m,m) - H_{0,\mathrm{q}}(n,n)$. Then, we have

$$[H_{0,\mathrm{q}}, \rho](n,m) = -\omega(n,m)\rho(n,m).$$

Therefore, we can rewrite (4) as follows

$$\partial_t \rho(n,m) = -\frac{1}{\varepsilon^2}(\mathrm{i}\omega(n,m) + \gamma(n,m))\rho(n,m) + \frac{i}{\varepsilon}\sum_{k\in\mathbb{N}}\Big[V^\varepsilon(n,k)\rho(k,m) - V^\varepsilon(k,m)\rho(n,k)\Big]. \tag{6}$$

Here and below, we assume

(*HQ1*) $\qquad \gamma(n,m) \geq 0, \qquad \gamma(n,n) = 0, \qquad \gamma(n,m) = \gamma(m,n),$

(*HQ2*) $\qquad \omega(n,m) = -\omega(m,n) \in \mathbb{R},$

(*HQ3*) $\qquad V^\varepsilon(t;n,k) = V(t,t/\varepsilon^2;n,k), \qquad V(t,\tau;n,k) = \overline{V(t,\tau;k,n)},$

(*HQ4*) $\qquad \sup_{t,\tau}\sup_{n\in\mathbb{N}}\sum_{k\in\mathbb{N}}|V(t,\tau;n,k)| + \sup_{t,\tau}\sum_{n\in\mathbb{N}}\sup_{k\in\mathbb{N}}|V(t,\tau;n,k)| = M < \infty.$

We set

$$Z(n,m) = \gamma(n,m) + \mathrm{i}\omega(n,m).$$

which thus vanishes when $n = m$ and verifies $\overline{Z(n,m)} = Z(m,n)$, as a consequence of (HQ1), (HQ2).

As usual, we shall denote by ℓ^2 the space of sequences $u : \mathbb{N} \to \mathbb{C}$, which are square summable. We also consider the Hilbert space of sequences with double index

$$\boldsymbol{\ell}^2 = \Big\{u : \mathbb{N}\times\mathbb{N} \to \mathbb{C}, \sum_{n,m\in\mathbb{N}} |u(n,m)|^2 < \infty\Big\}.$$

We denote by δ the sequence defined by

$$\delta(n,n) = 1, \qquad \delta(n,m) = 0 \quad \text{if } n \neq m.$$

For $u \in \ell^2$, we obviously have $u(n)\delta(n,m) \in \boldsymbol{\ell}^2$. Finally, it is convenient to introduce the following notation

$$\Theta^\varepsilon(t)[\rho](n,m) = i[V^\varepsilon(t),\rho](n,m) = i\sum_{k\in\mathbb{N}}\Big[V^\varepsilon(t;n,k)\rho(k,m) - V^\varepsilon(t;k,m)\rho(n,k)\Big].$$

As a matter a fact, we observe that $\Theta^\varepsilon(t)$ is a well defined operator on $\boldsymbol{\ell}^2$.

Lemma 1 *Suppose (HQ4). Then, $\{\Theta^\varepsilon(t),\ \varepsilon > 0, t \geq 0\}$ is a family of bounded operators on $\boldsymbol{\ell}^2$, the bound being independent on ε and t: for any $\rho \in \boldsymbol{\ell}^2$, we have*

$$\|\Theta^\varepsilon(t)[\rho]\|_{\boldsymbol{\ell}^2} \leq 2M\ \|\rho\|_{\boldsymbol{\ell}^2}.$$

We also remark that the adjoint operator satisfies $\Theta^\varepsilon(t)^\star = -\Theta^\varepsilon(t)$.

Then, we can easily show that (6) is a well posed problem, thanks to a standard fixed point reasoning applied to the following Duhamel form of the equation:

$$\rho(t;n,m) = \mathrm{e}^{-Z(n,m)t/\varepsilon^2}\rho(0;n,m) + \frac{1}{\varepsilon}\int_0^t \mathrm{e}^{-Z(n,m)(t-\sigma)/\varepsilon^2}\ \Theta^\varepsilon(\sigma)[\rho(\sigma)](n,m)\,\mathrm{d}\sigma. \tag{7}$$

Moreover, estimates on the $\boldsymbol{\ell}^2$ norm of the solution can be obtained: the starting point of our analysis is the following statement.

Proposition 1 *Suppose (HQ1), (HQ2), (HQ3), (HQ4). Consider a sequence of initial data such that*

$$(HQ5) \qquad \rho_0^\varepsilon(n,m) = \overline{\rho_0^\varepsilon(m,n)}, \qquad \sup_{\varepsilon>0}\|\rho_0^\varepsilon\|_{\boldsymbol{\ell}^2} = \sup_{\varepsilon>0}\left(\sum_{n,m\in\mathbb{N}}|\rho_0^\varepsilon(n,m)|^2\right)^{1/2} = M_0 < \infty.$$

Then, for any $\varepsilon > 0$, the problem (6) with $\rho|_{t=0} = \rho_0^\varepsilon$ has a unique solution $\rho^\varepsilon \in C^0(\mathbb{R}^+;\boldsymbol{\ell}^2)$. It satisfies $\rho^\varepsilon(t;n,m) = \overline{\rho^\varepsilon(t;m,n)}$. Furthermore, the sequence $(\rho^\varepsilon)_{\varepsilon>0}$ is bounded in $L^\infty(\mathbb{R}^+;\boldsymbol{\ell}^2)$.

If we strengthen (HQ1) as follows

$(HQ1')$ *There exists $\gamma > 0$ such that for any $(n,m) \in \mathbb{N}^2$, $n \neq m$, $\gamma(n,m) \geq \gamma > 0$,*

then, we have

$$\sup_{\varepsilon>0}\left(\frac{1}{\varepsilon^2}\int_0^\infty \sum_{n\neq m}|\rho^\varepsilon(t;n,m)|^2\,\mathrm{d}t\right) < \infty. \tag{8}$$

The difficulty of the asymptotics and the role of the damping term can be understood by looking at the simplest possible system: the two-level system.

2.2. The Two-level Model

We consider a quantum system with only two energy levels: the ground state, referred to by index 1, and an excited state, referred to by index 2. We set

$$V_{12}^\varepsilon = \overline{V_{21}^\varepsilon}, \qquad \omega_{21} = \omega = -\omega_{12}, \qquad \gamma_{12} = \gamma = \gamma_{21},$$

and we readily verify that $\rho_{12}^\varepsilon = \overline{\rho_{21}^\varepsilon}$ and $\rho_{11}^\varepsilon + \rho_{22}^\varepsilon$ remains constant. Since the density matrix has unit trace, this constant is 1. Let us assume furthermore $V_{11}^\varepsilon = V_{22}^\varepsilon$ (which is actually 0 in the dipolar approximation), so that the system becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{11}^\varepsilon = -\frac{2}{\varepsilon}\mathrm{Im}(V_{12}^\varepsilon\rho_{21}^\varepsilon), \qquad \frac{\mathrm{d}}{\mathrm{d}t}\rho_{21}^\varepsilon = -\frac{1}{\varepsilon^2}(\mathrm{i}\omega+\gamma)\rho_{21}^\varepsilon + \frac{i}{\varepsilon}V_{21}^\varepsilon(2\rho_{11}^\varepsilon - 1).$$

We define the perturbation as

$$V_{12}^\varepsilon(t) = \exp\left(i(\Delta+\omega)t/\varepsilon^2\right).$$

For the sake of simplicity, we set $\rho_{21}^\varepsilon(0) = 0$. We readily obtain that ρ_{11}^ε satisfies the following integral relation

$$\begin{aligned}\rho_{11}^\varepsilon(t) \;&=\; \rho_{11}(0) - 2\int_0^t \frac{1}{\gamma^2+\Delta^2}\ (2\rho_{11}^\varepsilon(s) - 1)\\ &\qquad \Big(\gamma[1 - \mathrm{e}^{-\gamma(t-s)/\varepsilon^2}\cos(\Delta(t-s)/\varepsilon^2)] + \Delta\mathrm{e}^{-\gamma(t-s)/\varepsilon^2}\sin(\Delta(t-s)/\varepsilon^2)\Big)\,\mathrm{d}s.\end{aligned}$$

Thus, for $\gamma > 0$, we check that the behavior of ρ_{11}^ε is close, as $\varepsilon \to 0$, to those of the solutions of the following Einstein rate equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{11} = \frac{2\gamma}{\gamma^2+\Delta^2}(\rho_{22}-\rho_{11}), \qquad \frac{\mathrm{d}}{\mathrm{d}t}(\rho_{11}+\rho_{22}) = 0.$$

This conclusion applies for the resonant case $\Delta = 0$ as well.

However, when $\gamma = 0$, ρ_{11}^ε presents an oscillating behavior. Indeed, we obtain

$$\rho_{11}^\varepsilon(t) = \frac{4}{4+\Delta^2/\varepsilon^2}(\rho_{11}(0)-1/2)\cos(\sqrt{4+\Delta^2/\varepsilon^2}\ t/\varepsilon) + \frac{1}{4+\Delta^2/\varepsilon^2}\Big(\frac{\Delta^2}{\varepsilon^2}\rho_{11}(0)+2\Big),$$

and the solution oscillates between the states $\rho_{11}(0)$, and $(4\rho_{22}(0)+\Delta^2\rho_{11}(0)/\varepsilon^2)/(4+\Delta^2/\varepsilon^2)$. This formula applies to the resonant case $\Delta = 0$ as well (in which case the population can be transfered completely into the excited state). This is the so-called Rabi oscillations phenomena.

This simple example shows that (6) has essentially an oscillating behavior when $\gamma = 0$; however, oscillations can be smoothed out in the limit $\varepsilon \to 0$ by the damping terms, assuming (HQ1'). We shall see that another way for smoothing out the oscillating behavior, even with a vanishing damping rate $\gamma = 0$, relies on the introduction of short-memory stochastic effects in the definition of the coefficients V^ε.

2.3. The Quantum Model with a (Quasi-)Periodic Perturbation

In this Section, we restrict to a very particular framework concerning the variations of the perturbation V^ε. Precisely, let $\mathbb{Y}$ stand for the unit cube in $\mathbb{R}^d$, $d \in \mathbb{N}$. We suppose that

$$(HQ-P1) \qquad \begin{cases} \text{There exist } \Omega \in \mathbb{R}^d \setminus \{0\}, \text{with rationally independent components,} \\ \text{such that } V^\varepsilon(t;n,m) = \mathcal{V}(t,\Omega t/\varepsilon^2;n,m), \\ \text{where } \vartheta \longmapsto \mathcal{V}(t,\vartheta;n,m) \text{is } \mathbb{Y}\text{−periodic.} \end{cases}$$

The periodicity assumptions means that $\mathcal{V}(t,\vartheta;n,m), = \mathcal{V}(t,\vartheta+\xi;n,m)$, for any $t \in \mathbb{R}$, $n,m \in \mathbb{N}$, $\vartheta \in \mathbb{Y}$ and $\xi \in \mathbb{Z}^d$. The vector Ω collects the frequencies of the oscillations present in the perturbation V^ε; it satisfies $\Omega\cdot\xi = 0$ for $\xi \in \mathbb{Q}^d$ iff $\xi = 0$. The simplest case where $d = 1$ corresponds to the usual framework of periodic oscillations. Note that (HQ3) and (HQ4) can be recast as

$$\begin{cases} \mathcal{V}(t,\vartheta;n,k) = \overline{\mathcal{V}(t,\vartheta;k,n)}, \\ \sup\limits_{t\ge 0,\ \vartheta\in\mathbb{Y}}\left(\sup\limits_{n\in\mathbb{N}}\sum\limits_{k\in\mathbb{N}}|\mathcal{V}(t,\vartheta;n,k)|\right) + \sup\limits_{t\ge 0,\ \vartheta\in\mathbb{Y}}\left(\sum\limits_{n\in\mathbb{N}}\sup\limits_{k\in\mathbb{N}}|\mathcal{V}(t,\vartheta;n,k)|\right) \le M < \infty \end{cases}$$

We also assume that $\mathcal{V}$ depends smoothly on the slow time variable, and satisfies

$$(HQ-P2) \qquad \sup_{t\ge 0,\ \vartheta\in\mathbb{Y}}\left(\sup_{n\in\mathbb{N}}\sum_{k\in\mathbb{N}}|\partial_t\mathcal{V}(t,\vartheta;n,k)| + \sum_{n\in\mathbb{N}}\sup_{k\in\mathbb{N}}|\partial_t\mathcal{V}(t,\vartheta;n,k)|\right) \le M < \infty.$$

2.3.1. Formal Asymptotics. Let us formally describe the asymptotics. We shall see how the strengthened condition (HQ1') is crucial. We expect that the behavior of the solution is driven by the specific frequencies of the perturbation; in turn, this motivates us to expand the solution as a double scale series, in the spirit of [9],

$$\rho^\varepsilon(t;n,m) = \rho^{(0)}(t,\Omega t/\varepsilon^2;n,m) + \varepsilon\rho^{(1)}(t,\Omega t/\varepsilon^2;n,m) + \varepsilon^2\rho^{(2)}(t,\Omega t/\varepsilon^2;n,m) + \dots$$

with the periodicity condition

$$\rho^{(i)}(t,\vartheta;n,m) = \rho^{(i)}(t,\vartheta+\xi;n,m)$$

for any $t \geq 0$, $\vartheta \in \mathbb{Y}$, $\xi \in \mathbb{N}^d$, $n,m \in \mathbb{N}$. Then, using the relation

$$\partial_t\Big(\rho(t,\Omega t/\varepsilon^2)\Big) = (\partial_t\rho)(t,\Omega t/\varepsilon^2) + \frac{1}{\varepsilon^2}(\Omega\cdot\nabla_\vartheta\rho)(t,\Omega t/\varepsilon^2)$$

and identifying terms arising with the same power of ε, we are led to the following equations

$$1/\varepsilon^2 \text{ terms:} \quad \Omega\cdot\nabla_\vartheta\rho^{(0)}(t,\vartheta;n,m) + Z(n,m)\rho^{(0)}(t,\vartheta;n,m) = 0, \tag{9}$$

$$1/\varepsilon^1 \text{ terms:} \quad \Omega\cdot\nabla_\vartheta\rho^{(1)}(t,\vartheta;n,m) + Z(n,m)\rho^{(1)}(t,\vartheta;n,m) = \Theta(t,\vartheta)[\rho^{(0)}(t,\vartheta)](n,m), \tag{10}$$

$$\begin{aligned} 1/\varepsilon^0 \text{ terms:} \quad & \Omega\cdot\nabla_\vartheta\rho^{(2)}(t,\vartheta;n,m) + Z(n,m)\rho^{(2)}(t,\vartheta;n,m) \\ & = -\partial_t\rho^{(0)}(t,\vartheta;n,m) + \Theta(t,\vartheta)[\rho^{(1)}(t,\vartheta)](n,m), \dots \end{aligned} \tag{11}$$

where $\Theta(t,\vartheta)$ stands for the bounded operator on $\boldsymbol{\ell}^2$ defined by

$$\Theta(t,\vartheta)[\rho](n,m) = i\sum_{k\in\mathbb{N}}\Big(\mathcal{V}(t,\vartheta;n,k)\rho(k,m) - \mathcal{V}(t,\vartheta;k,m)\rho(n,k)\Big).$$

Indeed, by (HQ4), we have for any $\rho \in \boldsymbol{\ell}^2$,

$$\sup_{t\geq 0,\ \vartheta\in\mathbb{Y}} \|\Theta(t,\vartheta)[\rho]\|_{\boldsymbol{\ell}^2} \leq 2M\ \|\rho\|_{\boldsymbol{\ell}^2}.$$

Then, the time variable t being only a parameter, we are led to investigate the following transport equation

$$\Omega\cdot\nabla_\vartheta R(\vartheta;n,m) + Z(n,m)R(\vartheta;n,m) = h(\vartheta;n,m) \tag{12}$$

with a given right-hand side

$$h \in L^2_\#(\mathbb{Y};\ell^2) = \Big\{f : \mathbb{R}^d\times\mathbb{N}\times\mathbb{N}\to\mathbb{C},\ \mathbb{Y}-\text{periodic wrt the first variable such that} \int_{\mathbb{Y}}\sum_{n,m\in\mathbb{N}}|f(\vartheta;n,m)|^2\,\mathrm{d}\vartheta < \infty\Big\}.$$

These equations are completely different depending if we look at the populations $n = m$, in which case $Z(n,m)$ vanishes, or the coherences $n \neq m$ in which case we shall require that $Z(n,m)$ has a non vanishing real part. Therefore, we shall use the following claim.

Lemma 2 *i) Let $Z \in \mathbb{C}$ with $\mathrm{Re}(Z) > 0$. Then, for any $h \in L^2_\#(\mathbb{Y})$, the Hilbert space of $\mathbb{Y}-$periodic functions which are square integrable on $\mathbb{Y}$, there exists a unique solution $R \in L^2_\#(\mathbb{Y})$ of*

$$\Omega\cdot\nabla_\vartheta R + ZR = h. \tag{13}$$

Precisely, the solution is explicitely given by

$$R(\vartheta) = -\int_0^{+\infty} \mathrm{e}^{-Z\sigma}\ h(\vartheta - \Omega\sigma)\,\mathrm{d}\sigma. \tag{14}$$

ii) When $Z = 0$, then $R \in L^2_\#$ satisfies $\Omega\cdot\nabla_\vartheta R = 0$ iff R does not depend on ϑ.

Proof. Observe that (14) defines an element of $L^2_\#(\mathbb{Y})$ since $\mathrm{Re}(Z) > 0$. We obtain formula (14) by integrating (13) along the characteristic lines:

$$\frac{\mathrm{d}}{\mathrm{d}\sigma}\Big(\mathrm{e}^{Z\sigma}R(\vartheta+\Omega\sigma)\Big) = \mathrm{e}^{Z\sigma}\ (\mathrm{ZR} + \Omega\cdot\nabla_\vartheta\mathrm{R})(\vartheta+\Omega\sigma) = \mathrm{e}^{Z\sigma}\ \mathrm{h}(\vartheta+\Omega\sigma).$$

Integration over $\sigma \in (-\infty, 0)$ leads to the result. Uniqueness of the solution is a consequence of the following energy estimate: after multiplication of (13) by $\overline{R}$ and passage to complex conjugates, we get:

$$\begin{aligned}
&\int_{\mathbb{Y}} \Omega \cdot \nabla_\vartheta |R|^2 \,\mathrm{d}\vartheta + \int_{\mathbb{Y}} (ZR\,\overline{R} + \overline{ZR}\,R)\,\mathrm{d}\vartheta \\
&= 0 + 2\mathrm{Re}(Z) \int_{\mathbb{Y}} |R|^2 \,\mathrm{d}\vartheta = \int_{\mathbb{Y}} (h\,\overline{R} + \overline{h}\,R)\,\mathrm{d}\vartheta \le 2\|h\|_{L^2(\mathbb{Y})}\|R\|_{L^2(\mathbb{Y})},
\end{aligned}$$

where we used the periodic boundary condition and the Cauchy-Schwarz inequality.

Clearly, constants are solutions of $\Omega \cdot \nabla_\vartheta R = 0$. Then, the proof of ii) simply relies on the Fourier expansion

$$R(\vartheta) = \sum_{\xi \in \mathbb{Z}^d} \widehat{R}(\xi) \mathrm{e}^{-2\mathrm{i}\pi\xi\cdot\vartheta}, \qquad \widehat{R}(\xi) = \int_{\mathbb{Y}} R(\vartheta) \mathrm{e}^{2\mathrm{i}\pi\xi\cdot\vartheta}\,\mathrm{d}\vartheta.$$

For a solution R of $\Omega \cdot \nabla_\vartheta R = 0$, we obtain $2\mathrm{i}\pi\ \Omega \cdot \xi\ \widehat{R}(\xi) = 0$. Since the components of Ω are rationally independent, it implies $\widehat{R}(\xi) = 0$ for any $\xi \in \mathbb{Z}^d \setminus \{0\}$, Accordingly, R does not depend on ϑ. ∎

Corollary 1 *Assume that $\gamma(n,m)$ fulfills the strengthened condition (HQ1'). Let $h \in L^2_\#(\mathbb{Y};\boldsymbol{\ell}^2)$ such that $h(n,n) = 0$ for any $n \in \mathbb{N}$. Then, there exists a solution $R \in L^2_\#(\mathbb{Y};\boldsymbol{\ell}^2)$ of (12) which is unique when imposing $R(n,n) = 0$.*

Proof. The only point that deserves to be discussed is to estimate the $L^2_\#(\mathbb{Y};\boldsymbol{\ell}^2)$ norm of the solution. This requires the bound from below on the relaxation coefficients (HQ1'). Indeed, the Cauchy-Schwarz inequality yields

$$\begin{aligned}
&\int_{\mathbb{Y}} \sum_{n,m} \Big| \int_0^\infty \mathrm{e}^{-\gamma(n,m)\sigma}\ \mathrm{e}^{-\mathrm{i}\omega(\mathrm{n,m})\sigma}\ h(\vartheta - \Omega\sigma; n,m)\,\mathrm{d}\sigma \Big|^2 \mathrm{d}\vartheta \\
&\qquad \le \sum_{n,m} \frac{1}{\gamma(n,m)} \int_0^\infty \mathrm{e}^{-\gamma(n,m)\sigma} \left(\int_{\mathbb{Y}} |h(\vartheta - \Omega\sigma; n,m)|^2 \,\mathrm{d}\vartheta \right) \mathrm{d}\sigma \\
&\qquad \le \sum_{n,m} \frac{1}{\gamma(n,m)^2} \int_{\mathbb{Y}} |h(\vartheta; n,m)|^2 \,\mathrm{d}\vartheta \le \frac{1}{\gamma^2} \|h\|^2_{\boldsymbol{\ell}^2}
\end{aligned}$$

∎

Let us go back to (9), (10), (11). At leading order, we thus have

$$\rho^{(0)}(t,\vartheta;n,n) = \rho^{(0)}(t;n,n), \qquad \rho^{(0)}(t,\vartheta;n,m) = 0 \quad \text{if } n \neq m.$$

Using this information, (10) becomes

$$(\Omega \cdot \nabla_\vartheta + Z(n,m))\rho^{(1)}(t,\vartheta;n,m) = i\ \mathcal{V}(t,\vartheta;n,m)(\rho^{(0)}(t;m,m) - \rho^{(0)}(t;n,n)).$$

When $n = m$, the right hand side vanishes, and $Z(n,n) = 0$ too, so that Lemma 2-ii) applies and the diagonal part $\rho^{(1)}(t,\vartheta;n,n)$ actually does not depend on the fast variable ϑ. For $n \neq m$, the solution factorizes, and we get

$$\begin{cases}
\rho^{(1)}(t,\vartheta;n,m) = i\chi(t,\vartheta;n,m)\ (\rho^{(0)}(t;m,m) - \rho^{(0)}(t;n,n)), \\
\chi(t,\vartheta;n,m) = -\displaystyle\int_0^{+\infty} \mathrm{e}^{-Z(n,m)\sigma}\ \mathcal{V}(t,\vartheta - \Omega\sigma;n,m)\,\mathrm{d}\sigma, \qquad n \neq m.
\end{cases}$$

The properties of the auxiliary function can be summarized as follows.

Lemma 3 *Assume that (HQ1), (HQ2), (HQ3), (HQ4) and the strengthened condition (HQ1') hold. Then χ satisfies $\chi(t,\vartheta;n,k)=\overline{\chi(t,\vartheta;k,n)}$ and*

$$\sup_{t\geq 0,\,\vartheta\in\mathbb{Y}}\sum_{n\in\mathbb{N}}\sup_{k\in\mathbb{N}}|\chi(t,\vartheta;n,k)|^2\leq\frac{M^2}{\gamma^2}.$$

Assuming (HQ-P2), a similar estimate holds for $\partial_t\chi(t,\vartheta;n,m)$.

In particular, observe that for $u\in\ell^2$, we have $\chi(t,\vartheta;n,m)u(m)\in L^\infty(\mathbb{R}^+\times\mathbb{Y};\boldsymbol{\ell}^2)$. Then, we use (11) to obtain a closed equation on $\rho^{(0)}$. Indeed, for $n=m$, we have

$$\Omega\cdot\nabla_\vartheta\rho^{(2)}(t,\vartheta;n,n)=-\partial_t\rho^{(0)}(t;n,n)+\Theta(t,\vartheta)[\rho^{(1)}(t,\vartheta)](n,n).$$

The condition $\int_{\mathbb{Y}}h\,\mathrm{d}\vartheta=0$ is at least a necessary condition to solve the equation $\Omega\cdot\nabla_\vartheta R=h$ (we do not claim that it is sufficient: this is a well known fact that the advection operator does not satisfy the Fredholm alternative; we refer to [19] and references therein for a detailed discussion on that question). Therefore, the compatibility condition leads to the following Einstein rate equation

$$\begin{aligned}\partial_t\rho^{(0)}(t;n,n)&=\int_{\mathbb{Y}}\Theta(t,\vartheta)[\rho^{(1)}(t,\vartheta)](n,n)\,\mathrm{d}\vartheta\\&=i\int_{\mathbb{Y}}\sum_{k\in\mathbb{N}}\Big(\mathcal{V}(t,\vartheta;n,k)\rho^{(1)}(t,\vartheta;k,n)-\mathcal{V}(t,\vartheta;k,n)\rho^{(1)}(t,\vartheta;n,k)\Big)\,\mathrm{d}\vartheta\\&=\sum_{k\in\mathbb{N}}A(t;n,k)\Big(\rho^{(0)}(t;k,k)-\rho^{(0)}(t;n,n)\Big)\end{aligned}$$

where

$$\begin{aligned}A(t;n,k)&=\int_{\mathbb{Y}}\Big(\mathcal{V}(t,\vartheta;n,k)\chi(t,\vartheta;k,n)+\mathcal{V}(t,\vartheta;k,n)\chi(t,\vartheta;n,k)\Big)\,\mathrm{d}\vartheta\\&=2\mathrm{Re}\int_{\mathbb{Y}}\mathcal{V}(t,\vartheta;n,k)\chi(t,\vartheta;k,n)\,\mathrm{d}\vartheta.\end{aligned}\tag{15}$$

(Remark that the diagonal part of $\rho^{(1)}$ does not enter this definition.) Using the definition of χ, we readily check that

$$A(t;n,k)=2\mathrm{Re}(Z(n,k))\int_{\mathbb{Y}}|\chi(t,\vartheta;n,k)|^2\,\mathrm{d}\vartheta>0,$$

for any $n\neq k$. This formal discussion can be made rigorous, which leads to the following statement.

Theorem 1 *Assume that (HQ1), (HQ2), (HQ3), (HQ4) and (HQ1') hold. Let the initial data ρ_0^ε satisfy (HQ5). We suppose that the coefficients are defined by (HQ-P1), and fulfill (HQ-P2). Then, up to a subsequence, ρ^ε converges to $\rho(t;n,n)\delta(n,m)$ weakly in $L^2(\mathbb{R}^+;\boldsymbol{\ell}^2)$; furthermore, the diagonal part $\rho^\varepsilon(t;n,n)$ converges to $\rho(t;n,n)$ in $C^0([0,T];\ell^2-weak)$‡, and the limit satisfies the Einstein rate equation*

$$\begin{cases}\partial_t\rho(t;n,n)=\displaystyle\sum_{k\in\mathbb{N}}A(t;n,k)(\rho(t;k,k)-\rho(t;n,n)),\\ \rho(0;n,n)=\displaystyle\lim_{\varepsilon\to 0}\rho_0^\varepsilon(n,n)\qquad\text{weakly in }\ell^2,\end{cases}\tag{16}$$

where the coefficients $A(t;n,k)$ are defined by (15). Since the solution of the limit problem is unique, if moreover $\rho_0^\varepsilon(n,n)\rightharpoonup\rho_0(n)$ weakly in ℓ^2, then the entire sequence converges.

‡ For a given Hilbert space H, a sequence of continuous functions $u_n:[0,T]\to H$ is said to converge to u in $C^0([0,T];H-weak)$, iff for any $\varphi\in H$, $\big(u_n(t),\varphi\big)_H$ converges to $\big(u(t),\varphi\big)_H$ as $n\to\infty$ uniformly on $[0,T]$.

2.3.2. Rigorous Proof. We propose a rigorous proof of Theorem 1 which is based on double scale convergence arguments. This tool has been introduced in [44] and [3] as an efficient way to obtain explicit formulae when dealing with homogenization problems with periodic variations of the coefficients, since it make a "zoom" on the specific frequencies present within the equation. The theory can be extended to more general oscillations, as in [15] or [45]. Considering quasi-periodic framework, we shall use the following claim.

Proposition 2 *Let u_ε be a bounded sequence in $L^2(\mathbb{R})$. Let $\Omega \in \mathbb{R}^d \setminus \{0\}$ the components of which are rationally independent. Then, there exists a subsequence, still labelled by ε, and a function $U \in L^2_\#(\mathbb{R} \times \mathbb{Y})$ such that for any trial function $\psi \in L^2(\mathbb{R}; C^0_\#(\mathbb{Y}))$,§ we have*

$$\lim_{\varepsilon\to 0} \int_{\mathbb{R}} u_\varepsilon(t)\ \psi(t, \Omega t/\varepsilon^2)\,\mathrm{d}t = \int_{\mathbb{R}}\int_{\mathbb{Y}} U(t,\vartheta)\ \psi(t,\vartheta)\ \mathrm{d}\vartheta\,\mathrm{d}t.$$

A detailed proof can be found in [19]. It adapts the arguments in [3], which are combined to the condition "Ω has rationally independent components"; this condition plays the role of an ergodic condition. Coming back to the problem under consideration, we have the following compactness statement.

Lemma 4 *There exists a function $R \in L^2_\#(\mathbb{R}^+ \times \mathbb{Y}; \boldsymbol{\ell}^2)$ and a subsequence still denoted by ρ^ε such that for any $\varphi \in C^0_{c\#}(\mathbb{R}^+ \times \mathbb{Y}; \boldsymbol{\ell}^2)$ ‖*

$$\lim_{\varepsilon\to 0} \int_0^\infty \sum_{n,m\in\mathbb{N}} \rho^\varepsilon(t;n,m)\ \overline{\varphi(t,\Omega t/\varepsilon^2;n,m)}\,\mathrm{d}t = \int_0^\infty \sum_{n,m\in\mathbb{N}} \int_{\mathbb{Y}} R(t,\vartheta;n,m)\ \overline{\varphi(t,\vartheta;n,m)}\,\mathrm{d}\vartheta\,\mathrm{d}t.$$

Let us multiply (6) by $\varphi(t,\Omega t/\varepsilon^2;n,m)$, where $\varphi \in C^\infty_c(\mathbb{R}^+ \times \mathbb{R}^d; \boldsymbol{\ell}^2)$ is a $\mathbb{Y}-$periodic function with respect to its second argument. We get

$$\begin{aligned} &\frac{\mathrm{d}}{\mathrm{d}t} \sum_{n,m\in\mathbb{N}} \rho^\varepsilon(t;n,m)\ \overline{\varphi(t,\Omega t/\varepsilon^2;n,m)} \\ &= \sum_{n,m\in\mathbb{N}} \rho^\varepsilon(t;n,m)\Big(\partial_t\overline{\varphi} + \frac{1}{\varepsilon^2}\Omega\cdot\nabla_\vartheta\overline{\varphi} - \frac{1}{\varepsilon^2}Z\overline{\varphi} - \frac{1}{\varepsilon}\overline{\Theta[\varphi]}\Big)(t,\Omega t/\varepsilon^2;n,m). \end{aligned}$$

After multiplication by ε^2, the limit $\varepsilon \to 0$ yields

$$\sum_{n,m\in\mathbb{N}} \int_0^\infty \int_{\mathbb{Y}} R(t,\vartheta;n,m)\ (\Omega\cdot\nabla_\vartheta\overline{\varphi} - Z\overline{\varphi})\,\mathrm{d}\vartheta\,\mathrm{d}t = 0.$$

This holds true for any test function φ, so that Lemma 2 applies, and we deduce that the double scale limit has only a diagonal part, which does not depend on the fast variable

$$R(t,\vartheta;n,m) = R(t;n,n)\ \delta(n,m).$$

§ We recall that the test function should be picked in a suitable space of admissible functions so that $\psi(t,\Omega t/\varepsilon^2)$ makes sense, which might lead to subtle measurability questions. Roughly speaking, regularity with respect to one variable, either the "slow" or the "fast" one, is required. Referring to [3], sp. paragraph 5, $L^2(\mathbb{R}; C^0_\#(\mathbb{Y}))$ is the space of (classes of) functions $\psi : \mathbb{R}\times\mathbb{R}^d \to \mathbb{R}$ which are measurable and square integrable with respect to the variable $t \in \mathbb{R}$, with values in the Banach space of continuous and $\mathbb{Y}-$periodic functions.

‖ the space of continuous functions $\varphi : \mathbb{R}^+ \times \mathbb{R}^d \to \boldsymbol{\ell}^2$ which are $\mathbb{Y}-$periodic with respect to the second variable and such that $\varphi(t,\vartheta;n,m)$ vanishes for t large enough.

Next, we use $\varphi(t,\vartheta;n,m) = \phi(n)\delta(n,m) + \varepsilon\psi(t,\vartheta;n,m)$ as a test function, with $\phi \in \ell^2$. The leading term is now $\mathrm{O}(1/\varepsilon)$, and we obtain

$$\sum_{n,m\in\mathbb{N}} \int_0^\infty \int_{\mathbb{Y}} R(t,\vartheta;n,m)(\Omega\cdot\nabla_\vartheta\overline{\psi} - Z\overline{\psi} - \overline{\Theta[\phi\delta]})(t,\vartheta;n,m)\,\mathrm{d}\vartheta\,\mathrm{d}t = 0.$$

However, we can get rid of the singular term by choosing $\psi(t,\vartheta;n,m)$ in such a way that

$$(\Omega\cdot\nabla_\vartheta - \overline{Z(n,m)})\psi(t,\vartheta;n,m) = \Theta[\phi\delta](t,\vartheta;n,m) = i\mathcal{V}(t,\vartheta;n,m)(\phi(m)-\phi(n)).$$

Namely, we set

$$\begin{aligned} &\psi(t,\vartheta;n,m) = i\widetilde{\chi}(t,\vartheta;n,m)\ (\phi(m)-\phi(n)),\\ &\widetilde{\chi}(t,\vartheta;n,m) = -\int_0^\infty \mathrm{e}^{\mathrm{i}\omega(\mathrm{n,m})\sigma}\mathrm{e}^{-\gamma(n,m)\sigma}\ \mathcal{V}(t,\vartheta+\Omega\sigma;n,m)\,\mathrm{d}\sigma, \qquad n\neq m. \end{aligned}$$

Of course $\widetilde{\chi}$ enjoys the same properties as χ in Lemma 3. In particular, ψ and $\partial_t\psi$ are admissible functions. For such a test function, we have

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\sum_{n,m\in\mathbb{N}} \rho^\varepsilon(t;n,m)\ &\overline{\phi(n)\delta(n,m) + \varepsilon\psi(t,\Omega t/\varepsilon^2;n,m)}\\ &= \sum_{n,m\in\mathbb{N}} \rho^\varepsilon(t;n,m)\ \overline{(-\Theta[\psi] + \varepsilon\partial_t\psi)(t,\Omega t/\varepsilon^2;n,m)}. \end{aligned} \tag{17}$$

First of all, combining this relation with the estimate in Lemma 3, we deduce that

$$\frac{\mathrm{d}}{\mathrm{d}t}\sum_{n,m\in\mathbb{N}} \rho^\varepsilon(t;n,m)\ \overline{\phi(n)\delta(n,m) + \varepsilon\psi(t,\Omega t/\varepsilon^2;n,m)}$$

is bounded in $L^\infty(0,T)$ for any $\phi\in\ell^2$. Hence, by virtue of the Arzela-Ascoli theorem,

$$\sum_{n,m\in\mathbb{N}} \rho^\varepsilon(t;n,m)\ \overline{\phi(n)\delta(n,m) + \varepsilon\psi(t,\Omega t/\varepsilon^2;n,m)}$$

lies in a compact set of $C^0([0,T])$. Using Lemma 3 again this is close, up to $\mathrm{O}(\varepsilon)$, to

$$\sum_{n\in\mathbb{N}} \rho^\varepsilon(t;n,n)\overline{\phi(n)}$$

which therefore lies in a compact set of $C^0([0,T])$ too. Combining this information with the separability of ℓ^2 and a diagonal argument, we show that we can extract a subsequence such that, for any $\phi\in\ell^2$,

$$\lim_{\varepsilon\to 0}\sum_{n\in\mathbb{N}} \rho^\varepsilon(t;n,n)\overline{\phi(n)} = \sum_{n\in\mathbb{N}} \rho(t;n,n)\overline{\phi(n)},$$

uniformly on $[0,T]$. Of course, we have

$$\rho(t;n,n) = \int_{\mathbb{Y}} R(t,\vartheta;n,n)\,\mathrm{d}\vartheta = R(t;n,n).$$

Eventually, as $\varepsilon\to 0$ in (17), we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\sum_{n\in\mathbb{N}} \rho(t;n,n)\ \overline{\phi(n)} = -\sum_{n,m\in\mathbb{N}} \int_{\mathbb{Y}} \rho(t;n,n)\delta(n,m)\ \overline{\Theta[\psi](t,\vartheta;n,m)}\,\mathrm{d}\vartheta$$

which corresponds to a "weak" formulation of (16). Indeed, we compute

$$\begin{aligned}
\int_{\mathbb{Y}} \Theta[\psi](t,\vartheta;n,n)\,\mathrm{d}\vartheta &= \mathrm{i}\sum_{k\in\mathbb{N}} \int_{\mathbb{Y}} \Big(\mathcal{V}(t,\vartheta;n,k) i\widetilde{\chi}(t,\vartheta;k,n)(\phi(n)-\phi(k)) \\
&\qquad -\mathcal{V}(t,\vartheta;k,n) i\widetilde{\chi}(t,\vartheta;n,k)(\phi(k)-\phi(n))\Big)\,\mathrm{d}\vartheta \\
&= \sum_{k\in\mathbb{N}} \widetilde{A}(t;n,k)\ (\phi(k)-\phi(n)),
\end{aligned}$$

where

$$\begin{aligned}
\widetilde{A}(t;n,k) &= \int_{\mathbb{Y}} (\mathcal{V}(t,\vartheta;n,k)\widetilde{\chi}(t,\vartheta;k,n) + \mathcal{V}(t,\vartheta;k,n)\widetilde{\chi}(t,\vartheta;n,k))\,\mathrm{d}\vartheta \\
&= 2\mathrm{Re}\int_{\mathbb{Y}} \mathcal{V}(t,\vartheta;n,k)\widetilde{\chi}(t,\vartheta;k,n)\,\mathrm{d}\vartheta.
\end{aligned}$$

Then, using the definition of the auxiliary functions $\widetilde{\chi}$ and χ, we check that

$$\begin{aligned}
\widetilde{A}(t;n,k) &= 2\mathrm{Re}\int_{\mathbb{Y}} (\Omega\cdot\nabla_{\vartheta}\chi + Z(n,k))\chi(t,\vartheta;n,k) i\widetilde{\chi}(t,\vartheta;k,n)\,\mathrm{d}\vartheta \\
&= 2\mathrm{Re}\int_{\mathbb{Y}} \chi(t,\vartheta;n,k)(-\Omega\cdot\nabla_{\vartheta}\chi + Z(n,k))\widetilde{\chi}(t,\vartheta;k,n)\,\mathrm{d}\vartheta \\
&= 2\mathrm{Re}\int_{\mathbb{Y}} \chi(t,\vartheta;n,k)(-\mathcal{V}(t,\vartheta;k,n))\,\mathrm{d}\vartheta = -A(t;n,k).
\end{aligned}$$

This ends the proof of Theorem 1. ∎

2.4. The Quantum Model with a Random Perturbation

2.4.1. Random Potential; Statement of the Results. In this Section we shall consider random variations of the perturbation V^ε. To this aim, we need to recall a few definitions. Let $(\Omega,\mathcal{P},\mu)$ be a probability space (with μ a $\sigma-$finite measure). A random variable X is a measurable function on Ω. The expectation of such a random variable X is defined by

$$\text{For } X:\Omega\longrightarrow\mathbb{R},\qquad \mathbb{E}(X) = \int_{\Omega} X(\omega)\,\mathrm{d}\mu(\omega),$$

which makes sense when X is an integrable random variable. A quantity is said deterministic when it does not depend on the alea variable $\omega\in\Omega$.

Now, we suppose that

$$V^\varepsilon(t;n,m) = \mathcal{V}(t/\varepsilon^2;n,m)$$

is an integrable random variable (for the sake of simplicity, we assume that V^ε depends on time only through the "fast" variable). Accordingly, the solution of (6) depends on the realization of the event $\omega\in\Omega$ and the solution ρ^ε is a random function too. Our analysis relies on the following assumptions

$(HQ-R1)$ $\mathcal{V}(\tau;n,m)$ is a bounded random variable with $\mathbb{E}(\mathcal{V}(\tau;n,m))=0$,

$(HQ-R2)$ There exists a smooth function $\mathcal{R}:\mathbb{R}\times\mathbb{N}^4\to\mathbb{C}$, such that for every $k,l,m,n\in\mathbb{N}$, $\tau,\sigma\in[0,\infty)$:
$$\mathbb{E}(\mathcal{V}(\tau;k,l)\ \mathcal{V}(\sigma;m,n))=\mathcal{R}(\tau-\sigma;k,l,m,n).$$

$(HQ-R3)$ There exists a constant $\mathcal{T}>0$ such that for any $k,l,m,n\in\mathbb{N}$, and $\tau,\sigma\in[0,\infty)$, if $|\tau-\sigma|\geq\mathcal{T}$ then $\mathcal{V}(\tau;k,l)$ and $\mathcal{V}(\sigma;m,n)$ are independent random variables.

The basic assumptions (HQ3) and (HQ4) can be reformulated as follows

There exists a constant $M>0$ such that
$$\sup_\tau\sup_{n\in\mathbb{N}}\sum_{k\in\mathbb{N}}|\mathcal{V}(\tau;n,k)|+\sup_\tau\sum_{n\in\mathbb{N}}\sup_{k\in\mathbb{N}}|\mathcal{V}(\tau;n,k)|=M<\infty,$$
holds almost surely and we have $\mathcal{V}(\tau;n,k)=\overline{\mathcal{V}(\tau;k,n)}$.

Assumptions (HQ-R1) and (HQ-R2) mean that $\mathcal{V}$ is a centered and stationary random variable, respectively: the covariances of $\mathcal{V}$ evaluated at different times depend only on the differences between these times. Assumption (HQ-R3) is a cornerstone of the analysis; it can be seen as a Markov like assumption which plays a time-mixing role and excludes long-memory effects. This is reminiscent of the classical Kubo analysis, [39]. Notice that (HQ-R3) implies that $\tau\longmapsto\mathcal{R}(\tau;k,l,m,n)$ is supported in $[-\mathcal{T},+\mathcal{T}]$. When dealing with such a perturbation, the strong condition (HQ1') can be weakened, and we can consider relaxation coefficients $\gamma(n,m)$ that vanish, up to a suitable non degeneracy condition. Precisely, we shall prove the following statement.

Theorem 2 *Assume that (HQ1), (HQ2), (HQ3) and (HQ4) hold. Let the initial data ρ_0^ε be a deterministic quantity satisfying (HQ5). We suppose that $V^\varepsilon(t;n,m)=\mathcal{V}(t/\varepsilon^2;n,m)$ with $\mathcal{V}$ verifying (HQ-R1), (HQ-R2), (HQ-R3). We also require that*

$(HQ1'')$ $Z(n,m)=\gamma(n,m)+\mathrm{i}\omega(n,m)$ vanishes iff $n=m$

Let $0<T<\infty$. Then, up to a subsequence, $\mathbb{E}\rho^\varepsilon(t;n,m)$ converges in $L^\infty(\mathbb{R}^+,\boldsymbol{\ell}^2)$ weakly-$\star$ to $\rho(t;n,n)\delta(n,m)$ and $\mathbb{E}\rho^\varepsilon(t;n,n)$ converges in $C^0([0,T],\ell^2-weak)$ to $\rho(t;n,n)\in L^\infty(\mathbb{R}^+;\ell^2)$, solution of the following Einstein rate equation
$$\begin{cases}\partial_t\rho(t;n,n)=\displaystyle\sum_{k\in\mathbb{N}}A(n,k)(\rho(t;k,k)-\rho(t;n,n)),\\ \rho(0;n,n)=\displaystyle\lim_{\varepsilon\to0}\rho^\varepsilon(0;n,n)\qquad\text{weakly in }\ell^2,\end{cases}\tag{18}$$
where the coefficients are given by
$$A(n,k)=2\mathrm{Re}\int_0^{\mathcal{T}}\mathcal{R}(\tau;n,k,k,n)\ \mathrm{e}^{-Z(k,n)\tau}\,\mathrm{d}\tau.\tag{19}$$

The new assumption (HQ1") is a non degeneracy hypothesis. In particular, it holds when the energy levels are non degenerate: $\omega(n,m)\neq0$ for any $n\neq m$, in which case we can assume that all the $\gamma(n,m)$'s vanish. However, this situation is questionable in view of applications: recall that $\omega(n,m)=H_0(m,m)-H_0(n,n)$ where the $H_0(n,n)$ are eigenvalues of a certain differential operator.

Assuming that all the energy levels are non degenerate means that all eigenspaces have dimension one. In fact (HQ1”) tells us that we should consider positive relaxations for degenerate energy levels which correspond to multi-dimensional eigenspaces. This hypothesis is crucial to conclude that the behavior as $\varepsilon \to 0$ is governed by the evolution of populations only. Another possibility would be to consider $\varepsilon-$dependent coefficients $\gamma^\varepsilon(n,m) > 0$ that might tend to 0 as we do in the following Theorem.

Theorem 3 *Assume that (HQ2), (HQ3) and (HQ4) hold. Let the initial data ρ_0^ε be a deterministic quantity satisfying (HQ5). We suppose that $V^\varepsilon(t;n,m)$ reads $\mathcal{V}(t/\varepsilon^2;n,m)$ with $\mathcal{V}$ verifying (HQ-R1), (HQ-R2), (HQ-R3). We consider the problem (4) with a sequence of coefficients verifying $\gamma^\varepsilon(n,n) = 0$ and for any $n \neq m$*

$$(HQ1''') \quad \begin{cases} 0 < \gamma_\star^\varepsilon \le \gamma^\varepsilon(n,m) = \gamma^\varepsilon(m,n) \le \Gamma < \infty, & \displaystyle\lim_{\varepsilon\to 0} \frac{\varepsilon^2}{\gamma_\star^\varepsilon} = 0, \\ \displaystyle\lim_{\varepsilon\to 0} \gamma^\varepsilon(n,m) = \gamma(n,m) \ge 0. \end{cases}$$

Let $0 < T < \infty$. Then, the off-diagonal part $\rho^\varepsilon(t;n,m)(1-\delta(n,m))$ tends strongly to 0 in $L^2(\mathbb{R}^+, \boldsymbol{\ell}^2)$ while, up to a subsequence, $\mathbb{E}\rho^\varepsilon(t;n,n)$ converges in $C^0([0,T];\ell^2-weak)$ to the solution $\rho(t;n,n) \in L^\infty(\mathbb{R}^+;\ell^2)$ of the Einstein rate equation (18), (19).

2.4.2. Proof of Theorem 2. From now on we suppose that (HQ-R1), (HQ-R2), (HQ-R3) are fulfilled. Let us integrate (6) over the time interval (s,t). We get for $t, s \ge 0$

$$\rho^\varepsilon(t;n,m) = \mathrm{e}^{-Z(n,m)(t-s)/\varepsilon^2}\rho^\varepsilon(s;n,m) + \frac{1}{\varepsilon}\int_s^t \mathrm{e}^{-Z(n,m)(t-\sigma)/\varepsilon^2}\ \Theta^\varepsilon(\sigma)[\rho^\varepsilon(\sigma)](n,m)\,\mathrm{d}\sigma. \tag{20}$$

First, using this formula with $s = 0$ (see (7)), and assuming that the initial data is deterministic, we remark that $\rho^\varepsilon(t)$ only depends on the realizations of $V^\varepsilon(\sigma)$ for $0 \le \sigma \le t$. Consequently, we obtain the following key property.

Lemma 5 *Suppose that the initial data ρ_0^ε is deterministic. Then, $V^\varepsilon(t')$ and $\rho^\varepsilon(t)$ are independent provided $t' \ge t + \varepsilon^2\mathcal{T}$.*

Secondly, combining (20) and Lemma 1 leads to the following continuity estimate.

Lemma 6 *Suppose that $0 \le \gamma(n,m) \le \Gamma \le \infty$. For any t, $t+h \ge 0$, we have*

$$\|\rho^\varepsilon(t;n,m) - \mathrm{e}^{Z(n,m)h/\varepsilon^2}\rho^\varepsilon(t+h;n,m)\|_{\boldsymbol{\ell}^2} \le 2M\ M_0\ \mathrm{e}^{\Gamma\max(0,h)/\varepsilon^2}\ \frac{|h|}{\varepsilon}.$$

We point out that this estimate is not uniform with respect to ε, and thus does not provide any compactness on ρ^ε. However, it will be very useful when estimating some remainder terms in the evolution of $\mathbb{E}\rho^\varepsilon$. Eventually, we can insert (20), with $s = t - \varepsilon^2\mathcal{T}$ into (6). It is convenient to introduce the multiplication operator

$$\mathrm{e}^{-Z\tau} : \rho \in \boldsymbol{\ell}^2 \longmapsto \mathrm{e}^{-Z(n,m)\tau}\rho(n,m) \in \boldsymbol{\ell}^2,$$

and we obtain

$$\begin{aligned} \partial_t\rho^\varepsilon(t;n,m) \ &= \ -\frac{1}{\varepsilon^2}Z(n,m)\rho^\varepsilon(t;n,m) \\ &\quad \left.+\frac{1}{\varepsilon}\Theta^\varepsilon(t)[\mathrm{e}^{-Z\mathcal{T}}\rho^\varepsilon(t-\varepsilon^2\mathcal{T})](n,m) \right\} = D^\varepsilon(t;n,m) \\ &\quad \left.+\frac{1}{\varepsilon^2}\Theta^\varepsilon(t)\left[\int_{t-\varepsilon^2\mathcal{T}}^t \mathrm{e}^{-Z(t-\sigma)/\varepsilon^2}\Theta^\varepsilon(\sigma)[\rho^\varepsilon(\sigma)]\,\mathrm{d}\sigma\right](n,m) \right\} = I^\varepsilon(t;n,m), \end{aligned}$$

for $t \geq \varepsilon^2 \mathcal{T}$. We rewrite the last term as the sum

$$
\begin{aligned}
I^\varepsilon(t;n,m) = {}& \frac{1}{\varepsilon^2}\left(\int_{t-\varepsilon^2\mathcal{T}}^t \Theta^\varepsilon(t)\mathrm{e}^{-Z(t-\sigma)/\varepsilon^2}\Theta^\varepsilon(\sigma)\,\mathrm{d}\sigma\right)\mathrm{e}^{Z(t-\sigma)/\varepsilon^2}[\mathbb{E}\rho^\varepsilon(t)](n,m) \quad \Big\} = L^\varepsilon(t;n,m)\\
&+\frac{1}{\varepsilon^2}\left(\int_{t-\varepsilon^2\mathcal{T}}^t \Theta^\varepsilon(t)\mathrm{e}^{-Z(t-\sigma)/\varepsilon^2}\Theta^\varepsilon(\sigma)[\rho(\sigma)-\mathrm{e}^{Z(t-\sigma)/\varepsilon^2}\mathbb{E}\rho^\varepsilon(t)]\,\mathrm{d}\sigma\right)(n,m) \quad \Big\} = R^\varepsilon(t;n,m).
\end{aligned}
$$

($D^\varepsilon(t)$ as "Delayed term", $L^\varepsilon(t)$ as "Leading term" and $R^\varepsilon(t)$ as "Remainder term"). The crucial observation is that taking the expectation makes the singular quantities vanish.

Proposition 3 *Let the assumptions of Theorem 2 be fulfilled. The following properties hold:*
i) $\mathbb{E}D^\varepsilon(t) = 0$,
ii) There exists a constant $C > 0$, depending only on M, M_0 and $\mathcal{T}$, such that

$$\sup_{t\geq\varepsilon^2\mathcal{T}} \|\mathbb{E}I^\varepsilon(t)\|_{\boldsymbol{\ell}^2} \leq C,$$

iii) There exists a constant $C > 0$, depending only on M, M_0 and $\mathcal{T}$, such that

$$\sup_{t\geq 2\varepsilon^2\mathcal{T}} \|\mathbb{E}R^\varepsilon(t)\|_{\boldsymbol{\ell}^2} \leq C\ \varepsilon,$$

iv) The expectation of the leading term can be recast as

$$\mathbb{E}L^\varepsilon(t;n,m) = \mathcal{Q}[\mathbb{E}\rho^\varepsilon(t)](n,m)$$

where $\mathcal{Q}$ is a bounded operator on $\boldsymbol{\ell}^2$ (which does not depend on ε).

Proof. Claim i) relies directly on Lemma 5, combined to Assumption (HQ-R1). Next, we get

$$\|I^\varepsilon(t)\|_{\boldsymbol{\ell}^2} \leq \frac{1}{\varepsilon^2}\ (2M)^2\ \|\rho^\varepsilon\|_{L^\infty(\mathbb{R}^+;\boldsymbol{\ell}^2)} \int_{t-\varepsilon^2\mathcal{T}}^t \mathrm{d}\sigma,$$

which proves ii). To prove property iii), we remark that, for $t-\varepsilon^2\mathcal{T} \leq \sigma \leq t$ and ζ given in $\mathbb{C}$, $\rho^\varepsilon(\sigma-\varepsilon^2\mathcal{T})$ and $V^\varepsilon(t)\mathrm{e}^{-\zeta(t-\sigma)/\varepsilon^2}V^\varepsilon(\sigma)$ are independent since $t,\sigma \geq \sigma-\varepsilon^2\mathcal{T}+\varepsilon^2\mathcal{T}$. This is a consequence of Lemma 5 again. In turn, we have

$$
\begin{aligned}
&\mathbb{E}\left(\int_{t-\varepsilon^2\mathcal{T}}^t \Theta^\varepsilon(t)\mathrm{e}^{-Z(t-\sigma)/\varepsilon^2}\Theta^\varepsilon(\sigma)\mathrm{e}^{-Z\mathcal{T}}\rho^\varepsilon(\sigma-\varepsilon^2\mathcal{T})\,\mathrm{d}\sigma\right)\\
&\qquad = \int_{t-\varepsilon^2\mathcal{T}}^t \mathbb{E}\Big(\Theta^\varepsilon(t)\mathrm{e}^{-Z(t-\sigma)/\varepsilon^2}\Theta^\varepsilon(\sigma)\Big)\ \mathrm{e}^{-Z\mathcal{T}}\ \mathbb{E}\rho^\varepsilon(\sigma-\varepsilon^2\mathcal{T})\,\mathrm{d}\sigma,
\end{aligned}
$$

for any $t \geq 2\varepsilon^2\mathcal{T}$. Hence, we get

$$
\begin{aligned}
\mathbb{E}R^\varepsilon(t) \ = \ & \frac{1}{\varepsilon^2}\mathbb{E}\int_{t-\varepsilon^2\mathcal{T}}^t \Theta^\varepsilon(t)\mathrm{e}^{-Z(t-\sigma)/\varepsilon^2}\Theta^\varepsilon(\sigma)[\rho^\varepsilon(\sigma)-\mathrm{e}^{-Z\mathcal{T}}\rho^\varepsilon(\sigma-\varepsilon^2\mathcal{T})]\,\mathrm{d}\sigma\\
&+\frac{1}{\varepsilon^2}\mathbb{E}\int_{t-\varepsilon^2\mathcal{T}}^t \Theta^\varepsilon(t)\mathrm{e}^{-Z(t-\sigma)/\varepsilon^2}\Theta^\varepsilon(\sigma)[\mathrm{e}^{-Z\mathcal{T}}\mathbb{E}\rho^\varepsilon(\sigma-\varepsilon^2\mathcal{T})-\mathrm{e}^{Z(t-\sigma)/\varepsilon^2}\mathbb{E}\rho^\varepsilon(t)]\,\mathrm{d}\sigma.
\end{aligned}
$$

We conclude by using Lemma 6, which allows us to estimate the $\boldsymbol{\ell}^2$ norm of both terms by

$$2M_0\ (2M)^3\ \frac{1}{\varepsilon^2}\ \frac{\varepsilon^2\mathcal{T}}{\varepsilon}\ \int_{t-\varepsilon^2\mathcal{T}}^t \mathrm{d}\sigma = 2M_0\ (2M)^3\ \mathcal{T}^2\ \varepsilon.$$

Eventually, we prove iii) by using the following computation: since

$$\mathbb{E}\Big(V^\varepsilon(t;j,k)V^\varepsilon(\sigma;l,m)\Big) = \mathcal{R}\Big(\frac{t-\sigma}{\varepsilon^2};j,k,l,m\Big),$$

for any $\zeta \in \mathbb{C}$ we are led to

$$\begin{aligned}
&\frac{1}{\varepsilon^2}\ \mathbb{E}\left(\int_{t-\varepsilon^2\mathcal{T}}^{t} V^\varepsilon(t;j,k)\mathrm{e}^{-\zeta(t-\sigma)/\varepsilon^2} V^\varepsilon(\sigma;l,m)\ \mathbb{E}\rho^\varepsilon(t;n,r)\,\mathrm{d}\sigma\right)\\
&= \int_{t-\varepsilon^2\mathcal{T}}^{t} \mathbb{E}\Big(V^\varepsilon(t;j,k)V^\varepsilon(\sigma;l,m)\Big)\ \mathrm{e}^{-\zeta(t-\sigma)/\varepsilon^2}\,\frac{\mathrm{d}\sigma}{\varepsilon^2}\ \mathbb{E}\rho^\varepsilon(t;n,r)\\
&= \int_0^{\mathcal{T}} \mathcal{R}(\tau;j,k,l,m)\ \mathrm{e}^{-\zeta\tau}\,\mathrm{d}\tau\ \mathbb{E}\rho^\varepsilon(t;n,r).
\end{aligned}$$

Hence, we check that

$$\begin{cases}
\mathbb{E}L^\varepsilon(t;n,m) \;=\; \mathcal{Q}[\mathbb{E}\rho^\varepsilon(t)](n,m),\\
\mathcal{Q}[\rho](n,m) = -\displaystyle\sum_{k,l\in\mathbb{N}}\Big(\int_0^{\mathcal{T}} \mathcal{R}(\tau;n,k,k,l)\ \mathrm{e}^{(Z(l,m)-Z(k,m))\tau}\,\mathrm{d}\tau\ \rho(l,m)\\
\qquad -\displaystyle\int_0^{\mathcal{T}} \mathcal{R}(\tau;n,k,l,m)\ \mathrm{e}^{(Z(k,l)-Z(k,m))\tau}\,\mathrm{d}\tau\ \rho(k,l)\\
\qquad -\displaystyle\int_0^{\mathcal{T}} \mathcal{R}(\tau;k,m,n,l)\ \mathrm{e}^{(Z(l,k)-Z(n,k))\tau}\,\mathrm{d}\tau\ \rho(l,k)\\
\qquad +\displaystyle\int_0^{\mathcal{T}} \mathcal{R}(\tau;k,m,l,k)\ \mathrm{e}^{(Z(n,l)-Z(n,k))\tau}\,\mathrm{d}\tau\ \rho(n,l)\Big).
\end{cases}$$

∎

Summarizing, we have obtained the following equation for $\mathbb{E}\rho^\varepsilon$, when $t \geq \varepsilon^2\mathcal{T}$,

$$\partial_t\mathbb{E}\rho^\varepsilon(t;n,m) + \frac{1}{\varepsilon^2}Z(n,m)\mathbb{E}\rho^\varepsilon(t;n,m) = \mathbb{E}I^\varepsilon(t;n,m) = \mathcal{Q}[\mathbb{E}\rho^\varepsilon(t)](n,m) + \mathbb{E}R^\varepsilon(t;n,m). \tag{21}$$

Recall that $Z(n,m) = \mathrm{i}\omega(n,m) + \gamma(n,m)$ vanishes iff $n = m$ by the non degeneracy condition (HQ1”). Thus, restricting (21) to the diagonal part of the density matrix, the singular term vanishes, while for $n \neq m$ we obtain

$$\lim_{\varepsilon\to 0} Z(n,m)\mathbb{E}\rho^\varepsilon(t;n,m) = 0 \qquad \text{in } \mathcal{D}'((0,\infty)).$$

We deduce the following compactness properties.

Lemma 7 *Possibly at the cost of extracting subsequences, we can suppose that $\mathbb{E}\rho^\varepsilon$ converges to some $\rho(t,n,m)$ in $L^\infty(\mathbb{R}^+;\boldsymbol{\ell}^2)$ weak$-\star$, which satifies $\rho(t;n,m) = 0$ if $n \neq m$. Furthermore, after a possible further extraction, we have*

$$\lim_{\varepsilon\to 0}\sum_{n\in\mathbb{N}} \mathbb{E}\rho^\varepsilon(t;n,n)\phi(n) = \sum_{n\in\mathbb{N}} \rho(t;n,n)\phi(n)\,,$$

for any $\phi \in \ell^2$, uniformly on any finite interval $[0,T]$.

Proof. A few words deserve to be said for proving the compactness since (21) applies for $t \geq \varepsilon^2\mathcal{T}$ only. Combining (21) to the Arzela-Ascoli proves that, for any fixed $\phi \in \ell^2$,

$$\Big\{\mathbb{E}\sum_{n\in\mathbb{N}} \rho^\varepsilon(t+\varepsilon^2\mathcal{T};n,n)\phi(n), \quad \varepsilon > 0\Big\}$$

lies in a compact set of $C^0([0,T])$, for any $0 < T < \infty$. However, since $Z(n,n) = 0$, reasoning as in Lemma 6 we obtain

$$\begin{aligned}
\|\rho^\varepsilon(t+\varepsilon^2\mathcal{T};n,n) - \rho^\varepsilon(t;n,n)\|_{\ell^2} &= \frac{1}{\varepsilon}\Big\|\int_t^{t+\varepsilon^2\mathcal{T}} \Theta^\varepsilon(\sigma)[\rho^\varepsilon(\sigma)](n,n)\,\mathrm{d}\sigma\Big\|_{\ell^2}\\
&\leq \frac{2M}{\varepsilon}\int_t^{t+\varepsilon^2\mathcal{T}} \|\rho^\varepsilon(\sigma)\|_{\boldsymbol{\ell}^2}\,\mathrm{d}\sigma \leq 2M\ M_0\ \mathcal{T}\ \varepsilon.
\end{aligned}$$

We deduce that $\{\mathbb{E}\sum_{n\in\mathbb{N}}\rho^\varepsilon(t;n,n)\phi(n),\ \varepsilon>0\}$ lies in a compact set of $C^0([0,T])$ too. We conclude by using the separability of ℓ^2 and a classical diagonal argument. ∎

We can now finish the proof of Theorem 2. Choosing $n=m$ in (21) and letting ε go to 0 yield

$$\partial_t\rho(t;n,n)=\mathcal{Q}[\rho(t)](n,n).$$

However, since the off-diagonal part of the limit density matrix vanishes, this is actually a closed equation for the populations, which reads as follows

$$\begin{aligned}\partial_t\rho(n,n) &= \sum_{k\in\mathbb{N}}\int_0^{\mathcal{T}}\Big(\mathcal{R}(\tau;n,k,k,n)\ \mathrm{e}^{-Z(k,n)\tau}+\mathcal{R}(\tau;k,n,n,k)\ \mathrm{e}^{-Z(n,k)\tau}\Big)\,\mathrm{d}\tau\ \rho(k,k)\\ &\quad -\rho(n,n)\sum_{k\in\mathbb{N}}\int_0^{\mathcal{T}}\Big(\mathcal{R}(\tau;n,k,k,n)\ \mathrm{e}^{-Z(k,n)\tau}+\mathcal{R}(\tau;k,n,n,k)\ \mathrm{e}^{-Z(n,k)\tau}\Big)\,\mathrm{d}\tau.\end{aligned}$$

Then, we remark that

$$\begin{aligned}\mathcal{R}(\tau;k,n,n,k)\mathrm{e}^{-Z(n,k)\tau} &= \mathbb{E}(\mathcal{V}(s+\tau;k,n)\mathcal{V}(s;n,k))\ \mathrm{e}^{-\mathrm{i}\omega(n,k)\tau}\ \mathrm{e}^{-\gamma(n,k)\tau}\\ &= \mathbb{E}(\overline{\mathcal{V}(s+\tau;n,k)}\ \overline{\mathcal{V}(s;k,n)})\ \mathrm{e}^{+\mathrm{i}\omega(k,n)\tau}\ \mathrm{e}^{-\gamma(k,n)\tau}\\ &= \overline{\mathcal{R}(\tau;n,k,k,n)\ \mathrm{e}^{-Z(k,n)\tau}}.\end{aligned}$$

Thus, we set

$$A(n,k)=2\mathrm{Re}\int_0^{\mathcal{T}}\mathcal{R}(\tau;n,k,k,n)\ \mathrm{e}^{-Z(k,n)\tau}\,\mathrm{d}\tau,$$

and we recognize the Einstein rate equation (18). ∎

We end this Section by discussing the non-negativity of the effective coefficients.

Lemma 8 *The coefficents $A(n,k)$ are non negative.*

Proof. The proof relies on the following observation, due to [47]: for any $F\in L^1(\mathbb{R})$, we have

$$\int_{\mathbb{R}}F(\tau)\,\mathrm{d}\tau=\lim_{R\to\infty}\frac{1}{2R}\int_{-R}^{+R}\int_{-R}^{+R}F(\sigma-\tau)\,\mathrm{d}\sigma\,\mathrm{d}\tau. \tag{22}$$

Indeed, remark that

$$\mathcal{R}(\tau;n,k,k,n)=\mathbb{E}\mathcal{V}(\tau;n,k)\mathcal{V}(0;k,n)=\mathbb{E}\mathcal{V}(0;k,n)\mathcal{V}(\tau;n,k)=\mathcal{R}(-\tau;k,n,n,k)=\overline{\mathcal{R}(\tau;k,n,n,k)}.$$

Hence, recalling (HQ1) and (HQ2), we can write

$$\begin{aligned}A(n,k) &= 2\mathrm{Re}\int_0^{\mathcal{T}}\mathcal{R}(\tau;n,k,k,n)\mathrm{e}^{-Z(k,n)\tau}\,\mathrm{d}\tau\\ &= 2\mathrm{Re}\int_{-\mathcal{T}}^0\mathcal{R}(\tau;k,n,n,k)\mathrm{e}^{Z(k,n)\tau}\,\mathrm{d}\tau=2\mathrm{Re}\int_{-\mathcal{T}}^0\mathcal{R}(\tau;n,k,k,n)\mathrm{e}^{Z(n,k)\tau}\,\mathrm{d}\tau\\ &= \mathrm{Re}\int_{-\mathcal{T}}^{+\mathcal{T}}\mathcal{R}(\tau;n,k,k,n)\mathrm{e}^{-\mathrm{i}\omega(k,n)\tau}\Big(\mathrm{e}^{-\gamma(k,n)\tau}\mathbb{1}_{\tau>0}+\mathrm{e}^{+\gamma(k,n)\tau}\mathbb{1}_{\tau<0}\Big)\,\mathrm{d}\tau.\end{aligned}$$

Note that the integral is taken over the interval $[-\mathcal{T},+\mathcal{T}]$ only, by virtue of (HQ-R3). Coming back to (22), we are led to compute $A(n,k)=\mathrm{Re}(\lim_{R\to+\infty} I_R/(2R))$, with

$$\begin{aligned}
I_R &= \int_{-R}^{+R}\int_{-R}^{+R} \mathcal{R}(\sigma-\tau;n,k,k,n)\mathrm{e}^{-\mathrm{i}\omega(k,n)(\sigma-\tau)}(\mathrm{e}^{-\gamma(k,n)(\sigma-\tau)}\mathbb{1}_{\sigma>\tau}+\mathrm{e}^{+\gamma(k,n)(\sigma-\tau)}\mathbb{1}_{\sigma<\tau})\,\mathrm{d}\sigma\,\mathrm{d}\tau\\
&= \int_{-R}^{+R}\int_{-R}^{+R} \mathbb{E}\mathcal{V}(\sigma;n,k)\mathcal{V}(\tau,k,n)\mathrm{e}^{-\mathrm{i}\omega(k,n)(\sigma-\tau)}(\mathrm{e}^{-\gamma(k,n)(\sigma-\tau)}\mathbb{1}_{\sigma>\tau}+\mathrm{e}^{+\gamma(k,n)(\sigma-\tau)}\mathbb{1}_{\sigma<\tau})\,\mathrm{d}\sigma\,\mathrm{d}\tau\\
&= \mathbb{E}\int_{-R}^{+R}\mathcal{V}(\sigma;n,k)\mathrm{e}^{-\mathrm{i}\omega(k,n)\sigma}\Big(\int_{-R}^{\sigma}\mathcal{V}(\tau;k,n)\mathrm{e}^{\mathrm{i}\omega(k,n)\tau}\mathrm{e}^{\gamma(k,n)\tau}\,\mathrm{d}\tau\Big)\mathrm{e}^{-\gamma(k,n)\sigma}\,\mathrm{d}\sigma\\
&\quad+\mathbb{E}\int_{-R}^{+R}\mathcal{V}(\tau;k,n)\mathrm{e}^{\mathrm{i}\omega(k,n)\tau}\Big(\int_{-R}^{\tau}\mathcal{V}(\sigma;n,k)\mathrm{e}^{-\mathrm{i}\omega(k,n)\sigma}\mathrm{e}^{\gamma(k,n)\sigma}\,\mathrm{d}\sigma\Big)\mathrm{e}^{-\gamma(k,n)\tau}\,\mathrm{d}\tau.
\end{aligned}$$

Let us set

$$\mathcal{U}(\sigma)=\int_{-R}^{\sigma}\mathcal{V}(\tau;k,n)\mathrm{e}^{\mathrm{i}\omega(k,n)\tau}\mathrm{e}^{\gamma(k,n)\tau}\,\mathrm{d}\tau,\qquad \overline{\mathcal{U}(\sigma)}=\int_{-R}^{\sigma}\mathcal{V}(\tau;n,k)\mathrm{e}^{-\mathrm{i}\omega(k,n)\tau}\mathrm{e}^{\gamma(k,n)\tau}\,\mathrm{d}\tau.$$

We recognize that I_R is nothing but

$$\begin{aligned}
&\mathbb{E}\int_{-R}^{+R}\Big(\overline{\mathcal{U}'(\sigma)}\mathcal{U}(\sigma)+\mathcal{U}'(\sigma)\overline{\mathcal{U}(\sigma)}\Big)\mathrm{e}^{-2\gamma(k,n)\sigma}\,\mathrm{d}\sigma\\
&=\mathbb{E}\Big\{\frac{|\mathcal{U}(R)|^2}{2}\mathrm{e}^{-2\gamma(k,n)R}+\gamma(k,n)\int_{-R}^{+R}|\mathcal{U}(\sigma)|^2\mathrm{e}^{-2\gamma(k,n)\sigma}\,\mathrm{d}\sigma\Big\},
\end{aligned}$$

which is therefore non negative.

The proof of (22) starts with the following simple remark

$$\int_{\mathbb{R}}F(s)\,\mathrm{d}s=\frac{1}{2R}\int_{-R}^{+R}\int_{\mathbb{R}}F(s)\,\mathrm{d}s\,\mathrm{d}t=\frac{1}{2R}\int_{-R}^{+R}\Big(\int_{\mathbb{R}}F(\sigma-t)\,\mathrm{d}\sigma\Big)\,\mathrm{d}t.$$

Therefore, it suffices to show that

$$\lim_{R\to\infty}\frac{1}{2R}\Big(\int_{-R}^{+R}\int_{|\sigma|\geq R}|F(\sigma-t)|\,\mathrm{d}\sigma\Big)\,\mathrm{d}t=0.$$

Changing variables again, we reduce the problem to investigating the behavior of

$$\frac{1}{2R}\Big(\int_{-R}^{+R}\int_{s+t\geq R}|F(s)|\,\mathrm{d}s\Big)\,\mathrm{d}t,$$

for large R, and similarly for the quantity obtained by replacing $s+t\geq R$ by $s+t\leq -R$. The Fubini theorem allows us to rewrite this integral as

$$\frac{1}{2R}\int_0^\infty|F(s)|\Big(\int_{\mathbb{R}}\mathbb{1}_{-R\leq t\leq R}\mathbb{1}_{R-s\leq t}\,\mathrm{d}t\Big)\,\mathrm{d}s=\frac{1}{2R}\int_0^{2R}|F(s)|\Big(\int_{R-s}^{R}\mathrm{d}t\Big)\,\mathrm{d}s=\int_0^{2R}|F(s)|\frac{s}{2R}\,\mathrm{d}s.$$

A simple application of the Lebesgue theorem ends the proof. ∎

2.5. Proof of Theorem 3

We only sketch the main arguments, since the proof remains quite close to the previous one. First of all, we readily obtain the following estimates, for any $t\geq 0$,

$$\begin{cases}
\displaystyle\sum_{n,m\in\mathbb{N}}|\rho^\varepsilon(t;n,m)|^2+\int_0^t\sum_{n,m\in\mathbb{N}}|h^\varepsilon(s;n,m)|^2\,\mathrm{d}s\leq\sum_{n,m\in\mathbb{N}}|\rho^\varepsilon(0;n,m)|^2\leq M_0<\infty,\\
\displaystyle h^\varepsilon(t;n,m)=\frac{\sqrt{\gamma^\varepsilon(n,m)}}{\varepsilon}\,\rho^\varepsilon(t;n,m).
\end{cases}$$

This motivates to split the solution as follows

$$\rho^\varepsilon(t;n,m) = \rho^\varepsilon(t;n,n)\delta(n,m) + \frac{\varepsilon}{\sqrt{\gamma_\star^\varepsilon}}\,\widetilde{\rho}^\varepsilon(t;n,m)$$

where $\widetilde{\rho}^\varepsilon(t;n,m) = \frac{\sqrt{\gamma_\star^\varepsilon}}{\varepsilon}\rho^\varepsilon(t;n,m)(1-\delta(n,m))$ is thus bounded in $L^2(\mathbb{R}^+;\boldsymbol{\ell}^2)$. Therefore, the scaling assumption (HQ1"') implies that, up to a subsequence, $\rho^\varepsilon(t;n,m)$ converges to some $\rho(t;n,n)\delta(n,m)$ weakly in $L^2(0,T;\boldsymbol{\ell}^2)$, $0<T<\infty$. Then, we observe that

$$\partial_t\rho^\varepsilon(t;n,n) = \frac{1}{\sqrt{\gamma_\star^\varepsilon}}\Theta^\varepsilon(t)[\widetilde{\rho}^\varepsilon(t)](n,n), \tag{23}$$

while the evolution of the remainder is driven by

$$\partial_t\widetilde{\rho}^\varepsilon(t;n,m) + \frac{Z^\varepsilon(n,m)}{\varepsilon^2}\widetilde{\rho}^\varepsilon(t;n,m) = \frac{\sqrt{\gamma_\star^\varepsilon}}{\varepsilon^2}\Theta^\varepsilon(t)[\rho^\varepsilon(t)](n,m),$$

with the obvious notation $Z^\varepsilon(n,m) = \mathrm{i}\omega(n,m)+\gamma^\varepsilon(n,m)$. We deduce that, for $t\geq\varepsilon^2\mathcal{T}$,

$$\widetilde{\rho}^\varepsilon(t;n,m) = \mathrm{e}^{-Z^\varepsilon(n,m)\mathcal{T}}\widetilde{\rho}^\varepsilon(t-\varepsilon^2\mathcal{T};n,m) + \frac{\sqrt{\gamma_\star^\varepsilon}}{\varepsilon^2}\int_{t-\varepsilon^2\mathcal{T}}^t \mathrm{e}^{-Z^\varepsilon(n,m)(t-\sigma)/\varepsilon^2}\;\Theta^\varepsilon(\sigma)[\rho^\varepsilon(\sigma)](n,m)\,\mathrm{d}\sigma$$

holds for $t\geq\varepsilon^2\mathcal{T}$; we insert this formula into (23) and get

$$\begin{aligned}\partial_t\rho^\varepsilon(t;n,n) \;&=\; \frac{1}{\sqrt{\gamma_\star^\varepsilon}}\Theta^\varepsilon(t)\Big[\mathrm{e}^{-Z^\varepsilon\mathcal{T}}\widetilde{\rho}^\varepsilon(t-\varepsilon^2\mathcal{T})\Big](n,n)\\ &\quad+\frac{1}{\varepsilon^2}\int_{t-\varepsilon^2\mathcal{T}}^t\Theta^\varepsilon(t)\Big[\mathrm{e}^{-Z^\varepsilon(t-\sigma)/\varepsilon^2}\Theta^\varepsilon(\sigma)[\rho^\varepsilon(\sigma)]\Big](n,n)\,\mathrm{d}\sigma.\end{aligned}\tag{24}$$

(The notation $\mathrm{e}^{Z^\varepsilon t}$ still stands for the multiplication operator in $\boldsymbol{\ell}^2$ $\rho(n,m)\mapsto\mathrm{e}^{Z^\varepsilon(n,m)t}\rho(n,m)$; similarly, we shall use the operator $\mathrm{e}^{\mathrm{i}\omega t}:\rho(n,m)\mapsto\mathrm{e}^{\mathrm{i}\omega(n,m)t}\rho(n,m)$.) Of course, the decorrelation property Lemma 5 still holds so that the expectation of the first term at the right hand side of (24) vanishes, while the $\boldsymbol{\ell}^2$ norm of the second one is clearly dominated by

$$(2M)^2\;M_0\;\frac{1}{\varepsilon^2}\int_{t-\varepsilon^2\mathcal{T}}^t\mathrm{d}\sigma = (2M)^2\;M_0\mathcal{T}.$$

Reasoning like in the previous Section, this provides the compactness of $\mathbb{E}\rho^\varepsilon(t;n,n)$ in $C^0([0,T];\ell^2-$*weak*), since we also have

$$\|\rho^\varepsilon(t;n,n)-\rho^\varepsilon(s;n,n)\|_{\ell^2} = \left\|\frac{1}{\varepsilon}\int_s^t\Theta^\varepsilon(\sigma)[\rho^\varepsilon(\sigma)](n,n)\,\mathrm{d}\sigma\right\|_{\ell^2}\leq 2M\;M_0\;\frac{|t-s|}{\varepsilon}.$$

To conclude, we need further continuity estimates. To this end, we rewrite (4) as follows

$$\partial_t\rho^\varepsilon(t;n,m)+\frac{i}{\varepsilon^2}\omega(n,m)\rho^\varepsilon(t;n,m) = +\frac{1}{\varepsilon}\Theta^\varepsilon(t)[\rho^\varepsilon(t)](n,m) - \frac{\sqrt{\gamma^\varepsilon(n,m)}}{\varepsilon}\;h^\varepsilon(t;n,m),$$

which yields

$$\begin{aligned}&\left\|\rho^\varepsilon(t;n,m)-\mathrm{e}^{-\mathrm{i}\omega(n,m)(t-s)/\varepsilon^2}\rho^\varepsilon(s;n,m)\right\|_{\boldsymbol{\ell}^2}\\ &=\frac{1}{\varepsilon}\left\|\int_s^t\mathrm{e}^{-\mathrm{i}\omega(n,m)(t-\sigma)/\varepsilon^2}\Big(\Theta^\varepsilon(\sigma)[\rho^\varepsilon(\sigma)](n,m)-\sqrt{\gamma^\varepsilon(n,m)}h^\varepsilon(\sigma;n,m)\Big)\,\mathrm{d}\sigma\right\|_{\boldsymbol{\ell}^2}\\ &\leq\frac{|t-s|}{\varepsilon}\;2MM_0+\frac{\sqrt{|t-s|}}{\varepsilon}\sqrt{\Gamma}\left(\int_s^t\|h^\varepsilon(\sigma)\|_{\boldsymbol{\ell}^2}^2\,\mathrm{d}\sigma\right)^{1/2}.\end{aligned}\tag{25}$$

Then, we expand the second integral in the right hand side of (24)

$$\begin{cases} \dfrac{1}{\varepsilon^2}\displaystyle\int_{t-\varepsilon^2\mathcal{T}}^{t} \Theta^\varepsilon(t)\Big[\mathrm{e}^{-Z^\varepsilon(t-\sigma)/\varepsilon^2}\Theta^\varepsilon(\sigma)[\rho^\varepsilon(\sigma)]\Big](n,m)\,\mathrm{d}\sigma = L^\varepsilon(t;n,m)+R^\varepsilon(t;n,m), \\ L^\varepsilon(t;n,m) = \dfrac{1}{\varepsilon^2}\displaystyle\int_{t-\varepsilon^2\mathcal{T}}^{t} \Theta^\varepsilon(t)\Big[\mathrm{e}^{-Z^\varepsilon(t-\sigma)/\varepsilon^2}\Theta^\varepsilon(\sigma)[\mathbb{E}\rho^\varepsilon(t)]\Big](n,m)\,\mathrm{d}\sigma, \\ R^\varepsilon(t;n,m) = \dfrac{1}{\varepsilon^2}\displaystyle\int_{t-\varepsilon^2\mathcal{T}}^{t} \Theta^\varepsilon(t)\Big[\mathrm{e}^{-Z^\varepsilon(t-\sigma)/\varepsilon^2}\Theta^\varepsilon(\sigma)[\rho^\varepsilon(\sigma)-\mathbb{E}\rho^\varepsilon(t)]\Big](n,m)\,\mathrm{d}\sigma. \end{cases}$$

By using the decorrelation properties again, we can write the expectation of the remainder as follows, for any $t \geq 2\varepsilon^2\mathcal{T}$,

$$\begin{aligned} \mathbb{E}R^\varepsilon(t;n,m) \;&=\; \mathbb{E}\frac{1}{\varepsilon^2}\int_{t-\varepsilon^2\mathcal{T}}^{t} \Theta^\varepsilon(t)\Big[\mathrm{e}^{-Z^\varepsilon(t-\sigma)/\varepsilon^2}\Theta^\varepsilon(\sigma)[\mathrm{e}^{-\mathrm{i}\omega\mathcal{T}}\mathbb{E}\rho^\varepsilon(\sigma-\varepsilon^2\mathcal{T}) - \mathrm{e}^{-\mathrm{i}\omega(\sigma-t)}\mathbb{E}\rho^\varepsilon(t)]\Big](n,m)\,\mathrm{d}\sigma \\ &\quad +\mathbb{E}\frac{1}{\varepsilon^2}\int_{t-\varepsilon^2\mathcal{T}}^{t} \Theta^\varepsilon(t)\Big[\mathrm{e}^{-Z^\varepsilon(t-\sigma)/\varepsilon^2}\Theta^\varepsilon(\sigma)[\rho^\varepsilon(\sigma) - \mathrm{e}^{-\mathrm{i}\omega\mathcal{T}}\rho^\varepsilon(\sigma-\varepsilon^2\mathcal{T})]\Big](n,m)\,\mathrm{d}\sigma. \end{aligned}$$

This can be evaluated by using (25); we get,

$$\begin{aligned} \|\mathbb{E}R^\varepsilon(t)\|_{\boldsymbol{\ell}^2} \;&\leq\; \frac{1}{\varepsilon^2}(2M)^2\int_{t-\varepsilon^2\mathcal{T}}^{t}\mathbb{E}\left(\Big\|\mathrm{e}^{-\mathrm{i}\omega\mathcal{T}}\Big(\rho^\varepsilon(\sigma-\varepsilon^2\mathcal{T}) - \mathrm{e}^{-\mathrm{i}\omega(\sigma-\varepsilon^2\mathcal{T}-t)}\rho^\varepsilon(t)\Big)\Big\|_{\boldsymbol{\ell}^2} \right. \\ &\qquad\qquad \left. + \Big\|\rho^\varepsilon(\sigma) - \mathrm{e}^{-\mathrm{i}\omega\mathcal{T}}\rho^\varepsilon(\sigma-\varepsilon^2\mathcal{T})\Big\|_{\boldsymbol{\ell}^2}\right)\,\mathrm{d}\sigma \\ &\leq\; \frac{1}{\varepsilon^2}(2M)^2\int_{t-\varepsilon^2\mathcal{T}}^{t}\left(6MM_0\frac{\varepsilon^2\mathcal{T}}{\varepsilon} + \frac{\sqrt{2\varepsilon^2\mathcal{T}}}{\varepsilon}\sqrt{\Gamma}\mathbb{E}\Big(\int_{\sigma-\varepsilon^2\mathcal{T}}^{t}\|h^\varepsilon(\sigma')\|_{\boldsymbol{\ell}^2}^2\,\mathrm{d}\sigma'\Big)^{1/2}\right. \\ &\qquad\qquad \left. + \frac{\sqrt{\varepsilon^2\mathcal{T}}}{\varepsilon}\sqrt{\Gamma}\mathbb{E}\Big(\int_{\sigma-\varepsilon^2\mathcal{T}}^{\sigma}\|h^\varepsilon(\sigma')\|_{\boldsymbol{\ell}^2}^2\,\mathrm{d}\sigma'\Big)^{1/2}\right)\,\mathrm{d}\sigma \\ &\leq\; C\left(\varepsilon + \frac{1}{\varepsilon^2}\int_{t-\varepsilon^2\mathcal{T}}^{t}\mathbb{E}\Big(\int_{t-2\varepsilon^2\mathcal{T}}^{t}\|h^\varepsilon(\sigma')\|_{\boldsymbol{\ell}^2}^2\,\mathrm{d}\sigma'\Big)^{1/2}\mathrm{d}\sigma\right) \\ &\leq\; C\left(\varepsilon + \mathbb{E}\Big(\int_{t-2\varepsilon^2\mathcal{T}}^{t}\|h^\varepsilon(\sigma')\|_{\boldsymbol{\ell}^2}^2\,\mathrm{d}\sigma'\Big)^{1/2}\right) \end{aligned}$$

where the constant $C>0$ depends on $\mathcal{T}$, M, M_0 but does not depend on ε. For any $t \geq 2\varepsilon^2\mathcal{T}$, this quantity is bounded uniformly with respect to ε. Actually, it tends to 0 in L^2 norm since

$$\int_{2\varepsilon^2\mathcal{T}}^{\infty}\Big(\int_{t-2\varepsilon^2\mathcal{T}}^{t}\|h^\varepsilon(\sigma')\|_{\boldsymbol{\ell}^2}^2\,\mathrm{d}\sigma'\Big)\,\mathrm{d}t = \int_0^\infty\|h^\varepsilon(\sigma')\|_{\boldsymbol{\ell}^2}^2\Big(\int_{\sigma'}^{\sigma'+2\varepsilon^2\mathcal{T}}\mathrm{d}t\Big)\,\mathrm{d}\sigma' \leq M_0\,\varepsilon^2\mathcal{T}.$$

It remains to compute the leading order term, namely

$$\begin{aligned} \mathbb{E}L^\varepsilon(t;n,n) \;&=\; \frac{1}{\varepsilon^2}\int_{t-\varepsilon^2\mathcal{T}}^{t}\mathbb{E}\Theta^\varepsilon(t)\Big[\mathrm{e}^{-Z^\varepsilon(t-\sigma)/\varepsilon^2}\Theta^\varepsilon(\sigma)[\mathrm{e}^{-\mathrm{i}\omega(\sigma-t)}\mathbb{E}\rho^\varepsilon(t)]\Big](n,n)\,\mathrm{d}\sigma \\ &=\; \sum_{k,l\in\mathbb{N}}\Big(-\int_0^{\mathcal{T}}\mathcal{R}(\tau;n,k,k,l)\;\mathrm{e}^{(\mathrm{i}\omega(l,n)-Z^\varepsilon(k,n))\tau}\,\mathrm{d}\tau\;\mathbb{E}\rho^\varepsilon(t;l,n) \\ &\qquad + \int_0^{\mathcal{T}}\mathcal{R}(\tau;n,k,l,n)\;\mathrm{e}^{(\mathrm{i}\omega(k,l)-Z^\varepsilon(k,n))\tau}\,\mathrm{d}\tau\;\mathbb{E}\rho^\varepsilon(t;k,l) \\ &\qquad + \int_0^{\mathcal{T}}\mathcal{R}(\tau;k,n,n,l)\;\mathrm{e}^{(\mathrm{i}\omega(l,k)-Z^\varepsilon(n,k))\tau}\,\mathrm{d}\tau\;\mathbb{E}\rho^\varepsilon(t;l,k) \\ &\qquad - \int_0^{\mathcal{T}}\mathcal{R}(\tau;k,n,l,k)\;\mathrm{e}^{(\mathrm{i}\omega(n,l)-Z^\varepsilon(n,k))\tau}\,\mathrm{d}\tau\;\mathbb{E}\rho^\varepsilon(t;n,l)\Big). \end{aligned}$$

As ε goes to 0, this converges to

$$\sum_{k\in\mathbb{N}}\int_0^{\mathcal{T}}\Big(\mathcal{R}(\tau;n,k,k,n)\mathrm{e}^{-Z(k,n)\tau}+\mathcal{R}(\tau;k,n,n,k)\ \mathrm{e}^{-Z(n,k)\tau}\Big)\,\mathrm{d}\tau\ \rho(t;k,k)$$
$$-\sum_{k\in\mathbb{N}}\int_0^{\mathcal{T}}\Big(\mathcal{R}(\tau;n,k,k,n)\ \mathrm{e}^{-Z(k,n)\tau}+\mathcal{R}(\tau;k,n,n,k)\ \mathrm{e}^{-Z(n,k)\tau}\Big)\,\mathrm{d}\tau\ \rho(t;n,n),$$

and we recover the announced Einstein rate equations. ∎

3. Classical Model

3.1. Modeling Issues and Mathematical Preliminaries

Let us describe the specific relaxation operator that we use in (3). The operator is intended to mimic, at the classical level, the relaxation effect of the quantum relaxation operator. The classical counterpart of the quantum population is the number of particles on a given energy surface $\{(x,p)\in\mathbb{R}^{2D},\ H_0(x,p)=\text{Constant}\}$. Hence, we shall assume that this number is well defined and finite for almost all energy. Precisely, let us introduce the following requirements on the free Hamiltonian H_0.

(HC1) $\qquad H_0\in C^\infty(\mathbb{R}^{2D}),\ H_0(x,p)\geq -C_0$ for some $C_0\geq 0$, $\lim_{|(x,p)|\to\infty} H_0(x,p)=+\infty.$

(HC2) For almost all $E\in\mathbb{R}$, the set $\Sigma_E=\{(x,p)\in\mathbb{R}^{2D}$such that $H_0(x,p)=E\}$ is a smooth orientable $(2D-1)$ submanifold of $\mathbb{R}^{2D}$. For any such E, let $\mathrm{d}\Sigma_E(x,p)$ denote the induced euclidean surface measure. We define
$$\delta(H_0(x,p)-E):=\frac{\mathrm{d}\Sigma_E(x,p)}{|\nabla_{x,p}H_0(x,p)|}.$$
For any E, we suppose that Σ_E has finite measure
$$h_0(E):=\int_{\Sigma_E}\delta(H_0(x,p)-E)<+\infty,\qquad \text{a.e. } E\in\mathbb{R}.$$

These assumptionsℙ are fulfilled e.g. by the harmonic potential $H_{\text{harm}}(x,p)=(x^2+p^2)/2$, in which case energy shells simply reduce to spheres. Hypothesis (HC1) allows us to define the measure $\delta(H_0(x)-E)$ which is actually nothing but the microcanonical measure, or Liouville measure, on the energy shell $\Sigma_E=\{H_0(x,p)=E\}$.

The integral
$$\Pi f(E):=\frac{1}{h_0(E)}\int_{\Sigma_E}f(x,p)\ \delta(H_0(x,p)-E). \tag{26}$$
gives the number of particles in the energy shell Σ_E. Now, let us set
$$P:f\longmapsto Pf(x,p):=\Pi f(H_0(x,p)). \tag{27}$$
Going on with the analogy between classical and quantum mechanics leads to the following definition of the relaxation operator to be used in (3)
$$Q(f)=\gamma(Pf-f), \tag{28}$$

ℙ It would be more rigorous to consider $E\in H_0(\mathbb{R}^{2D})=\{H_0(x,p),\ (x,p)\in\mathbb{R}^{2D}\}$ instead of $E\in\mathbb{R}$, but we shall make the slight abuse of notation of considering $E\in\mathbb{R}$.

with $\gamma \geq 0$. This operator models relaxation phenomena that make the distribution of particles uniform on any energy shells. We will go back to the derivation of such an operator from the quantum equation via semi-classical limits in a forthcoming work (see [46] for a related question). For further purposes, let us collect the basic properties of the operator P.

Lemma 9 *The operator P satisfies:*
(i) P is a continuous projection operator on L^r spaces: $P(Pf) = Pf$ and $\|Pf\|_{L^r(\mathbb{R}^{2D})} \leq \|f\|_{L^r(\mathbb{R}^{2D})}$ for any $1 \leq r \leq \infty$.
(ii) P is conservative in the sense that for any integrable function, we get

$$\int_{\mathbb{R}^{2D}} Pf \,\mathrm{d}p\,\mathrm{d}x = \int_{\mathbb{R}^{2D}} f \,\mathrm{d}p\,\mathrm{d}x.$$

(iii) P is self-adjoint in $L^2(\mathbb{R}^{2D})$. Consequently, the following orthogonality property holds: for any function $f \in L^2(\mathbb{R}^{2D})$ and $\varphi : \mathbb{R} \to \mathbb{R}$ such that $(x,p) \longmapsto \varphi(H_0(x,p))$ lies in $L^2(\mathbb{R}^{2D})$, we have

$$\int_{\mathbb{R}^{2D}} \varphi(H_0(x,p))(I-P)f \,\mathrm{d}p\,\mathrm{d}x = 0.$$

(iv) P is a non negative operator: if $f \geq 0$ a.e., then $Pf \geq 0$ a.e. (x,p) too. Moreover, if $f \geq 0$ and $Pf = 0$ a.e. then $f = 0$ a.e.
(v) The operators $f \longmapsto Pf$ and $f \longmapsto \{H_0, f\}$ are orthogonal, in the sense that $P\{H_0, f\} = 0$, holds for any $f \in L^2(\mathbb{R}^{2D})$ such that $\{H_0, f\} \in L^2(\mathbb{R}^{2D})$. Consequently, for any $f, g \in L^2(\mathbb{R}^{2D})$ such that $\{H_0, f\}$ and $\{H_0, g\}$ belong to $L^2(\mathbb{R}^{2D})$, we have $P(\{H_0, f\}g) = -P(f\{H_0, g\})$.
(vi) The operator Q is a bounded operator on $L^2(\mathbb{R}^{2D})$ and for any $f \in L^2(\mathbb{R}^{2D})$, we have

$$-\int_{\mathbb{R}^{2D}} Q(f)f \,\mathrm{d}p\,\mathrm{d}x = \gamma \int_{\mathbb{R}^{2D}} |Pf - f|^2 \,\mathrm{d}p\,\mathrm{d}x \geq 0.$$

We refer to [19] for proofs, which are more or less direct consequences of the coarea formula

$$\int_{\mathbb{R}^{2D}} f(x,p) \,\mathrm{d}p\,\mathrm{d}x = \int_{\mathbb{R}} \left(\int_{\Sigma_E} f(x,p)\, \delta(H_0(x,p) - E) \right) dE, \tag{29}$$

for any function $f \in L^1(\mathbb{R}^{2D})$. In particular, we have

$$\int_{\mathbb{R}^{2D}} f(x,p) \,\mathrm{d}p\,\mathrm{d}x = \int_{\mathbb{R}} \Pi f(E)\, h_0(E)\, dE. \tag{30}$$

The starting point of our analysis relies on the following statement (which is the classical analog of Proposition 1).

Proposition 4 *Suppose (HC1), (HC2) and let $\gamma \geq 0$. Let V^ε be a smooth potential, say $V^\varepsilon \in C^2(\mathbb{R} \times \mathbb{R}^{2D})$ with bounded second order derivatives. Consider a sequence of initial data such that*

$$(HC3) \qquad f_0^\varepsilon(x,p) \geq 0, \qquad \sup_{\varepsilon > 0} \int_{\mathbb{R}^{2D}} |f_0^\varepsilon(x,p)|^2 \,\mathrm{d}p\,\mathrm{d}x = M_0 < \infty.$$

Then, for any $\varepsilon > 0$, the problem

$$\partial_t f^\varepsilon + \frac{1}{\varepsilon^2}\{H_0, f^\varepsilon\} + \frac{1}{\varepsilon}\{V^\varepsilon, f^\varepsilon\} = \frac{1}{\varepsilon^2}\gamma(Pf^\varepsilon - f^\varepsilon), \tag{31}$$

with $f|_{t=0} = f_0^\varepsilon$ has a unique (non-negative) solution $f^\varepsilon \in C^0(\mathbb{R}^+; L^2(\mathbb{R}^{2D}))$. Furthermore, the sequence $(f^\varepsilon)_{\varepsilon>0}$ is bounded in $L^\infty(\mathbb{R}^+; L^2(\mathbb{R}^{2D}))$. If $\gamma > 0$, then we also have

$$\sup_{\varepsilon>0} \left(\frac{\gamma}{\varepsilon^2} \int_0^\infty \int_{\mathbb{R}^{2D}} |(f^\varepsilon - Pf^\varepsilon)(t;x,p)|^2 \,\mathrm{d}p\,\mathrm{d}x\,\mathrm{d}t \right) \leq M_0 < \infty.$$

Actually, we can obtain more estimates. Indeed, for any convex function $\Psi : \mathbb{R}^+ \to \mathbb{R}^+$, $t \mapsto \int_{\mathbb{R}^{2D}} \Psi(f^\varepsilon)\,\mathrm{d}p\,\mathrm{d}x$ is a non increasing quantity and we can establish uniform estimates in any $L^r(\mathbb{R}^{2D})$ space, $1 \leq r \leq \infty$.

Our aim is to show that, up to some physically relevant assumptions on V^ε, the phase space density $f^\varepsilon(t; x, p)$ behaves like $F(t; H_0(x, p))$, where $F(t, E)$ satisfies a diffusion equation

$$\partial_t(h_0 F) - \partial_E(h_0 d\, \partial_E F) = 0, \tag{32}$$

with h_0 defined in (HC2). Coming back to the physical meaning, $h_0 F(E)\, dE$ can be interpreted as the number of particles having their energy in the interval $(E, E + dE)$ while $h_0 d\, \partial_E F(E)$ gives the density of the flux of particles through the energy surface Σ_E. The expression of the effective coefficient d, that will indeed be checked to be nonnegative, highly depends on the oscillating features of the potential V^ε. We shall describe the two different frameworks:
- either we deal with (quasi-)periodic oscillations, in which case the relaxation operator is crucial for smoothing out too sharp resonance effects.
- or V^ε is defined through a random variable with short-time memory, in which case we can neglect the relaxation effects (at least in the limit $\varepsilon \to 0$).

3.2. Liouville Equation with an Oscillating Potential: an explicit example

The solution of the kinetic equation

$$\partial_t f^\varepsilon + \frac{1}{\varepsilon^2}\{H_0, f^\varepsilon\} + \frac{1}{\varepsilon}\{V(t/\varepsilon^2), f^\varepsilon\} = 0,$$

with

$$H_0(x, p) = (x^2 + p^2)/2, \qquad V(t; x) = x \cos(\omega t)$$

can be explicitely computed. Indeed, let us consider the characteristics $(X^\varepsilon, P^\varepsilon)$ associated to the full Hamiltonian $H_0(x, p)/\varepsilon^2 + V(t/\varepsilon^2; x)/\varepsilon$. We have

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}s} X^\varepsilon(s; t, x, p) = \dfrac{1}{\varepsilon^2} P^\varepsilon(s; t, x, p), & X^\varepsilon(t; t, x, p) = x, \\[2ex] \dfrac{\mathrm{d}}{\mathrm{d}s} P^\varepsilon(s; t, x, p) = -\dfrac{1}{\varepsilon^2} X^\varepsilon(s; t, x, p) + \dfrac{1}{\varepsilon}\cos(\omega s/\varepsilon^2), & P^\varepsilon(t; t, x, p) = p. \end{cases}$$

Since the microscopic density is conserved along these curves, we get

$$f^\varepsilon(t; x, p) = f_0(X^\varepsilon(0; t, x, p), P^\varepsilon(0; t, x, p)).$$

Hence, we observe that f^ε has a very different behavior than that of a solution of a diffusion equation, see [19]. This illustrates the crucial role of the relaxation in the deterministic framework, or of the stochastic effects.

3.3. The Classical Model with a (Quasi-)Periodic Perturbation

We consider a perturbation V^ε which oscillates in a quasi-periodic way. Let $\mathbb{Y}$ be the unit cube in $\mathbb{R}^d$, for some integer $d \geq 1$. We assume that

$$\begin{cases} \text{There exists a vector } \Omega \in \mathbb{R}^d \setminus \{0\} \text{ and a smooth function} \\ \qquad\qquad \mathcal{V} : \mathbb{R}^d \times \mathbb{R}^{2D} \to \mathbb{R}, \\ \text{which is } \mathbb{Y}\text{-periodic with respect to the first argument, such that} \\ \qquad\qquad V^\varepsilon(t; x, p) = \mathcal{V}(t, \Omega t/\varepsilon^2; x, p). \end{cases}$$

Such a function can be written by means of its Fourier series

$$\mathcal{V}(t, \vartheta; x, p) = \sum_{\xi \in \mathbb{Z}^d} \widehat{\mathcal{V}}(t, \xi; x, p)\, \mathrm{e}^{2i\pi\xi\cdot\vartheta}, \qquad \widehat{\mathcal{V}}(t, \xi; x, p) = \int_{\mathbb{Y}} \mathcal{V}(t, \vartheta; x, p)\, \mathrm{e}^{-2i\pi\xi\cdot\vartheta}\, \mathrm{d}\vartheta.$$

Taking into account the oscillation frequencies of the perturbation, we expand the solution of (4)

$$f^\varepsilon(t; x, p) = F^{(0)}(t, \Omega t/\varepsilon^2; x, p) + \varepsilon F^{(1)}(t, \Omega t/\varepsilon^2; x, p) + \varepsilon^2 F^{(2)}(t, \Omega t/\varepsilon^2; x, p) + \ldots$$

where all functions $F^{(i)}$ are supposed $\mathbb{Y}-$periodic with respect to the second variable. Since

$$\partial_t \Big(F^{(i)}(t, \Omega t/\varepsilon^2; x, p) \Big) = \Big(\partial_t F^{(i)} + \frac{1}{\varepsilon^2}\, \Omega \cdot \nabla_\vartheta F^{(i)} \Big)(t, \Omega t/\varepsilon^2; x, p),$$

we introduce the operator

$$\mathcal{T} F = \Omega \cdot \nabla_\vartheta f F + \{H_0, F\} - Q(F),$$

the adjoint of which is $\mathcal{T}^\star \varphi = -\Omega \cdot \nabla_\vartheta \varphi - \{H_0, \varphi\} - Q(\varphi)$. We are led to the following system

$$1/\varepsilon^2 \text{ term:} \qquad \mathcal{T} F^{(0)} = 0, \tag{33}$$

$$1/\varepsilon \text{ term:} \qquad \mathcal{T} F^{(1)} = -\{\mathcal{V}, F^{(0)}\}, \tag{34}$$

$$\varepsilon^0 \text{ term:} \qquad \mathcal{T} F^{(2)} = -\partial_t F^{(0)} - \{\mathcal{V}, F^{(1)}\} \tag{35}$$

and so on... They are the analogs of (9), (10) and (11).

The general form of these equation, where the time variable t appears only as a parameter, reads $\mathcal{T} F = h$. Clearly

$$\int_{\mathbb{Y}} Ph\, \mathrm{d}\vartheta = 0 \tag{36}$$

is a necessary condition if we want to solve the cell equation, and we might wonder if it is also sufficient. This is a quite subtle question and we refer to [19] for details on the solvability of the cell equations. However, the situation simplifies when the data h satisfies the pointwise relation $Ph = 0$. Indeed, applying the operator P to the equation yields $\Omega \cdot \nabla_\vartheta PF + 0 = Ph = 0$. Hence, passing to Fourier coefficients, we obtain $\Omega \cdot \xi\ \widehat{Pf}(\xi; x, p) = 0$. Since the components of Ω are rationally independent, we deduce that $\widehat{Pf}(\xi; x, p) = 0$ for any $\xi \neq 0$ and therefore Pf does not depend on ϑ. Requiring $\int_{\mathbb{Y}} PF\, \mathrm{d}\vartheta = 0$ gives $PF = 0$. Therefore, when $Ph = 0$, we are led to solve

$$\Omega \cdot \nabla_\vartheta F + \{H_0, F\} + \gamma F = h, \qquad PF = 0.$$

Let us introduce the characteristics $\Theta \in \mathbb{R}^d$, $(\mathcal{X}, \mathcal{P}) \in \mathbb{R}^{2D}$, the solutions of the ODE system

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}s}\Theta(s) = \Omega, & \dfrac{\mathrm{d}}{\mathrm{d}s}\mathcal{X}(s) = \nabla_p H_0(\mathcal{X}(s), \mathcal{P}(s)), & \dfrac{\mathrm{d}}{\mathrm{d}s}\mathcal{P}(s) = -\nabla_x H_0(\mathcal{X}(s), \mathcal{P}(s)), \\ \Theta(0) = \vartheta, & \mathcal{X}(0) = x, & \mathcal{P}(0) = p. \end{cases}$$

Note in particular that $\Theta(s) = \vartheta + s\Omega$ and $(\mathcal{X}, \mathcal{P})$ are well defined by (HC1). Hence, we get

$$\frac{\mathrm{d}}{\mathrm{d}s}\Big(\mathrm{e}^{\gamma s}\ F(\Theta(s), \mathcal{X}(s), \mathcal{P}(s))\Big) = \mathrm{e}^{\gamma s}\ h(\Theta(s), \mathcal{X}(s), \mathcal{P}(s)).$$

Integration with respect to s yields the following statement.

Lemma 10 *Assume (HC1), (HC2) and let $\gamma > 0$. Let us denote by $L^2_\#(\mathbb{Y} \times \mathbb{R}^{2D})$ the space of functions from $\mathbb{R}^d \times \mathbb{R}^{2D}$ to $\mathbb{R}$, which are $\mathbb{Y}-$periodic with respect to the first variable and square integrable on $\mathbb{Y}\times\mathbb{R}^{2D}$. We set $H_\# = \{u \in L^2_\#(\mathbb{Y}\times\mathbb{R}^{2D}),\ \mathcal{T}u \in L^2_\#(\mathbb{Y}\times\mathbb{R}^{2D})\}$. Let $h \in L^2_\#(\mathbb{Y}\times\mathbb{R}^{2D})$ be such that $Ph = 0$. Then the solution $F \in H_\#$ of $\mathcal{T}F = h$ with $PF = 0$ is given by*

$$F(\vartheta; x, p) = -\int_0^\infty \mathrm{e}^{-\gamma s}\ h(\vartheta - s\Omega; \mathcal{X}(-s; x, p), \mathcal{P}(-s; x, p))\,\mathrm{d}s. \tag{37}$$

Accordingly, if h lies in $C^0(\mathbb{Y}; L^2(\mathbb{R}^{2D}))$, then, so does F.

The crucial role of the relaxation coefficient $\gamma > 0$ becomes clear and this statement has to be compared to Lemma 2 and Corollary 1. Coming back to (33), we get $F^{(0)}(t, \vartheta; x, p) = F(t; H_0(x, p))$, Therefore, (34) becomes

$$\mathcal{T}F^{(1)} = -\{\mathcal{V}, H_0\}\ \partial_E F(t; H_0(x, p)),$$

which can be solved by $F^{(1)}(t, \vartheta; x, p) = -\chi(t, \vartheta; x, p)\ \partial_E F(t; H_0(x, p))$, with

$$\chi(t, \vartheta; x, p) = -\int_0^\infty \mathrm{e}^{-\gamma s}\ \{\mathcal{V}, H_0\}(t, \vartheta - \Omega s; \mathcal{X}(-s; x, p), \mathcal{P}(-s; x, p))\,\mathrm{d}s, \tag{38}$$

a formula which makes sense under suitable regularity assumption on $\mathcal{V}$. For the time being, let us use (38) formally. We obtain a closed equation for $F(t; H_0(x, p))$ by applying the compatibility relation (36) to (35). We get

$$\begin{aligned}
0 &= \partial_t \int_{\mathbb{Y}} P\Big(F(t; H_0(x, p))\Big)\,\mathrm{d}\vartheta + \int_{\mathbb{Y}} P\Big(\{\mathcal{V}, F^{(1)}\}\Big)(t, \vartheta; x, p)\,\mathrm{d}\vartheta \\
&= \partial_t F(t; H_0(x, p)) - \left(\int_{\mathbb{Y}} P\Big(\{\mathcal{V}, \chi\}(t, \vartheta; x, p)\Big)\,\mathrm{d}\vartheta\right) \partial_E F(t; H_0(x, p)) \\
&\qquad - \left(\int_{\mathbb{Y}} P\Big(\{\mathcal{V}, H_0\}\ \chi(t, \vartheta; x, p)\Big)\,\mathrm{d}\vartheta\right) \partial^2_{EE} F(t; H_0(x, p)).
\end{aligned}$$

By using the coarea formula (30), we deduce that $F(t; E)$ verifies the following drift-diffusion equation

$$\partial_t(h_0(E)F(t, E)) = h_0(E)a(t; E)\partial_E F(t; E) + h_0(E)d(t; E)\partial^2_{EE} F(t; E),$$

with coefficients defined by

$$\begin{cases}
a(t; E) = \Pi\Big(\displaystyle\int_{\mathbb{Y}} \{\mathcal{V}, \chi\}\,\mathrm{d}\vartheta\Big)(E), \\
d(t; E) = \Pi\Big(\displaystyle\int_{\mathbb{Y}} \{\mathcal{V}, H_0\}\ \chi\,\mathrm{d}\vartheta\Big)(E).
\end{cases}$$

However, using the coarea formula, we will show that

$$h_0(E)a(t; E) = \partial_E\Big(h_0(E)d(t; E)\Big),$$

so that (32) can be finally deduced. These manipulations require some regularity assumptions for expression (38) to make sense as well as those involving derivatives of χ. To this aim, we assume

$$(HC4)\left\{\begin{array}{l}\text{Let } (\mathcal{X},\mathcal{P}) : (t;x,p)\in\mathbb{R}\times\mathbb{R}^{2D}\longmapsto(\mathcal{X}(t;x,p),\mathcal{P}(t;x,p))\in\mathbb{R}^{2D}\text{ stand for}\\ \text{the solution of the ODE system}\\ \qquad\qquad\left\{\begin{array}{ll}\dfrac{\mathrm{d}}{\mathrm{d}t}\mathcal{X}(t)=\nabla_p H_0(\mathcal{X}(t),\mathcal{P}(t)), & \dfrac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}(t)=-\nabla_x H_0(\mathcal{X}(t),\mathcal{P}(t)),\\ \mathcal{X}(0)=x, & \mathcal{P}(0)=p.\end{array}\right.\\ \text{We assume that for any } 0<R<\infty\text{, there exist } C_R,\ q_R\geq 0\text{ verifying}\\ \text{for any } t\in\mathbb{R}\text{:}\ \displaystyle\sup_{|(x.p)|\leq R}|\nabla_{x,p}(\mathcal{X}(t;x,p),\mathcal{P}(t;x,p))|\leq C_R\ (1+|t|)^{q_R}.\end{array}\right.$$

Next, we specify the assumptions on the perturbation.

$$(HC-P1)\left\{\begin{array}{l}\text{We assume that } V^\varepsilon(t;x,p)=\mathcal{V}(t,\Omega t/\varepsilon^2;x,p)\text{ where}\\ \ \vartheta\in\mathbb{R}^d\mapsto\mathcal{V}(t,\vartheta;x,p)\text{ is }\mathbb{Y}-\text{periodic},\\ \ \Omega\in\mathbb{R}^d\text{ has rationally independent components},\\ \ \mathcal{V}\in C^0(\mathbb{R}\times\mathbb{Y}\times\mathbb{R}^{2D}),\ \partial^\alpha_{t,x,p}\mathcal{V}\in C^0\cap L^\infty(\mathbb{R}\times\mathbb{Y}\times\mathbb{R}^{2D}),\quad|\alpha|=1,2.\\ \text{Furthermore, there exists some }\beta\geq 0\text{ such that}\\ \qquad\displaystyle\sup_{t\in\mathbb{R}\vartheta\in\mathbb{Y}}\int_{\mathbb{R}^{2D}}\frac{\{\mathcal{V}(t,\vartheta;x,p),H_0(x,p)\}^2}{w(x,p)^\beta}\,\mathrm{d}p\,\mathrm{d}x<\infty,\\ \text{where } w(x,p)=(1+H_0(x,p)^2)^{1/2}.\end{array}\right.$$

Of course, hypothesis (HC4) is satisfied globally, with exponent $q=0$, by the harmonic oscillator Hamiltonian. It is a strong stability assumption on H_0, which actually plays a crucial role in the estimates that allow to justify the asymptotics. For instance the following property is useful.

Lemma 11 *Add (HC4) to the hypothesis of Lemma 10. If, furthermore $\nabla_{x,p}h$ lies in $C^0(\mathbb{Y};L^2_{\mathrm{loc}}(\mathbb{R}^{2D}))$, then, so does F.*

In particular, we can make the definition of the auxiliary function χ rigorous.

Corollary 2 *Assume Hypothesis (HC1), (HC2), (HC4) and (HC-P1). Then, there exists a unique function $\chi:\mathbb{R}\times\mathbb{Y}\times\mathbb{R}^{2D}\to\mathbb{R}$ such that*

$$\mathcal{T}\chi=\{\mathcal{V},H_0\},\qquad\int_{\mathbb{Y}\times\mathbb{R}^{2D}}|\chi(t,\vartheta;x,p)|^2\,\frac{\mathrm{d}p\,\mathrm{d}x\,\mathrm{d}\vartheta}{w(x,p)^\beta}<\infty,\qquad\int_{\mathbb{Y}}P\chi\,\mathrm{d}\vartheta=0.$$

χ is defined by the formula (38). For any $0<R<\infty$, χ, $\partial_t\chi$ and $\nabla_{x,p}\chi$ belong to $C^0(\mathbb{R}\times\mathbb{Y};L^2(B(0,R)))$, where $B(0,R)=\{(x,p)\in\mathbb{R}^{2D},|(x,p)|\leq R\}$, and $P\chi=0$. Similar conclusions hold considering the solution $\chi^\star$ of $\mathcal{T}^\star\chi^\star=\{\mathcal{V},H_0\}$.

The role of Hypothesis (HC4) is to guarantee enough regularity on χ (or $\chi^\star$) to justify the formal manipulations made above. Remark that assuming $H_0\in W^{2,\infty}(\mathbb{R}^{2D})$, we readily obtain the estimate $|\nabla_{x,p}(\mathcal{X},\mathcal{P})(s)|\leq\mathrm{e}^{Cs}\ (1+|(x,p)|)$ for some $C>0$. Then, the same proof can be adapted, at the price of considering large enough values of the parameter γ (which should be $>C$), which is not satisfactory from a physical viewpoint. To conclude, the asymptotic behavior of (31) with (quasi-)periodic perturbation as $\varepsilon\to 0$ is described by the following statement.

Theorem 4 *Let $f_0^\varepsilon \geq 0$ satisfying (HC3) be the initial data for (31). We suppose that Hypothesis (HC1), (HC2), (HC4) and (HC-P1) are satisfied. Then, $f^\varepsilon = Pf^\varepsilon + \varepsilon g_\varepsilon$ where g_ε is bounded in $L^2((0,T)\times\mathbb{R}^{2D})$ and, up to a subsequence, $Pf^\varepsilon(t;x,p)$ converges to $F(t;H_0(x,p))$ in $C^0([0,T];L^2(\mathbb{R}^{2D})-weak)$, where $F:\mathbb{R}^+\times\mathbb{R}\to\mathbb{R}^+$ satisfies the diffusion equation (32) with the initial data $F(t=0;E)$ given by the weak limit of $\Pi f_0^\varepsilon(E)$ in $L^2(\mathbb{R},h_0(E)\,dE)$.*

We skip the details of the proof which remains in the spirit of Section 2.3.2, and we refer to [19] instead. The arguments rely on a convenient choice of oscillating test functions: multiplying (3) by $\varepsilon^2\psi(t,\Omega t/\varepsilon^2;x,p)$ and letting $\varepsilon\to 0$, we prove that f^ε converges to a function that depends on the energy only, and we identify the limit equation by using the following test function

$$\begin{cases} \phi(H_0(x,p)) + \varepsilon\chi^\star(t,\Omega t/\varepsilon^2;x,p)\partial_E\phi(H_0(x,p))\,, \quad \text{where} \\ \chi^\star(t,\vartheta;x,p) = -\displaystyle\int_0^\infty \mathrm{e}^{-\gamma s}\ \{\mathcal{V},H_0\}(t,\vartheta+\Omega s;\mathcal{X}(s;x,p),\mathcal{P}(s;x,p))\,\mathrm{d}s \end{cases}$$

Here, we only check that d is non negative (see [19] for details). Indeed, for any $\varphi\in C_c^\infty(\mathbb{R})$, we have

$$\int_{\mathbb{R}^{2D}} d(T;H_0(x,p))\varphi^2(H_0(x,p))\,\mathrm{d}p\,\mathrm{d}x = \gamma\int_{\mathbb{R}^{2D}}\int_{\mathbb{Y}} |P\chi\varphi(H_0)-\chi\varphi(H_0)|^2\,\mathrm{d}\vartheta\,\mathrm{d}p\,\mathrm{d}x \geq 0.$$

Moreover, due to the coarea formula, we obtain

$$-\int_{\mathbb{R}} h_0(E)d(t;E)\psi'(E)\,\mathrm{d}E = \int_{\mathbb{R}^{2D}} \{\mathcal{V},\chi\}\ \psi(H_0)\,\mathrm{d}p\,\mathrm{d}x = \int_{\mathbb{R}} a(t;E)\psi(E)h_0(E)\,\mathrm{d}E$$

which shows that $h_0(E)a(t;E) = \partial_E(h_0(E)d(t;E))$.

3.4. The Classical Model with a Random Perturbation

We now consider the case where the perturbation oscillates randomly, in the spirit of Section 2.4. Namely, we deal with $V^\varepsilon(t;x,p) = \mathcal{V}(t/\varepsilon^2;x,p)$, with $\mathcal{V}(s;x,p)$ a random variable. This Section is organized as follows. First, we set up some notations and definitions and we state the main results precisely. Then, we study the free relaxation case and we end this section with the analysis of the case of possibly vanishing relaxations.

3.4.1. Random Potential; Statement of the Results. Throughout this section, in addition to (HC1) and (HC2), we assume that H_0 verifies

$$(HC4') \qquad \sup_{y\in\mathbb{R}^{2D}} |\partial^\alpha H_0(y)| \leq C \quad \text{for } |\alpha| = 2,3,$$

where we have used the shortened notation $y=(x,p)\in\mathbb{R}^{2D}$. We also introduce the following $2D\times 2D$ matrix

$$J = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix},$$

I being the $D\times D$ identity matrix. Given two vectors $a,b\in\mathbb{R}^{2D}$, we denote $a\cdot b$ the usual euclidean product in $\mathbb{R}^{2D}$ and $a\otimes b$ stands for the $2D\times 2D$ matrix with components a_ib_j. We shall make use of the following relations

$$\{a,b\} = J\nabla b\cdot\nabla a, \qquad\qquad Ja\cdot b\ Jc\cdot d = b\otimes d : Ja\otimes Jc, \tag{39}$$

where for two $2D \times 2D$ matrices A, B, we denote $A : B = \sum_{i,j=1}^{2D} A_{ij} B_{ij}$.

We shall make use of the characteristic curves

$$\begin{array}{rlcl} \mathcal{Y}: & \mathbb{R} \times \mathbb{R}^{2D} & \longrightarrow & \mathbb{R}^D \times \mathbb{R}^D \\ & (t, y) & \longmapsto & \mathcal{Y}(t; y) = (\mathcal{X}(t; x, p), \mathcal{P}(t; x, p)), \end{array}$$

the solutions of the differential system

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{Y} = J\nabla H_0(\mathcal{Y}), \qquad \mathcal{Y}(0; y) = y.$$

Since the differential system is autonomous, the solution of the ODE with initial data equal to y at time s is given by $\mathcal{Y}(t-s; y)$. Moreover, energy is conserved

$$H_0(\mathcal{Y}(t; y)) = H_0(y).$$

This implies, due to (HC1), that $\mathcal{Y}(t; y)$ remains in a bounded set when $t \in \mathbb{R}$ and y lies in a bounded set of $\mathbb{R}^{2D}$. As a consequence of (HC4'), $\mathcal{Y}$ is, at least, a C^2 function of its arguments, and we check that

$$\left\{ \begin{array}{l} \text{There exist constants } C_1, C_2 > 0, \text{ depending on (HC4'), such that} \\ |\mathcal{Y}(t; y)| \leq C_1(1 + |t|)\mathrm{e}^{C_2|t|}\ (1 + |y|), \qquad |\partial^\alpha \mathcal{Y}(t; y)| \leq C_1\ \mathrm{e}^{C_2|t|} \quad \text{for } |\alpha| = 1, 2. \end{array} \right. \tag{40}$$

In some sense, (HC4') strongly weakens (HC4) that appeared in the deterministic framework. Let us introduce the family of operators, parametrized by $t \in \mathbb{R}$, defined by

$$S_t[\varphi](y) = \varphi(\mathcal{Y}(t; y)).$$

Since $\mathrm{div}(J\nabla H_0) = 0$, $\{S_t,\ t \in \mathbb{R}\}$ defines a group of isometries on $C^0(\mathbb{R}^{2D})$ or $L^p(\mathbb{R}^{2D})$ spaces. It will be also useful to consider the action on Sobolev spaces; we get

$$\left\{ \begin{array}{l} \text{There exists constants } C_1, C_2 > 0, \text{ depending on (HC4'), such that} \\ \|S_t\varphi\|_{H^k(\mathbb{R}^{2D})} \leq C_1 \mathrm{e}^{C_2|t|}\ \|\varphi\|_{H^k(\mathbb{R}^{2D})} \quad \text{for } k = 1, 2 \end{array} \right. \tag{41}$$

Furthermore, the adjoint operators are defined by

$$S_t^\star[\varphi](y) = S_{-t}[\varphi](y),$$

and we note that

$$S_t[Pf] = Pf = PS_t[f]. \tag{42}$$

Indeed, by virtue of the energy conservation, for any smooth trial function, we get

$$\int_{\mathbb{R}^{2D}} S_t[f](y)\ \phi(H_0(y))\,\mathrm{d}y = \int_{\mathbb{R}^{2D}} f(y)\ S_{-t}[\phi(H_0(y))]\,\mathrm{d}y = \int_{\mathbb{R}^{2D}} f(y)\ \phi(H_0(y))\,\mathrm{d}y$$

Let us now collect the necessary assumptions on the potential. We suppose that

$$V^\varepsilon(t; y) = \mathcal{V}(t/\varepsilon^2; y)$$

is an integrable random variable which is required to satisfy:

$(HC-R1)$ $\qquad \nabla\mathcal{V}(\tau;y)$ is a bounded random variable with $\mathbb{E}(\nabla\mathcal{V}(\tau;y)) = 0$,

$(HC-R2)$ $\qquad$ There exists a smooth function $\mathcal{R} : \mathbb{R}\times\mathbb{R}^{2D}\times\mathbb{R}^{2D} \to \mathbb{R}^{2D\times 2D}$, such that for any $i,j\in\{1,\dots,2D\}$, $\tau,\sigma\in[0,\infty)$, $y,z\in\mathbb{R}^{2D}$:

$$\mathbb{E}(\partial_{y_i}\mathcal{V}(\tau;y)\ \partial_{z_j}\mathcal{V}(\sigma;z)) = \mathcal{R}_{ij}(\tau-\sigma;y,z).$$

$(HC-R3)$ $\qquad$ There exists a constant $\mathcal{T}>0$ such that for any $i,j\in\{1,\dots,2D\}$, $\tau,\sigma\in[0,\infty)$, $y,z\in\mathbb{R}^{2D}$, if $|\tau-\sigma|\ge\mathcal{T}$ then $\partial_{y_i}\mathcal{V}(\tau;y)$ and $\partial_{z_j}\mathcal{V}(\sigma;z)$ are independent random variables,

$(HC-R4)$ $\qquad$ There exists a constant $M>0$ such that, for $1\le|\alpha|\le 3$

$$\sup_{\tau\in\mathbb{R},\ y\in\mathbb{R}^{2D}} |\partial_y^\alpha\mathcal{V}(\tau;y)| = M < \infty,$$

holds almost surely.

It would be tempting to completely remove the relaxation operator when dealing with random perturbations. With respect to this question, we are able to prove the following result.

Theorem 5 *Let $\gamma=0$, i.e. let the equation under consideration be*

$$\partial_t f^\varepsilon + \frac{1}{\varepsilon^2}\{H_0,f^\varepsilon\} + \frac{1}{\varepsilon}\{V^\varepsilon,f^\varepsilon\} = 0, \tag{43}$$

Assume that H_0 fulfills (HC1), (HC2), and (HC4'). We also suppose that H_0 is such that

$(HC5)$ $\qquad \{H_0,f\}=0$ *iff* $f(y)=F(H_0(y))$ *is a function of the energy only.*

Assume that (HC-R1), (HC-R2), (HC-R3), and (HC-R4) hold. Let the initial data f_0^ε be a deterministic quantity satisfying (HC3). Let $0<T<\infty$. Then, up to a subsequence, $\mathbb{E}Pf^\varepsilon$ converges to $F(t;H_0(y))\in L^\infty(\mathbb{R}^+;L^2(\mathbb{R}^{2D}))$ in $C^0([0,T];L^2(\mathbb{R}^{2D})-weak)$, with $F(t;E)$ being the solution of the following diffusion equation

$$\begin{cases} \partial_t(h_0F) = \partial_E(h_0 d\partial_E F), \\ F(0;E) = \lim\limits_{\varepsilon\to 0}\Pi f^\varepsilon(0;y) \qquad \text{weakly in } L^2(\mathbb{R},\ h_0(E)\,\mathrm{d}E), \end{cases} \tag{44}$$

and where the effective coefficient is given by

$$d(E) = \Pi\left(\int_0^{\mathcal{T}} \mathcal{R}(\tau;\mathcal{Y}(\tau;y),y) : J\nabla H_0(\mathcal{Y}(\tau;y))\otimes J\nabla H_0(y)\,\mathrm{d}\tau\right)(E).$$

Condition (HC5) is questionable since it may be not satisfied when $D\ge 2$, in particular for systems presenting symmetries. Of course, in the one-dimension case it is fulfilled by the harmonic oscillator $H_0(x,p)=(x^2+p^2)/2$, but even this simple Hamiltonian fails in verifying (HC5) when $D\ge 2$ (since $F(x,p)=x\wedge p$ satisfies $\{H_0,F\}=0$). Clearly (HC5) is related to ergodic properties of the flow associated to H_0: as a matter of fact, ergodicity of the free Hamiltonian on the energy shells $\{H_0=\text{Cst.}\}$ guarantees (HC5). Therefore, it is not obvious at all that we are able to find a smooth Hamiltonian H_0 such that (HC5) holds, as discussed in [10], [36], [22]. Coming back to the analogy with the quantum case, condition (HC5) is not surprising: it has to be compared to

(HQ1") when $\gamma(n,m)=0$. Note also that the analogy with quantum modeling leads to consider the following natural generalization of the interaction operator

$$Q(f)(x,p) = \int_{\Sigma_{H_0(x,p)}} B(x,p;y,q)\ \big(f(y,q)-f(x,p)\big)\ \delta(H_0(y,q)-H_0(x,p)),$$

for a certain kernel $B \geq 0$. However, the analysis of the classical model remains much more involved than for the quantum case, due to the following reasons. The analog of the operators $\mathrm{e}^{-Z(n,m)t/\varepsilon^2}$ would be the semi-group associated to the operator $\frac{1}{\varepsilon^2}\{H_0,\cdot\}+\frac{1}{\varepsilon^2}\gamma Q(\cdot)$. Then, the difficulty is two-fold:
- First, the operator Q is non local: evaluating Qf at (x,p) involves the values of the unknown f on many other points (y,q) while in the quantum case, the relaxation operator evaluated on (n,m) does not depend on other energy indices;
- Second, the operator Q is well defined as an endomorphism of $L^2(\mathbb{R}^{2D})$, but its action on Sobolev spaces and commutation with derivatives is far from clear. Hence, this leads to difficulties when considering the action of the semi-group on the Poisson bracket $\{V^\varepsilon, f\}$.
Nevertheless, we are able to consider sequences of relaxation coefficients γ^ε, that are positive functions of the energy and that might tend to 0, at least for some energy levels, when $\varepsilon \to 0$. We assume

$$(HC5') \qquad \begin{cases} \text{Let } \gamma^\varepsilon:\mathbb{R}\to\mathbb{R} \text{ be a sequence of } C^1 \text{ functions verifying} \\ \qquad 0<\gamma^\varepsilon_\star \leq \gamma^\varepsilon(E) \leq \Gamma < \infty, \qquad \lim\limits_{\varepsilon\to 0}\dfrac{\varepsilon^2}{\gamma^\varepsilon_\star}=0, \\ \qquad \sup\limits_{\varepsilon>0,\ E\in\mathbb{R}} \left|\dfrac{\mathrm{d}}{\mathrm{d}E}\gamma^\varepsilon(E)\right| \leq \Gamma < \infty, \\ \lim\limits_{\varepsilon\to 0}\gamma^\varepsilon(E)=\gamma(E)\geq 0 \qquad \text{uniformly on compact sets,} \end{cases}$$

and we consider the problem

$$\partial_t f^\varepsilon + \frac{1}{\varepsilon^2}\{H_0,f^\varepsilon\} + \frac{1}{\varepsilon}\{V^\varepsilon,f^\varepsilon\} + \frac{1}{\varepsilon^2}\ \gamma^\varepsilon(H_0)(Pf^\varepsilon - f^\varepsilon) = 0. \tag{45}$$

Theorem 6 *Assume that H_0 fulfills (HC1), (HC2), and (HC4'). Let γ^ε be defined as in (HC5'). Assume that (HC-R1), (HC-R2), (HC-R3), and (HC-R4) hold. Let the initial data f_0^ε be a deterministic quantity satisfying (HC3) and let f^ε be the corresponding solution of (45). Let $0<T<\infty$. Then, up to a subsequence, $\mathbb{E}Pf^\varepsilon$ converges to $F(t;H_0(y)) \in L^\infty(\mathbb{R}^+;L^2(\mathbb{R}^{2D}))$ in $C^0([0,T];L^2(\mathbb{R}^{2D})-weak)$, with $F(t;E)$ being the solution of the diffusion equation (44) where the effective coefficient is given by*

$$d(E) = \Pi\left(\int_0^{\mathcal{T}} \mathrm{e}^{-\gamma(H_0)\tau}\ \mathcal{R}(\tau;\mathcal{Y}(\tau;y),y) : J\nabla H_0(\mathcal{Y}(\tau;y))\otimes J\nabla H_0(y)\,\mathrm{d}\tau\right)(E).$$

3.4.2. The Relaxation-Free Case. Using the characteristics, the solution of (43) can be seen as a fixed point of the following Duhamel formula

$$f^\varepsilon(t;y) = S_{(s-t)/\varepsilon^2}[f^\varepsilon(s)](y) - \frac{1}{\varepsilon}\int_s^t S_{(\sigma-t)/\varepsilon^2}[\{V^\varepsilon(\sigma),f^\varepsilon(\sigma)\}](y)\,\mathrm{d}\sigma. \tag{46}$$

Using this formula with $s=0$ shows that $f^\varepsilon(t)$ depends only on the realizations of $V^\varepsilon(\sigma)$ for $0\leq\sigma\leq t$, and we deduce the following claim.

Lemma 12 *Assume (HC1), (HC2), (HC4'), and (HC-R1), (HC-R2), (HC-R3), (HC-R4). Suppose that the initial data f_0^ε is deterministic. Then, $f^\varepsilon(t)$ and $V^\varepsilon(t')$ are independent random variables when $t' \geq t + \varepsilon^2 \mathcal{T}$.*

Next, we obtain the following continuity estimate.

Lemma 13 *Assume (HC1), (HC2), (HC4'), and (HC-R1), (HC-R2), (HC-R3), (HC-R4). Then, for any $\varphi \in C_c^\infty(\mathbb{R}^{2D})$, we have*

$$\Big| \int_{\mathbb{R}^{2D}} (f^\varepsilon(t;y) - S_{(s-t)/\varepsilon^2}[f^\varepsilon(s)](y))\varphi(y)\,\mathrm{d}y \Big| \leq C \ \mathrm{e}^{C_2|t-s|/\varepsilon^2} \ \frac{|t-s|}{\varepsilon} \ \|\varphi\|_{H^1(\mathbb{R}^{2D})},$$

where C depends on (HC3), (HC-R4) and (HC4').

Proof. By using (46), and integrating by parts, we are led to evaluate

$$\begin{aligned}
&\frac{1}{\varepsilon}\Big| \int_s^t \int_{\mathbb{R}^{2D}} f^\varepsilon(\sigma) \ \{V^\varepsilon(\sigma), S_{(t-\sigma)/\varepsilon^2}\varphi\}\,\mathrm{d}y \Big| \\
&\leq \frac{1}{\varepsilon} \ \|f^\varepsilon\|_{L^\infty(\mathbb{R}^+;L^2(\mathbb{R}^{2D}))} \ \|\nabla_{x,p} V^\varepsilon\|_{L^\infty(\mathbb{R}\times\mathbb{R}^{2D})} \ \Big| \int_s^t \|\nabla_{x,p}(S_{(t-\sigma)/\varepsilon^2}[\varphi])\|_{L^2(\mathbb{R}^{2D})}\,\mathrm{d}\sigma \Big| \\
&\leq M M_0 C_1 \ \frac{|t-s|}{\varepsilon} \ \mathrm{e}^{C_2|t-s|/\varepsilon^2} \ \|\varphi\|_{H^1(\mathbb{R}^{2D})},
\end{aligned}$$

where we used (41). This proves the Lemma. ∎

By using (46) with $s = t - \varepsilon^2\mathcal{T}$, we get, for $t \geq \varepsilon^2\mathcal{T}$,

$$\begin{aligned}
\partial_t f^\varepsilon + \frac{1}{\varepsilon^2}\{H_0, f^\varepsilon\} &= -\frac{1}{\varepsilon} \ \{V^\varepsilon(t), f^\varepsilon(t)\} \\
&= -\frac{1}{\varepsilon} \ \{V^\varepsilon(t), S_{-\mathcal{T}}[f^\varepsilon(t-\varepsilon^2\mathcal{T})]\} && \Big\} := D^\varepsilon(t) \\
&\quad -\frac{1}{\varepsilon^2} \ \Big\{V^\varepsilon(t), \int_{t-\varepsilon^2\mathcal{T}}^t S_{(\sigma-t)/\varepsilon^2}[\{V^\varepsilon(\sigma), S_{(t-\sigma)/\varepsilon^2} f^\varepsilon(\sigma)\}]\Big\} && \Big\} := I^\varepsilon(t).
\end{aligned}$$

Then, we split the last term as follows

$$\begin{aligned}
&\frac{1}{\varepsilon^2} \ \Big\{V^\varepsilon(t), \int_{s-\varepsilon^2\mathcal{T}}^t S_{(\sigma-t)/\varepsilon^2}[\{V^\varepsilon(\sigma), S_{(t-\sigma)/\varepsilon^2}[\mathbb{E} f^\varepsilon(t)]\}]\Big\}\,\mathrm{d}\sigma && \Big\} := L^\varepsilon(t) \\
&+\frac{1}{\varepsilon^2} \ \Big\{V^\varepsilon(t), \int_{s-\varepsilon^2\mathcal{T}}^t S_{(\sigma-t)/\varepsilon^2}[\{V^\varepsilon(\sigma), f^\varepsilon(\sigma) - S_{(t-\sigma)/\varepsilon^2}[\mathbb{E} f^\varepsilon(t)]\}]\Big\}\,\mathrm{d}\sigma && \Big\} := R^\varepsilon(t).
\end{aligned}$$

Lemma 14 *Assume (HC3), (HC4'), (HC-R2), (HC-R3) and (HC-R4). Then, the following properties hold:*
i) $\mathbb{E} D^\varepsilon(t) = 0$,
ii) There exists a constant $C > 0$, depending on (HC3), (HC4'), (HC-R4), and $\mathcal{T}$, such that for any $\varphi \in C_c^\infty(\mathbb{R}^{2D})$, $t \geq \varepsilon^2\mathcal{T}$,

$$\Big|\mathbb{E} \int_{\mathbb{R}^{2D}} I^\varepsilon(t)\varphi(x,p)\,\mathrm{d}p\,\mathrm{d}x\Big| \leq C \ \|\varphi\|_{H^2(\mathbb{R}^{2D})}.$$

iii) There exists a constant $C > 0$, depending on (HC3), (HC4'), (HC-R4), and $\mathcal{T}$, such that for any $\varphi \in C_c^\infty(\mathbb{R}^{2D})$, and $t \geq 2\varepsilon^2\mathcal{T}$,

$$\Big|\mathbb{E} \int_{\mathbb{R}^{2D}} R^\varepsilon(t)\varphi(x,p)\,\mathrm{d}p\,\mathrm{d}x\Big| \leq C \ \varepsilon \ \|\varphi\|_{H^3(\mathbb{R}^{2D})}.$$

iii) There exists an operator $\mathcal{Q}$, which does not depend on ε, nor on t, such that

$$\mathbb{E}L^\varepsilon(t) = \mathcal{Q}(\mathbb{E}f^\varepsilon(t)), \qquad \Big|\int_{\mathbb{R}^{2D}} \mathcal{Q}(f)\varphi\,\mathrm{d}p\,\mathrm{d}x\Big| \le C\ \|f\|_{L^2(\mathbb{R}^{2D})}\ \|\varphi\|_{H^3(\mathbb{R}^{2D})}$$

holds for any $\varphi \in C_c^\infty(\mathbb{R}^{2D})$, the constant $C > 0$ depending only on (HC3), (HC4'), (HC-R4), and $\mathcal{T}$.

Proof. Throughout the proof we denote by C a quantity which depends only on (HC3), (HC4'), (HC-R4), even if the value of C may change from a line to another. The expectation of $D^\varepsilon(t)$ vanishes since $f^\varepsilon(t-\varepsilon^2\mathcal{T})$ and $V^\varepsilon(t)$ are independent, by virtue of Lemma 12, while $\mathbb{E}V^\varepsilon(t) = 0$. Next, the estimate on I^ε follows from (HC-R4) and (41) which imply

$$\begin{aligned}\Big|\int_{\mathbb{R}^{2D}} I^\varepsilon(t)\varphi(x,p)\,\mathrm{d}p\,\mathrm{d}x\Big| \ \le\ & \|D^2_{x,p}V^\varepsilon\|_{L^\infty(\mathbb{R}\times\mathbb{R}^{2D})}\ \|\nabla_{x,p}V^\varepsilon\|_{L^\infty(\mathbb{R}\times\mathbb{R}^{2D})}\ \|\varphi\|_{H^2(\mathbb{R}^{2D})}\\ & \times\|f^\varepsilon\|_{L^\infty(\mathbb{R}^+;L^2(\mathbb{R}^{2D}))}\ \frac{1}{\varepsilon^2}\int_{t-\varepsilon^2\mathcal{T}}^t C\,\mathrm{d}\sigma,\end{aligned}$$

and proves ii).

Now, we remark that for any $\sigma \in (t-\varepsilon^2\mathcal{T}, t)$, $f(\sigma-\varepsilon^2\mathcal{T})$ and $V^\varepsilon(t)$, $V^\varepsilon(\sigma)$ are independent since $t, \sigma \ge \sigma - \varepsilon^2\mathcal{T} + \varepsilon^2\mathcal{T}$. Hence, we get for $t \ge 2\varepsilon^2\mathcal{T}$,

$$\begin{aligned}&\mathbb{E}\int_{t-\varepsilon^2\mathcal{T}}^t S_{-\mathcal{T}}[f^\varepsilon(\sigma-\varepsilon^2\mathcal{T})]\ \Big\{V^\varepsilon(\sigma), S_{(t-\sigma)/\varepsilon^2}[\{V^\varepsilon(t),\varphi\}]\Big\}\,\mathrm{d}\sigma\\ &\qquad = \int_{t-\varepsilon^2\mathcal{T}}^t \mathbb{E}\Big(S_{-\mathcal{T}}[f^\varepsilon(\sigma-\varepsilon^2\mathcal{T})]\Big)\ \mathbb{E}\Big\{V^\varepsilon(\sigma), S_{(t-\sigma)/\varepsilon^2}[\{V^\varepsilon(t),\varphi\}]\Big\}\,\mathrm{d}\sigma\\ &\qquad = \mathbb{E}\int_{t-\varepsilon^2\mathcal{T}}^t \mathbb{E}\Big(S_{-\mathcal{T}}[f^\varepsilon(\sigma-\varepsilon^2\mathcal{T})]\Big)\ \Big\{V^\varepsilon(\sigma), S_{(t-\sigma)/\varepsilon^2}[\{V^\varepsilon(t),\varphi\}]\Big\}\,\mathrm{d}\sigma.\end{aligned}$$

This allows us to write

$$\begin{aligned}&\mathbb{E}\int_{\mathbb{R}^{2D}} R^\varepsilon(t)\varphi(y)\,\mathrm{d}y\\ &= \frac{1}{\varepsilon^2}\mathbb{E}\int_{\mathbb{R}^{2D}}\int_{t-\varepsilon^2\mathcal{T}}^t \Big(f^\varepsilon(\sigma) - S_{-\mathcal{T}}[f^\varepsilon(\sigma-\varepsilon^2\mathcal{T})]\Big)\ \Big\{V^\varepsilon(\sigma), S_{(t-\sigma)/\varepsilon^2}[\{V^\varepsilon(t),\varphi\}]\Big\}\,\mathrm{d}\sigma\,\mathrm{d}y\\ &+\frac{1}{\varepsilon^2}\mathbb{E}\int_{\mathbb{R}^{2D}}\int_{t-\varepsilon^2\mathcal{T}}^t \Big(\mathbb{E}S_{-\mathcal{T}}[f^\varepsilon(\sigma-\varepsilon^2\mathcal{T})] - S_{(t-\sigma)/\varepsilon^2}[\mathbb{E}f^\varepsilon(t)]\Big)\ \Big\{V^\varepsilon(\sigma), S_{(t-\sigma)/\varepsilon^2}[\{V^\varepsilon(t),\varphi\}]\Big\}\,\mathrm{d}\sigma\,\mathrm{d}y.\end{aligned}$$

Note that in the last integral, we have

$$\mathbb{E}S_{-\mathcal{T}}[f^\varepsilon(\sigma-\varepsilon^2\mathcal{T})] - S_{(t-\sigma)/\varepsilon^2}[\mathbb{E}f^\varepsilon(t)] = \mathbb{E}S_{(t-\sigma)/\varepsilon^2}\Big[S_{(\sigma-\varepsilon^2\mathcal{T}-t)/\varepsilon^2}[f^\varepsilon(\sigma-\varepsilon^2\mathcal{T})] - f^\varepsilon(t)\Big].$$

Then, applying Lemma 13 and (41), we evaluate as follows

$$\begin{aligned}&\Big|\mathbb{E}\int_{\mathbb{R}^{2D}} R^\varepsilon(t)\varphi(x,p)\,\mathrm{d}y\Big|\\ &\le C\frac{1}{\varepsilon^2}\int_{t-\varepsilon^2\mathcal{T}}^t \frac{1}{\varepsilon}\ \mathrm{e}^{2C_2\mathcal{T}}\ \varepsilon^2\mathcal{T}\mathbb{E}\Big\|\Big\{V^\varepsilon(\sigma), S_{(t-\sigma)/\varepsilon^2}[\{V^\varepsilon(t),\varphi\}]\Big\}\Big\|_{H^1(\mathbb{R}^{2D})}\\ &\le C\frac{1}{\varepsilon^2}\ \mathrm{e}^{3C_2\mathcal{T}}\ \frac{\varepsilon^2\mathcal{T}}{\varepsilon}\ \varepsilon^2\mathcal{T}\ \|\varphi\|_{H^3(\mathbb{R}^{2D})}.\end{aligned}$$

This proves iii).

Finally, we check that $\mathbb{E}\int_{\mathbb{R}^{2D}} L^\varepsilon\varphi\,\mathrm{d}y$ can be recast as the sum of terms looking like

$$\begin{aligned}&\frac{1}{\varepsilon^2}\mathbb{E}\int_{\mathbb{R}^{2D}}\int_{t-\varepsilon^2\mathcal{T}}^t S_{(t-\sigma)/\varepsilon^2}[\mathbb{E}f^\varepsilon(t)](y)\quad \partial_i V^\varepsilon(\sigma;y)\ \partial_j V^\varepsilon(t;\mathcal{Y}((t-\sigma)/\varepsilon^2;y))\\ &\qquad\qquad \times(\partial^2_{kl}\varphi)(\mathcal{Y}((t-\sigma)/\varepsilon^2;y))\ \partial_m\mathcal{Y}_n((t-\sigma)/\varepsilon^2;y)\,\mathrm{d}\sigma\,\mathrm{d}p\,\mathrm{d}x\end{aligned}$$

or

$$\frac{1}{\varepsilon^2}\mathbb{E}\int_{\mathbb{R}^{2D}}\int_{t-\varepsilon^2\mathcal{T}}^{t} S_{(t-\sigma)/\varepsilon^2}[\mathbb{E}f^\varepsilon(t)](y) \quad \partial_i V^\varepsilon(\sigma;y)\ (\partial^2_{jk}V^\varepsilon)(t;\mathcal{Y}((t-\sigma)/\varepsilon^2;y))$$
$$\times(\partial_l\varphi)(\mathcal{Y}((t-\sigma)/\varepsilon^2;y))\ \partial_m\mathcal{Y}_n((t-\sigma)/\varepsilon^2;y)\,\mathrm{d}\sigma\,\mathrm{d}p\,\mathrm{d}x$$

where the indices $i,j,k,l,m,n,\in\{1,\dots,2D\}$ and ∂ stands for any first order derivative with respect to the variable y. As a consequence of (HC-R2), these expressions become

$$\int_{\mathbb{R}^{2D}}\int_{t-\varepsilon^2\mathcal{T}}^{t} S_{(t-\sigma)/\varepsilon^2}[\mathbb{E}f^\varepsilon(t)](y)\ \mathcal{R}_{ij}((\sigma-t)/\varepsilon^2;y,\mathcal{Y}((t-\sigma)/\varepsilon^2;y))$$
$$\times(\partial^2_{kl}\varphi)(\mathcal{Y}((t-\sigma)/\varepsilon^2;y))\ \partial_m\mathcal{Y}_n((t-\sigma)/\varepsilon^2;y)\frac{\mathrm{d}\sigma}{\varepsilon^2}\,\mathrm{d}p\,\mathrm{d}x$$
$$=\int_{\mathbb{R}^{2D}}\int_0^{\mathcal{T}} S_{-\tau}[\mathbb{E}f^\varepsilon(t)](y)\ \mathcal{R}_{ij}(\tau;y,\mathcal{Y}(-\tau;y))$$
$$\times(\partial^2_{kl}\varphi)(\mathcal{Y}(-\tau;y))\ \partial_m\mathcal{Y}_n(-\tau;y)\,\mathrm{d}\tau\,\mathrm{d}p\,\mathrm{d}x$$

or

$$\int_{\mathbb{R}^{2D}}\int_{t-\varepsilon^2\mathcal{T}}^{t} S_{(t-\sigma)/\varepsilon^2}[\mathbb{E}f^\varepsilon(t)](y)\ (\partial_{y_k}\mathcal{R}_{ij})((\sigma-t)/\varepsilon^2;y,\mathcal{Y}((t-\sigma)/\varepsilon^2;y))$$
$$\times(\partial_l\varphi)(\mathcal{Y}((t-\sigma)/\varepsilon^2;y))\ \partial_m\mathcal{Y}_n((t-\sigma)/\varepsilon^2;y)\frac{\mathrm{d}\sigma}{\varepsilon^2}\,\mathrm{d}p\,\mathrm{d}x$$
$$=\int_{\mathbb{R}^{2D}}\int_0^{\mathcal{T}} S_{-\tau}[\mathbb{E}f^\varepsilon(t)](y)\ (\partial_{y_k}\mathcal{R}_{ij})(\tau;y,\mathcal{Y}(-\tau;y))$$
$$\times(\partial_l\varphi)(\mathcal{Y}(-\tau;y))\ \partial_m\mathcal{Y}_n(-\tau;y)\,\mathrm{d}\tau\,\mathrm{d}p\,\mathrm{d}x$$

respectively, which define the operator $\mathcal{Q}$. ∎

Up to now, the non degeneracy assumption (HC5) does not play any role; it will appear when identifying the limit equation. The end of the proof of Theorem 5 splits into several steps.

Step 1. Projecting the Equation; Compactness.
By using Proposition 4, we can extract a subsequence such that

$$\mathbb{E}f^\varepsilon \rightharpoonup f \qquad \text{weakly in } L^2((0,T)\times\mathbb{R}^{2D}),\quad 0<T<\infty.$$

Furthermore, multiplying (43) by ε^2 yields

$$\mathbb{E}\{H_0,f^\varepsilon\}=\{H_0,\mathbb{E}f^\varepsilon\}=-\Big(\varepsilon^2\partial_t\mathbb{E}f^\varepsilon+\varepsilon\mathbb{E}\{V^\varepsilon,f^\varepsilon\}\Big).$$

Letting ε go to 0 leads to

$$\{H_0,f\}=0.$$

This is where Hypothesis (HC5) is used: it implies that $f(t;y)=F(t;H(y))$ only depends on the energy. Therefore, we realize that it suffices to determine the behavior of $\mathbb{E}Pf^\varepsilon$ as $\varepsilon\to 0$. Indeed, $\mathbb{E}Pf^\varepsilon$ satisfies

$$\partial_t\mathbb{E}Pf^\varepsilon=-\mathbb{E}P\Big(\frac{1}{\varepsilon}\{V^\varepsilon,f^\varepsilon\}\Big)=\mathbb{E}P(D^\varepsilon-L^\varepsilon-R^\varepsilon)=-\mathbb{E}P(L^\varepsilon+R^\varepsilon). \tag{47}$$

Thus, we obtain that $\mathbb{E}Pf^\varepsilon$ satisfies some compactness properties in a space of continuous functions with respect to the time variable.

Lemma 15 *We can extract a subsequence such that, for any $\varphi \in L^2(\mathbb{R}^{2D})$,*

$$\lim_{\varepsilon\to 0}\int_{\mathbb{R}^{2D}} \mathbb{E}Pf^\varepsilon(t;y)\ \varphi(y)\,\mathrm{d}y = \int_{\mathbb{R}^{2D}} F(t;H_0(y))\ \varphi(y)\,\mathrm{d}y.$$

uniformly on $[0,T]$.

Proof. Combining (47) to Lemma 14, we first deduce that, for any $\varphi \in C_c^\infty(\mathbb{R}^{2D})$, the set

$$\Big\{\int_{\mathbb{R}^{2D}} \mathbb{E}Pf^\varepsilon(t+\varepsilon^2\mathcal{T})\ \varphi\,\mathrm{d}y,\quad \varepsilon>0\Big\}$$

is relatively compact in $C^0([0,T])$, for any $0<T<\infty$, by virtue of the Arzela-Ascoli Theorem. Since P is self-adjoint, we can use Lemma 13 with $\varphi(y)=\phi(H_0(y))$, $\phi\in C_c^\infty(\mathbb{R})$, as test function. Indeed, we get

$$\begin{aligned}&\Big|\int_{\mathbb{R}^{2D}} (f^\varepsilon(t;y)-f^\varepsilon(s;y))\phi(H_0(y))\,\mathrm{d}y\Big|\\ &\qquad = \Big|\int_{\mathbb{R}^{2D}} (f^\varepsilon(t;y)-S_{(s-t)/\varepsilon^2}f^\varepsilon(s;y))\phi(H_0(y))\,\mathrm{d}y\Big|\\ &\qquad \le C\mathrm{e}^{C_2|t-s|/\varepsilon^2}\ \frac{|t-s|}{\varepsilon}\ \|\phi(H_0(y))\|_{H^1(\mathbb{R}^{2D})}.\end{aligned}$$

Consequently, using this information with $s=t+\varepsilon^2\mathcal{T}$, we deduce that

$$\Big\{\int_{\mathbb{R}^{2D}} \mathbb{E}Pf^\varepsilon(t;y)\ \phi(H_0(y))\,\mathrm{d}y,\quad \varepsilon>0\Big\}$$

is relatively compact in $C^0([0,T])$, too. Since we also have

$$\Big|\int_{\mathbb{R}^{2D}} \mathbb{E}Pf^\varepsilon\ \varphi\,\mathrm{d}y\Big| \le M_0\ \|\varphi\|_{L^2(\mathbb{R}^{2D})},$$

we can extend the compactness property to any test function $\varphi\in L^2(\mathbb{R}^{2D})$. Then, by standard arguments, we extract a subsequence, still labelled by ε, such that, for any $\varphi\in L^2(\mathbb{R}^{2D})$, $\int_{\mathbb{R}^{2D}}\mathbb{E}Pf^\varepsilon\ \varphi\,\mathrm{d}p\,\mathrm{d}x$ converges uniformly on $C^0([0,T])$. It is already known that $\mathbb{E}f^\varepsilon$ converges to a function which only depends on the energy, weakly in $L^2((0,T)\times\mathbb{R}^{2D})$, and we now identify the limits. ∎

Step 2. Computation of the Leading Order Term.

Since we consider the projected equation (47), it is enough to consider test functions only depending on the energy: $\varphi(y)=\phi(H_0(y))$. By Lemma 14, the contribution of $\mathbb{E}R^\varepsilon$ disappears as ε tends to 0, and we are left with the task of discussing $\mathbb{E}\int_{\mathbb{R}^{2D}} L^\varepsilon(t;y)\ \phi(H_0(y))\,\mathrm{d}y$. The energy conservation implies that $S_\tau[\phi(H_0(y))]=\phi(H_0(y))$, and thus we obtain

$$\begin{aligned}&\mathbb{E}\int_{\mathbb{R}^{2D}} L^\varepsilon(t;y)\ \phi(H_0(y))\,\mathrm{d}y\\ &= \frac{1}{\varepsilon^2}\mathbb{E}\int_{\mathbb{R}^{2D}}\int_{t-\varepsilon^2\mathcal{T}}^{t} \mathbb{E}f^\varepsilon(t;y)\ S_{(\sigma-t)/\varepsilon^2}\Big[\Big\{V^\varepsilon(\sigma),S_{(t-\sigma)/\varepsilon^2}[\{V^\varepsilon(t),\phi(H_0(y))\}]\Big\}\Big]\,\mathrm{d}y\\ &= \int_{\mathbb{R}^{2D}} \mathbb{E}f^\varepsilon(t;y)\Big(A^\varepsilon(t;y)\partial^2_{EE}\phi(H_0(y))+B^\varepsilon(t;y)\partial_E\phi(H_0(y))\Big)\,\mathrm{d}y\end{aligned}$$

with

$$\begin{aligned}A^\varepsilon(t;y) &= \frac{1}{\varepsilon^2}\int_{t-\varepsilon^2\mathcal{T}}^{t} \mathbb{E}S_{(\sigma-t)/\varepsilon^2}[\{V^\varepsilon(\sigma),H_0\}]\ \{V^\varepsilon(t),H_0\}\,\mathrm{d}\sigma,\\ B^\varepsilon(t;y) &= \frac{1}{\varepsilon^2}\int_{t-\varepsilon^2\mathcal{T}}^{t} \mathbb{E}S_{(\sigma-t)/\varepsilon^2}\Big[\Big\{V^\varepsilon(\sigma),S_{(t-\sigma)/\varepsilon^2}[\{V^\varepsilon(t),H_0\}]\Big\}\Big].\end{aligned}$$

In view of Lemma 14-iii), we can expect that these coefficients do not depend on t nor on ε.

Lemma 16 *The coefficients $A^\varepsilon(t;y)$ and $B^\varepsilon(t;y)$ are given by*

$$A(y) = \int_0^{\mathcal{T}} \mathcal{R}(\tau;\mathcal{Y}(\tau;y),y) : J\nabla H_0(\mathcal{Y}(\tau;y)) \otimes J\nabla H_0(y)\,\mathrm{d}\tau,$$
$$B(y) = -\int_0^{\mathcal{T}} S_\tau\Big[\mathrm{div}_z\Big(J\mathcal{R}(\tau;y,\mathcal{Y}(-\tau;z))J\nabla H_0(\mathcal{Y}(-\tau;z))\Big)\Big|_{z=y}\Big]\,\mathrm{d}\tau.$$

Proof. The proof relies on the following relation

$$\begin{aligned} S_{s-t}[\{\mathcal{V}(s),H_0\}]\ \{\mathcal{V}(t),H_0\}(y) &= J\nabla H_0(\mathcal{Y}(s-t;y))\cdot\nabla\mathcal{V}(s;\mathcal{Y}(s-t;y))\ J\nabla H_0(y)\cdot\nabla\mathcal{V}(t;y)\\ &= \nabla\mathcal{V}(s;\mathcal{Y}(s-t;y))\otimes\nabla\mathcal{V}(t;y) : J\nabla H_0(\mathcal{Y}(s-t;y))\otimes J\nabla H_0(y). \end{aligned}$$

Taking the expectation leads to

$$\begin{aligned} &\mathbb{E}S_{s-t}[\{\mathcal{V}(s),H_0\}]\ \{\mathcal{V}(t),H_0\}(y)\\ &\qquad = \mathcal{R}(s-t;\mathcal{Y}(s-t;y),y) : J\nabla H_0(\mathcal{Y}(s-t;y))\otimes J\nabla H_0(y). \end{aligned} \tag{48}$$

We apply this formula with t,s replaced by $t/\varepsilon^2, s/\varepsilon^2$. We get

$$\begin{aligned} A^\varepsilon(t;y) &= \int_{t-\varepsilon^2\mathcal{T}}^t \mathcal{R}((\sigma-t)/\varepsilon^2;\mathcal{Y}((\sigma-t)/\varepsilon^2;y),y) : J\nabla H_0(\mathcal{Y}((\sigma-t)/\varepsilon^2;y))\otimes J\nabla H_0(y)\frac{\mathrm{d}\sigma}{\varepsilon^2}\\ &= \int_0^{\mathcal{T}} \mathcal{R}(\tau;\mathcal{Y}(\tau;y),y) : J\nabla H_0(\mathcal{Y}(\tau;y),y)\otimes J\nabla H_0(y)\,\mathrm{d}\tau. \end{aligned}$$

We perform similar maniplulations for the second coefficient. Let us define

$$U(s,t;y,z) = \mathrm{div}_z\Big(J\nabla\mathcal{V}(s,y)\otimes\nabla\mathcal{V}(t;\mathcal{Y}(t-s;z))J\nabla H_0(\mathcal{Y}(t-s;z))\Big)$$

and

$$\mathcal{U}(\tau;y,z) = \mathrm{div}_z\Big(J\mathcal{R}(\tau;y,\mathcal{Y}(-\tau;z))J\nabla H_0(\mathcal{Y}(-\tau;z))\Big),$$

so that $\mathbb{E}U(s,t;y,z) = \mathcal{U}(s-t;y,z)$ holds. We have

$$\Big\{\mathcal{V}(s), S_{t-s}[\{\mathcal{V}(t),H_0]\}\Big\}(y) = J\nabla\Big(J\nabla H_0(\mathcal{Y}(t-s;y))\cdot\nabla\mathcal{V}(t;\mathcal{Y}(t-s;y))\Big)\cdot\nabla\mathcal{V}(s;y) = -U(s,t;y,y).$$

Therefore, taking the expectation yields

$$\mathbb{E}\Big\{\mathcal{V}(s), S_{t-s}[\{\mathcal{V}(t),H_0]\}\Big\}(y) = -\mathcal{U}(s-t;y,y). \tag{49}$$

Applying this formula with t,s replaced by $t/\varepsilon^2, s/\varepsilon^2$ leads to the asserted formula for $B^\varepsilon(t;y)$. ∎

Step 3. Passing to the Limit; Effective Coefficients.
As ε goes to 0 in (47), using the fact that $\mathbb{E}f^\varepsilon(t;y)$ converges weakly to $F(t;H_0(y))$, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}^{2D}} F(t;H_0(y))\ \phi(H_0(y))\,\mathrm{d}y = \int_{\mathbb{R}^{2D}} F(t;H_0(y))(A(y)\partial^2_{EE}\phi(H_0(y)) + B(y)\partial_E\phi(H_0(y)))\,\mathrm{d}y.$$

Since the limit F and the test function both depend on the energy only, using the coarea formula, this can be seen as a very weak formulation of the following drift-diffusion equation

$$\partial_t(h_0F) = \partial^2_{EE}(h_0dF) + \partial_E(h_0cF),$$

with $d(E) = \Pi A(E)$ and $c(E) = \Pi B(E)$.

Lemma 17 *The coefficient $d(E)$ belongs to $L^\infty_{\mathrm{loc}}(\mathbb{R})$ and satisfies $d(E)\geq 0$. Moreover, we have $\frac{\mathrm{d}}{\mathrm{d}E}(h_0(E)d(E)) = h_0(E)c(E)$.*

Proof. We start by remarking that

$\mathcal{R}_{ij}(\tau;y,z) = \mathbb{E}(\partial_i\mathcal{V}(\tau,y)\ \partial_j\mathcal{V}(0,z)) = \mathbb{E}(\partial_j\mathcal{V}(0,z)\ \partial_i\mathcal{V}(\tau,y)) = \mathcal{R}_{ji}(-\tau,z,y).$

In other words, $\mathcal{R}(\tau;y,z) =^T \mathcal{R}(-\tau;z,y)$. Then, we compute

$$\begin{aligned}
PA(y) &= P\int_0^{\mathcal{T}} \mathcal{R}(\tau;\mathcal{Y}(\tau;y),y) : J\nabla H_0(\mathcal{Y}(\tau;y)) \otimes J\nabla H_0(y)\,\mathrm{d}\tau \\
&= P\int_0^{\mathcal{T}} S_\tau\Big[\mathcal{R}(\tau;y,\mathcal{Y}(-\tau;y)) : J\nabla H_0(y) \otimes J\nabla H_0(\mathcal{Y}(-\tau;y))\Big]\,\mathrm{d}\tau \\
&= P\int_0^{\mathcal{T}} \mathcal{R}(\tau;y,\mathcal{Y}(-\tau;y)) : J\nabla H_0(y) \otimes J\nabla H_0(\mathcal{Y}(-\tau;y))\,\mathrm{d}\tau \\
&\qquad\qquad\qquad\text{using (42)} \\
&= P\int_{-\mathcal{T}}^{0} \mathcal{R}(-\tau;y,\mathcal{Y}(\tau;y)) : J\nabla H_0(y) \otimes J\nabla H_0(\mathcal{Y}(\tau;y))\,\mathrm{d}\tau \\
&\qquad\qquad\qquad\text{changing variables } \tau\to-\tau.
\end{aligned}$$

However, we have $\mathcal{R} : a\otimes b =^T \mathcal{R} : b\otimes a$ which yields

$$\begin{aligned}
PA(y) &= P\int_{-\mathcal{T}}^{0} \mathcal{R}(\tau;\mathcal{Y}(\tau;y),y) : J\nabla H_0(\mathcal{Y}(\tau;y)) \otimes J\nabla H_0(y)\,\mathrm{d}\tau \\
&= \frac{1}{2}\,P\int_{-\mathcal{T}}^{-\mathcal{T}} \mathcal{R}(\tau;\mathcal{Y}(\tau;y),y) : J\nabla H_0(\mathcal{Y}(\tau;y)) \otimes J\nabla H_0(y)\,\mathrm{d}\tau.
\end{aligned}$$

Now, recalling that $\tau\mapsto\mathcal{R}(\tau;y,y')$ is compactly supported in $[-\mathcal{T},+\mathcal{T}]$, we use (22) which leads to

$$\begin{aligned}
PA(y) &= \lim_{R\to\infty}\frac{1}{4R}P\int_{-R}^{+R}\int_{-R}^{+R} \mathcal{R}(t-s;\mathcal{Y}(t-s;y),y) : J\nabla H_0(\mathcal{Y}(t-s;y)) \otimes J\nabla H_0(y)\,\mathrm{d}t\,\mathrm{d}s \\
&= \lim_{R\to\infty}\frac{1}{4R}P\mathbb{E}\int_{-R}^{+R}\int_{-R}^{+R} \nabla\mathcal{V}(t;\mathcal{Y}(t-s;y)) \otimes \nabla\mathcal{V}(s,y) : J\nabla H_0(\mathcal{Y}(t-s;y)) \otimes J\nabla H_0(y)\,\mathrm{d}t\,\mathrm{d}s \\
&= \lim_{R\to\infty}\frac{1}{4R}P\mathbb{E}\int_{-R}^{+R}\int_{-R}^{+R} S_{-s}\Big[\nabla\mathcal{V}(t;\mathcal{Y}(t;y)) \otimes \nabla\mathcal{V}(s,\mathcal{Y}(s;y)) \\
&\qquad\qquad : J\nabla H_0(\mathcal{Y}(t;y)) \otimes J\nabla H_0(\mathcal{Y}(s;y))\Big]\,\mathrm{d}t\,\mathrm{d}s \\
&= \lim_{R\to\infty}\frac{1}{4R}P\mathbb{E}\int_{-R}^{+R}\int_{-R}^{+R} \nabla\mathcal{V}(t;\mathcal{Y}(t;y)) \otimes \nabla\mathcal{V}(s,\mathcal{Y}(s;y)) : J\nabla H_0(\mathcal{Y}(t;y)) \otimes J\nabla H_0(\mathcal{Y}(s;y))\,\mathrm{d}t\,\mathrm{d}s \\
&= \lim_{R\to\infty}\frac{1}{4R}P\mathbb{E}\left(\int_{-R}^{+R} S_t[\mathcal{V}(t;y)\cdot J\nabla H_0(y)]\,\mathrm{d}t\right)^2 \geq 0.
\end{aligned}$$

Finally, let us go back to (48) and (49) which tell us that

$$PA = P\mathbb{E}\int_0^{\mathcal{T}} S_\tau[\{\mathcal{V}(\tau),H_0\}]\ \{\mathcal{V}(0),H_0\}\,\mathrm{d}\tau.$$

and, using (42),

$$PB = P\mathbb{E}\int_0^{\mathcal{T}} \Big\{\mathcal{V}(\tau), S_{-\tau}[\{\mathcal{V}(0),H_0\}]\Big\}\,\mathrm{d}\tau.$$

Let $\psi \in C_c^\infty(\mathbb{R})$. Using the coarea formula, we obtain

$$\begin{aligned}
\int_{\mathbb{R}} \partial_E(h_0(E)d(E))\ \psi(E)\,\mathrm{d}E &= -\int_{\mathbb{R}} h_0(E)d(E)\ \partial_E\psi(E)\,\mathrm{d}E = -\int_{\mathbb{R}^{2D}} PA(y)\ \partial_E\psi(H_0(y))\,\mathrm{d}y \\
&= -P\mathbb{E}\int_0^{\mathcal{T}}\int_{\mathbb{R}^{2D}} S_\tau[\{\mathcal{V}(\tau),H_0\}]\ \{\mathcal{V}(0),H_0\}\ \partial_E\psi(H_0(y))\,\mathrm{d}y\,\mathrm{d}\tau \\
&= -P\mathbb{E}\int_0^{\mathcal{T}}\int_{\mathbb{R}^{2D}} S_\tau[\{\mathcal{V}(\tau),\psi(H_0)\}]\ \{\mathcal{V}(0),H_0\}\,\mathrm{d}y\,\mathrm{d}\tau \\
&= P\mathbb{E}\int_0^{\mathcal{T}}\int_{\mathbb{R}^{2D}} \Big\{\mathcal{V}(\tau),S_{-\tau}[\{\mathcal{V}(0),H_0\}]\Big\}\ \psi(H_0)\,\mathrm{d}y\,\mathrm{d}\tau \\
&= \int_{\mathbb{R}^{2D}} PB(y)\ \psi(H_0(y))\,\mathrm{d}y = \int_{\mathbb{R}} h_0(E)c(E)\ \psi(E)\,\mathrm{d}E.
\end{aligned}$$

∎

3.4.3. The Case With Relaxation. In this section we deal with a relaxation coefficient which depends on the energy, as presented in (HC5'). Of course, a noticeable case consists in assuming full relaxation, γ being a positive constant. But, we can also consider a sequence of coefficients that vanishes, not too fast, as ε goes to 0, see (HC5'). Our analysis heavily uses the additional information on $f^\varepsilon - Pf^\varepsilon$ which is offered by the relaxation. Indeed, we readily obtain the following adaptations of Proposition 4.

Proposition 5 *Suppose that H_0 verifies (HC1), (HC2), (HC4'). Consider a sequence of initial data such that (HC3) holds. Let V^ε be a smooth potential, say $V^\varepsilon \in C^2(\mathbb{R}\times\mathbb{R}^{2D})$ with bounded second order derivatives. Let γ^ε satisfy (HC5'). Then, for any $\varepsilon > 0$, the problem (45) with $f|_{t=0} = f_0^\varepsilon$ has a unique (non-negative) solution $f^\varepsilon \in C^0(\mathbb{R}^+; L^2(\mathbb{R}^{2D}))$. The sequence $(f^\varepsilon)_{\varepsilon>0}$ is bounded in $L^\infty(\mathbb{R}^+; L^2(\mathbb{R}^{2D}))$. Furthermore, let us set $h^\varepsilon(t;x,p) = \frac{\sqrt{\gamma^\varepsilon(H_0(x,p))}}{\varepsilon}(f^\varepsilon - Pf^\varepsilon)(t;x,p)$; then, we have*

$$\sup_{\varepsilon>0}\left(\int_0^\infty\int_{\mathbb{R}^{2D}} |h^\varepsilon(t;x,p)|^2\,\mathrm{d}p\,\mathrm{d}x\,\mathrm{d}t\right) \le M_0 < \infty.$$

Hence, we can expand the solution as

$$f^\varepsilon = Pf^\varepsilon + \frac{\varepsilon}{\sqrt{\gamma_\star^\varepsilon}}g^\varepsilon, \qquad g^\varepsilon = \sqrt{\frac{\gamma_\star^\varepsilon}{\varepsilon^2}}(f^\varepsilon - Pf^\varepsilon) \text{ is bounded in } L^2(\mathbb{R}^+\times\mathbb{R}^{2D}),$$

since $|g^\varepsilon| \le |h^\varepsilon|$. From now on we assume $\varepsilon^2/\gamma_\star^\varepsilon \to 0$, so that we already deduce that f^ε behaves like its projection Pf^ε. Accordingly, we can suppose that $\mathbb{E}f^\varepsilon$ converges to a function $F(t;H_0(y))$ depending on the energy only, weakly in $L^2((0,T)\times\mathbb{R}^{2D})$, and we shall derive the equation satisfied by the limit. To this end, we start by applying the projection operator to (45). We get

$$\partial_t Pf^\varepsilon = -\frac{1}{\varepsilon}\ P\{V^\varepsilon, f^\varepsilon\}.$$

The key observation is that the right hand side only depends on the remainder g^ε since

$$P\{V^\varepsilon, f^\varepsilon\} = P\{V^\varepsilon, Pf^\varepsilon\} + \frac{\varepsilon}{\sqrt{\gamma_\star^\varepsilon}}\{V^\varepsilon, g^\varepsilon\} = \frac{\varepsilon}{\sqrt{\gamma_\star^\varepsilon}}\ P\{V^\varepsilon, g^\varepsilon\}$$

holds by using Lemma 9-v). Hence, we deduce that

$$\partial_t Pf^\varepsilon = -\frac{1}{\sqrt{\gamma_\star^\varepsilon}}\ P\{V^\varepsilon, g^\varepsilon\}. \tag{50}$$

This will be combined with the following evolution equation for the remainder

$$\partial_t g^\varepsilon + \frac{1}{\varepsilon^2}\{H_0, g^\varepsilon\} + \frac{1}{\varepsilon^2}\gamma^\varepsilon(H_0) g^\varepsilon = -\frac{\sqrt{\gamma^\varepsilon_\star}}{\varepsilon^2}(I-P)\{V^\varepsilon, f^\varepsilon\}. \tag{51}$$

We shall use various formulations of (45) and (51) integrated along the characteristics $\mathcal{Y}$ associated to the free Hamiltonian in order to establish useful properties and estimates. Note that the energy conservation yields $\exp\Big(\int_s^t \gamma^\varepsilon(H_0(\mathcal{Y}(u))\,\mathrm{d}u\Big) = \exp\Big(\gamma^\varepsilon(H_0)(t-s)\Big)$

First, f^ε satisfies the following Duhamel formula

$$\begin{aligned} f^\varepsilon(t;y) \;&=\; \mathrm{e}^{-\gamma^\varepsilon(H_0)t/\varepsilon^2} S_{-t/\varepsilon^2}[f_0^\varepsilon](y) - \frac{1}{\varepsilon}\int_s^t \mathrm{e}^{-\gamma^\varepsilon(H_0)(t-\sigma)/\varepsilon^2} S_{(\sigma-t)/\varepsilon^2}[\{V^\varepsilon(\sigma), f^\varepsilon(\sigma)\}](y)\,\mathrm{d}\sigma \\ &+\frac{1}{\varepsilon^2}\int_s^t \mathrm{e}^{-\gamma^\varepsilon(H_0)(t-\sigma)/\varepsilon^2}\;\gamma^\varepsilon(H_0)\; S_{(\sigma-t)/\varepsilon^2}[Pf^\varepsilon(\sigma)](y)\,\mathrm{d}\sigma. \end{aligned}$$

This shows that $f^\varepsilon(t)$ depends on the realizations of $V^\varepsilon(\sigma)$ for $0\le\sigma\le t$ only. We deduce the following:

Lemma 18 *Suppose that the initial data f_0^ε is deterministic. Then, $f^\varepsilon(t)$ and $V^\varepsilon(t')$ are independent when $t' \ge t + \varepsilon^2\mathcal{T}$.*

Second, we also have

$$\begin{aligned} f^\varepsilon(t;y) \;&=\; S_{(s-t)/\varepsilon^2}[f^\varepsilon(s)](y) - \frac{1}{\varepsilon}\int_s^t S_{(\sigma-t)/\varepsilon^2}[\{V^\varepsilon(\sigma), f^\varepsilon(\sigma)\}](y)\,\mathrm{d}\sigma \\ &+\frac{1}{\varepsilon^2}\int_s^t \gamma^\varepsilon(H_0) S_{(\sigma-t)/\varepsilon^2}[Pf^\varepsilon(\sigma)-f^\varepsilon(\sigma)](y)\,\mathrm{d}\sigma. \end{aligned}$$

Let $\psi\in C_c^\infty(\mathbb{R}^{2D})$. We set

$$\begin{aligned} H^\varepsilon[\psi](t,s) \;&=\; \int_{\mathbb{R}^{2D}} \left(f^\varepsilon(t;y) - S_{(s-t)/\varepsilon^2}[f^\varepsilon(s)](y)\right)\,\psi(y)\,\mathrm{d}y \\ &= -\frac{1}{\varepsilon}\int_s^t\int_{\mathbb{R}^{2D}} f^\varepsilon(\sigma;y)\;\{V^\varepsilon(\sigma), S_{(t-\sigma)/\varepsilon^2}[\psi]\}(y)\,\mathrm{d}y\,\mathrm{d}\sigma \\ &+\frac{1}{\varepsilon^2}\int_s^t\int_{\mathbb{R}^{2D}} \gamma^\varepsilon(Pf^\varepsilon - f^\varepsilon)(\sigma;y)\; S_{(t-\sigma)/\varepsilon^2}[\psi](y)\,\mathrm{d}y\,\mathrm{d}\sigma. \end{aligned} \tag{52}$$

Lemma 19 *i) Let $0<R<\infty$. Then, there exists $C(R)>0$, depending on R, (HC4') and (HC-R4) such that for any $\psi\in C_c^\infty(\mathbb{R}^{2D})$, with supp$(\psi)\subset B(0,R)$ and for any $t,s\ge 0$ we have*

$$\begin{aligned} |H^\varepsilon[\psi](t,s)| \;&\le\; C(R)\;\|\psi\|_{W^{1,\infty}(\mathbb{R}^{2D})}\;\|f^\varepsilon\|_{L^\infty(\mathbb{R}^+;L^2(\mathbb{R}^{2D}))}\;\varepsilon\;\mathrm{e}^{C_2|t-s|/\varepsilon^2} \\ &+C(R)\sqrt{\Gamma}\|\psi\|_{L^\infty(\mathbb{R}^{2D})}\;\frac{\sqrt{|t-s|}}{\varepsilon}\left(\int_s^t \|h^\varepsilon(\sigma)\|^2_{L^2(\mathbb{R}^{2D})}\,\mathrm{d}\sigma\right)^{1/2}. \end{aligned}$$

ii) Furthermore, if $\psi(x,p)=\varphi(H_0(x,p))$ with $\varphi\in C_c^\infty(\mathbb{R})$, supp$(\varphi)\subset(-R,+R)$, then one has

$$|H^\varepsilon[\varphi(H_0)](t,s)| \le C(R)\;\|\partial_E\varphi\|_{L^\infty(\mathbb{R})}\;\|f^\varepsilon\|_{L^\infty(\mathbb{R}^+;L^2(\mathbb{R}^{2D}))}\;\frac{|t-s|}{\varepsilon}.$$

Proof. Estimate i) is an immediate consequence of (52), using (40) and (HC-R4). We show ii) by considering a test function which depends on the energy only

$$\begin{aligned} |H^\varepsilon[\varphi(H_0)](t,s)| \;&=\; \left|\int_{\mathbb{R}^{2D}} (f(t;y)-f(s;y))\varphi(H_0(y))\,\mathrm{d}y\right| \\ &= \frac{1}{\varepsilon}\left|\int_s^t\int_{\mathbb{R}D} f(\sigma;y)\;\{V^\varepsilon(\sigma),H_0\}\;\partial_E\varphi(H_0(y))\,\mathrm{d}y\,\mathrm{d}\sigma\right|. \end{aligned}$$

■

We perform similar manipulations on (51). Integrating on the time interval $(t-\varepsilon^2\mathcal{T},t)$, we get

$$\begin{aligned} g^\varepsilon(t;y) &= \mathrm{e}^{-\gamma^\varepsilon(H_0(y))\mathcal{T}} S_{-\mathcal{T}}[g^\varepsilon(t-\varepsilon^2\mathcal{T})](y) \\ &\quad -\frac{\sqrt{\gamma^\varepsilon_\star}}{\varepsilon^2}\int_{t-\varepsilon^2\mathcal{T}}^t \mathrm{e}^{-\gamma^\varepsilon(H_0(y))(t-\sigma)/\varepsilon^2} S_{(\sigma-t)/\varepsilon^2}\Big[(I-P)\{V^\varepsilon(\sigma),f^\varepsilon(\sigma)\}\Big](y)\,\mathrm{d}\sigma. \end{aligned} \tag{53}$$

Then, we insert (53) into (50). Using Proposition 9-v), we obtain

$$\begin{aligned} \partial_t P f^\varepsilon &= -\frac{1}{\sqrt{\gamma^\varepsilon_\star}}\ P\{V^\varepsilon(t),\mathrm{e}^{-\gamma^\varepsilon(H_0(y))\mathcal{T}}S_{-\mathcal{T}}[g^\varepsilon(t-\varepsilon^2\mathcal{T})]\} \\ &\quad +\frac{1}{\varepsilon^2}P\int_{t-\varepsilon^2\mathcal{T}}^t \Big\{V^\varepsilon(t),\mathrm{e}^{-\gamma^\varepsilon(H_0(y))(t-\sigma)/\varepsilon^2}\ S_{(\sigma-t)/\varepsilon^2}[\{V^\varepsilon(\sigma),f^\varepsilon(\sigma\}]\Big\}\,\mathrm{d}\sigma, \end{aligned} \tag{54}$$

for $t\geq\varepsilon^2\mathcal{T}$. Multiplying by $\varphi(H_0(x,p))$ where $\varphi\in C_c^\infty(\mathbb{R})$, $\mathrm{supp}(\varphi)\subset(-R,+R)$ yields

$$\begin{aligned} &\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}^{2D}} f^\varepsilon\varphi(H_0)\,\mathrm{d}y \\ &= \left.\frac{1}{\sqrt{\gamma^\varepsilon_\star}}\int_{\mathbb{R}^{2D}} g^\varepsilon(t-\varepsilon^2\mathcal{T})\ \mathrm{e}^{-\gamma^\varepsilon(H_0(y))\mathcal{T}}\ S_{\mathcal{T}}[\{V^\varepsilon(t),H_0\}]\ \partial_E\varphi(H_0)\,\mathrm{d}y\quad\right\}:=D^\varepsilon(t)[\varphi] \\ &\quad \left.+\frac{1}{\varepsilon^2}\int_{t-\varepsilon^2\mathcal{T}}^t\int_{\mathbb{R}^{2D}} f^\varepsilon(\sigma)\ \Phi^\varepsilon(t,\sigma)\,\mathrm{d}y\,\mathrm{d}\sigma\quad\right\}:=I^\varepsilon(t)[\varphi], \end{aligned} \tag{55}$$

where we have set

$$\Phi^\varepsilon(t,\sigma)=\Big\{V^\varepsilon(\sigma),\mathrm{e}^{-\gamma^\varepsilon(H_0(y))(t-\sigma)/\varepsilon^2}\ S_{(t-\sigma)/\varepsilon^2}[\{V^\varepsilon(t),H_0\}]\ \partial_E\varphi(H_0)\Big\}$$

Using Lemma 18, we observe that $\mathbb{E}D^\varepsilon(t)[\varphi]=0$ and we split

$$\begin{aligned} I^\varepsilon(t)[\psi] &= \left.\frac{1}{\varepsilon^2}\int_{t-\varepsilon^2\mathcal{T}}^t\int_{\mathbb{R}^{2D}} S_{(t-\sigma)/\varepsilon^2}[\mathbb{E}f^\varepsilon(t)]\ \Phi^\varepsilon(t,\sigma)\,\mathrm{d}y\,\mathrm{d}\sigma\quad\right\}:=L^\varepsilon(t)[\psi] \\ &\quad \left.+\frac{1}{\varepsilon^2}\int_{t-\varepsilon^2\mathcal{T}}^t\int_{\mathbb{R}^{2D}} (f^\varepsilon(\sigma)-S_{(t-\sigma)/\varepsilon^2}[\mathbb{E}f^\varepsilon(t)])\ \Phi^\varepsilon(t,\sigma)\,\mathrm{d}y\,\mathrm{d}\sigma\quad\right\}:=R^\varepsilon(t)[\psi] \end{aligned}$$

where, for $t\geq 2\varepsilon^2\mathcal{T}$

$$\begin{aligned} \mathbb{E}R^\varepsilon(t)[\psi] &= \mathbb{E}\frac{1}{\varepsilon^2}\int_{t-\varepsilon^2\mathcal{T}}^t\int_{\mathbb{R}^{2D}}\Big(f^\varepsilon(\sigma)-S_{-\mathcal{T}}[f^\varepsilon(\sigma-\varepsilon^2\mathcal{T})]\Big)\ \Phi^\varepsilon(t,\sigma)\,\mathrm{d}y\,\mathrm{d}\sigma \\ &\quad +\mathbb{E}\frac{1}{\varepsilon^2}\int_{t-\varepsilon^2\mathcal{T}}^t\int_{\mathbb{R}^{2D}} S_{(t-\sigma)/\varepsilon^2}\Big[f^\varepsilon(t)-S_{(\sigma-\varepsilon^2\mathcal{T}-t)/\varepsilon^2}[f^\varepsilon(\sigma-\varepsilon^2\mathcal{T})]\Big)\ \mathbb{E}\Phi^\varepsilon(t,\sigma)\,\mathrm{d}y\,\mathrm{d}\sigma, \end{aligned}$$

As a matter of fact, due to the regularity assumptions (HC4'), (HC-R4), (HC5'), we can evaluate

$$\left.\begin{array}{l} |\Phi^\varepsilon(t,\sigma)| \\ |\nabla_y\Phi^\varepsilon(t,\sigma)| \end{array}\right\}\leq C(R)\ \mathrm{e}^{C_2|t-\sigma|/\varepsilon^2}\ \Big(1+\frac{|t-\sigma|}{\varepsilon^2}\Big)\ \left\{\begin{array}{l} \|\varphi\|_{W^{2,\infty}(\mathbb{R})} \\ \|\varphi\|_{W^{3,\infty}(\mathbb{R})}. \end{array}\right. \tag{56}$$

This allows us to prove the following claim.

Lemma 20 *Let H_0 satisfy (HC1), (HC2), (HC4'), and let V^ε satisfy (HC-R1), (HC-R2), (HC-R3) and (HC-R4). Let f_0^ε be deterministic and satisfy (HC3). Let $0<R<\infty$ and pick $\varphi\in C_c^\infty(\mathbb{R})$, with supp($\varphi$) $\subset B(0,R)$. Then, the following properties hold:*
i) $\mathbb{E}D^\varepsilon(t)[\varphi]=0$,
ii) For any $t\geq\varepsilon^2\mathcal{T}$, $|I^\varepsilon(t)[\varphi]|\leq C$,

iii) For any $t \geq \varepsilon^2\mathcal{T}$, $|\mathbb{E}L^\varepsilon(t)[\varphi]| \leq C$,
iv) For any $t \geq 2\varepsilon^2\mathcal{T}$, $|\mathbb{E}R^\varepsilon(t)[\varphi]| \leq C$ *and moreover*

$$\int_{2\varepsilon^2\mathcal{T}}^T |\mathbb{E}R^\varepsilon(t)[\varphi]|^2 \,\mathrm{d}t \leq C\varepsilon^2,$$

for a constant $C > 0$ *which depends on the assumptions on the data,* R *and* $\|\varphi\|_{W^{2,\infty}(\mathbb{R})}$ *(or* $\|\varphi\|_{W^{3,\infty}(\mathbb{R})}$ *in iv)).*

Proof. Only iv) deserves to be discussed. Combining Lemma 19 to (56), we get

$$\begin{aligned}
&|\mathbb{E}R^\varepsilon(t)[\varphi]| \leq C\ \frac{1}{\varepsilon^2}\mathbb{E}\Bigg(\|f^\varepsilon\|_{L^\infty(\mathbb{R}^+;L^2(\mathbb{R}^{2D}))}\ \varepsilon\int_{t-\varepsilon^2\mathcal{T}}^t \mathrm{e}^{C_2(t-\sigma)/\varepsilon^2}\,\mathrm{d}\sigma \\
&\qquad +\frac{\sqrt{\varepsilon^2\mathcal{T}}}{\varepsilon}\int_{t-\varepsilon^2\mathcal{T}}^t \Big[\Big(\int_{\sigma-\varepsilon^2\mathcal{T}}^\sigma \|h^\varepsilon(\sigma')\|^2_{L^2(\mathbb{R}^{2D})}\,\mathrm{d}\sigma'\Big)^{1/2} + \Big(\int_{\sigma-\varepsilon^2\mathcal{T}}^t \|h^\varepsilon(\sigma')\|^2_{L^2(\mathbb{R}^{2D})}\,\mathrm{d}\sigma'\Big)^{1/2}\Big]\,\mathrm{d}\sigma\Bigg). \\
&\leq C\mathbb{E}\left(\|f^\varepsilon\|_{L^\infty(\mathbb{R}^+;L^2(\mathbb{R}^{2D}))}\ \varepsilon + \frac{2}{\varepsilon^2}\int_{t-\varepsilon^2\mathcal{T}}^t \Big(\int_{t-2\varepsilon^2\mathcal{T}}^t \|h^\varepsilon(\sigma')\|^2_{L^2(\mathbb{R}^{2D})}\,\mathrm{d}\sigma'\Big)^{1/2}\mathrm{d}\sigma\right) \\
&\leq C\mathbb{E}\left(\|f^\varepsilon\|_{L^\infty(\mathbb{R}^+;L^2(\mathbb{R}^{2D}))}\ \varepsilon + 2\Big(\int_{t-2\varepsilon^2\mathcal{T}}^t \|h^\varepsilon(\sigma')\|^2_{L^2(\mathbb{R}^{2D})}\,\mathrm{d}\sigma'\Big)^{1/2}\right)
\end{aligned}$$

which is uniformly bounded by virtue of Proposition 5. We deduce the sharp L^2 estimate by observing that

$$\int_{2\varepsilon^2\mathcal{T}}^\infty \Big(\int_{t-2\varepsilon^2\mathcal{T}}^\sigma \|h^\varepsilon(\sigma')\|^2_{L^2(\mathbb{R}^{2D})}\,\mathrm{d}\sigma'\Big)\,\mathrm{d}t = \int_0^\infty \|h^\varepsilon(\sigma')\|^2_{L^2(\mathbb{R}^{2D})}\Big(\int_{\sigma'}^{\sigma'+2\varepsilon^2\mathcal{T}}\mathrm{d}t\Big)\,\mathrm{d}\sigma' = \varepsilon^2\mathcal{T}\|h^\varepsilon\|^2_{L^2(\mathbb{R}^+\times\mathbb{R}^{2D})}.$$

∎

Coming back to (55), we deduce that, for any fixed $\varphi \in C_c^\infty(\mathbb{R})$, $\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}^{2D}} \mathbb{E}f^\varepsilon(t + \varepsilon^2\mathcal{T}; y)\varphi(H_0(y))\,\mathrm{d}y$ is bounded in $L^\infty(0,T)$. Using the Arzela-Ascoli theorem, and coming back to Lemma 19-ii), we show that $\int_{\mathbb{R}^{2D}} \mathbb{E}f^\varepsilon(t;y)\varphi(H_0(y))\,\mathrm{d}y$ lies in a compact set of $C^0([0,T])$. Thus, by using standard approximation and separability arguments, we extract a subsequence, still labelled by ε, such that

$$\lim_{\varepsilon\to 0}\int_{\mathbb{R}^{2D}} \mathbb{E}f^\varepsilon(t;y)\varphi(H_0(y))\,\mathrm{d}y = \int_{\mathbb{R}^{2D}} F(t;H_0(y))\varphi(H_0(y))\,\mathrm{d}y$$

uniformly on $[0,T]$ for any $\varphi \in L^2(\mathbb{R}; h_0(E)\,\mathrm{d}E)$. Finally, it remains to pass to the limit in

$$\mathbb{E}L^\varepsilon(t)[\varphi(H_0)] = \int_{\mathbb{R}^{2D}} \mathbb{E}f^\varepsilon(t)\left(\frac{1}{\varepsilon^2}\int_{t-\varepsilon^2\mathcal{T}}^t \mathbb{E}S_{(\sigma-t)/\varepsilon^2}[\Phi^\varepsilon(t,\sigma)]\,\mathrm{d}\sigma\right)\mathrm{d}y.$$

We conclude by reproducing the computations of Step 2 and 3 in Section 3.4.2. ∎

4. Concluding remarks

In this paper, we have performed a mathematically rigorous investigation of the behavior of confined particles subject to a fast time-varying perturbation potential. We have dealt with both the quantum and classical cases and, beyond the different modeling contexts, tried to outline the analogies between the two cases. In the quantum case, the large time behavior of the particles is ruled by an Einstein rate equation for the level populations of the confining potential, while in the classical case, a Fokker-Planck type diffusion equation is found for the energy distribution of the particles. Two different frameworks have been considered. First, a fully deteministic framework has been used, but the asymptotic limit depends on a particular relaxation operator that is needed to ensure that the density matrix is close to a diagonal one (in the quantum case) or the distribution function to a function of the total energy only (in the classical case). A second framework deals with random time-varying perturbation under some assumption on the time-decay of the pair correlations. In this random framework, the introduction of a relaxation operator is not needed and we show that the expectation of the solutions converges to the limit equations.

At this level, a remark is in order, because the analogy between the two cases conceals a small difference. Indeed, the fact that the density matrix is diagonal does not mean that it is a function of the Hamiltonian only. In the case with spherical symmetry for instance, the density matrix will depend on the Hamiltonian and on the components of the angular momentum. Therefore, a strict analogy with the quantum case would have been that the solutions of the classical equation $\{H_0, f\} = 0$ are of the form $f_0 = F(H_0, I_1, \ldots, I_K)$, where $\{I_1, \ldots, I_K\}$ is the set of all invariants of the trajectories (beyond the total energy H_0). Then, the relaxation operator should have been defined as a projection onto the manifold defined by constant $(H_0, I_1, \ldots, I_K)$ and the limiting model would have been a $K+1$-dimensional diffusion in the space spanned by $(H_0, I_1, \ldots, I_K)$. The diffusion matrix would have been constructed by a similar procedure as the one used in section 3. In this paper, we have restricted ourselves to the case of one single invariant H_0 just for the sake of simplicity since the whole theory would obviously extend to the more general case (possibly at the expense of some mathematical technicalities).

A last remark is about the connection between the two limit models. Indeed, since one can pass from the quantum kinetic model to the classical one by a semi-classical analysis (using the Wigner equation formalism, for instance), it is natural to wonder whether it is possible to make a connection between the Einstein rate equations on the one hand and the Fokker-Planck diffusion model on the other hand. Although this program seems natural, its mathematical realization is made difficult by the different functional analytic frameworks of the two situations. Work is currently undertaken to try to bypass these technical difficulties.

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