

# Asymptotics Problems for Wave-Particles Interactions; Quantum and Classical Models

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**Quantum Model:** Unknown=**Density Matrix**  $\rho(t; n, m)$ ,  $n, m \in \mathbb{N}$ ,

$$i\hbar \partial_t \rho + [H_q, \rho] = \frac{1}{\tau} Q_q(\rho), \quad \text{Bloch equation}$$

where  $[H_q, \rho](n, m) = \sum_{k \in \mathbb{N}} (H_q(n, k)\rho(k, m) - \rho(n, k)H_q(k, m))$ ,

**Classical Model:** Unknown=**Distribution Function**  $f(t; x, p) \geq 0$ ,  
 $x, p \in \mathbb{R}^N$

$$\partial_t f + \{H_c, f\} = \frac{1}{\tau} Q_c(f),$$

where  $\{H_c, f\} = \nabla_p H_c \cdot \nabla_x f - \nabla_x H_c \cdot \nabla_p f$ .

## Scaling Issues

$$\text{We split } H = \begin{cases} H_{0c}(x, p) + \epsilon V_c(t, t/\theta; x, p), \\ H_{0q}(n, m) + \epsilon V_q(t, t/\theta; n, m), \end{cases}$$

$H_0$  = time independent Hamiltonian corresponding to the **confining potential** of the atomic nucleus,

$\epsilon V$  = perturbations by external electro-magnetic waves

Scaling Assumptions:

$$\frac{TH_{0c}}{LP} \simeq \frac{1}{\epsilon^2} \gg 1, \quad \frac{TH_{0q}}{\hbar} \simeq \frac{1}{\epsilon^2} \gg 1, \quad \frac{T}{\theta} \simeq \frac{1}{\epsilon^2}, \quad \frac{T}{\tau} \simeq \frac{1}{\epsilon^2}.$$

## Cutting Edge Questions

$$i\partial_t \rho + \frac{1}{\epsilon^2} [H_{0q} + \epsilon V_q(t/\epsilon^2), \rho] = \frac{1}{\epsilon^2} Q_q(\rho),$$

$$\partial_t f + \frac{1}{\epsilon^2} \underbrace{\{H_{0c} + \epsilon V_c(t/\epsilon^2), f\}} = \underbrace{\frac{1}{\epsilon^2} Q_c(f)},$$

Free Hamiltonian  $H_0$

Damping

+ Small Oscillating Perturbation

or Relaxation term

- Derivation of a New Classical Model (Relaxation operator)
- Relaxation and Homogenization all together
- Random vs. Deterministic modelling

## Asymptotic Behavior

- Quantum Model:  $\rho_\epsilon(t; n, m) \rightarrow \rho(t; n, n) \delta(n, m)$  verifying the **Einstein Rate Equation**

$$\partial_t \rho(t; n, n) = \sum_k A(t; n, k) (\rho(t; k, k) - \rho(t; n, n))$$

- Classical Model:  $f_\epsilon(t; x, p) \rightarrow F(t; H_0(x, p))$  verifying the **Diffusion Eq.** wrt energy

$$\partial_t (h_0(E) F(t; E)) - \partial_E (d(E) h_0(E) \partial_E F(t; E)) = 0$$

$h_0(E) F(t; E) = \#$  of particles with energy  $E$ ,

$d(E) h_0(E) \partial_E F(t; E) =$  Flux through the energy surface  $\Sigma_E$ .

- Both limit eq. are **Irreversible Equations** (decay of  $L^2$  norms)

## Role of the Damping Term, Deterministic vs Random Perturbations

Two Difficulties:

- Homogeneization Limit (Fast Oscillations of  $V$ )
- Relaxation Limit that pushes towards  $\text{Ker}([H_0, \cdot] - Q_q)$  (resp.  $\text{Ker}(\{H_0, \cdot\} - Q_c) \sim$  “hydrodynamic limit”

Two Frameworks:

- (Quasi-)Periodic Oscillations and Damping is crucial
- Random Perturbation where Damping term can vanish

## Role of the Damping: Cell Problems

Let  $\Omega \in \mathbb{R}^D$  with **rationally independent components**. Consider

$$\lambda R + \Omega \cdot \nabla_{\vartheta} R = H,$$

with  $(0, 1)^N = \Theta$ -periodic boundary condition and  $\lambda \geq 0$ .

- If  $\lambda = 0$  then  $\int_{\Theta} H \, d\vartheta = 0$  is a *necessary* condition.
- If  $\lambda = 0$  and  $H = 0$  then  $\Omega \cdot \xi \widehat{R}(\xi) = 0$  and  **$R$  is constant**.
- But the Fredholm alternative *does not* apply to  $\Omega \cdot \nabla_{\vartheta}$  due to **Small Divisors** problems: set  $\widehat{R}(\xi) = -i\widehat{H}(\xi)/\Omega \cdot \xi$ ,

$$\text{If } |\Omega \cdot \xi| \geq C/|\xi|^\gamma \text{ then } \|R\|_{L^2} \leq C\|H\|_{H^\gamma}.$$

- With  **$\lambda > 0$**  we get

$$R(\vartheta) = \int_0^{+\infty} e^{-\lambda\sigma} H(\vartheta - \Omega\sigma) \, d\sigma \in L^2.$$

## How does randomness induce irreversibility ?

Toy Model:  $\frac{d}{dt}u_\epsilon(t) = i\frac{1}{\epsilon}a(t/\epsilon^2)u_\epsilon(t)$  with  $a$  random,  $\mathbb{E}a = 0$

Crucial assumption:  $a(t)$  and  $a(s)$  decorrelate when  $|t - s| \geq 1$

Duhamel's Formula:  $u_\epsilon(t) = u_\epsilon(t - \epsilon^2) + \frac{1}{\epsilon} \int_{t-\epsilon^2}^t ia(s/\epsilon^2)u_\epsilon(s) ds$

$$\frac{a(t/\epsilon^2)}{\epsilon}u_\epsilon(t) = \underbrace{\frac{a(t/\epsilon^2)}{\epsilon}u_\epsilon(t - \epsilon^2)}_{\mathbb{E}(\dots) = 0} + \underbrace{\frac{1}{\epsilon^2} \int_{t-\epsilon^2}^t ia(t/\epsilon^2)a(s/\epsilon^2)u_\epsilon(s) ds}_{\mathcal{O}(1)}$$

$$\mathbb{E}\frac{i}{\epsilon}a(t/\epsilon^2)u(t) = - \int_0^1 \mathbb{E}(a(t/\epsilon^2)a(t/\epsilon^2 - \tau)) d\tau \mathbb{E}u_\epsilon(t) + \text{small terms}$$

so that the limit eq. is

$$\frac{d}{dt}u = -\lambda u, \quad \lambda = \int_0^1 \mathbb{E}(a(0)a(-\tau)) d\tau > 0.$$

## The Quantum Model

$$\left\{ \begin{array}{l} \gamma(n, m) \geq 0, \quad \gamma(n, n) = 0, \quad \gamma(n, m) = \gamma(m, n), \\ \omega(n, m) = -\omega(m, n) \in \mathbb{R}, \\ V_\epsilon(t; n, k) = V(t, t/\epsilon^2; n, k), \quad V(n, k) = \overline{V(k, n)} + \text{bounds} \end{array} \right.$$

$$Q(\rho)(n, m) = i\gamma(n, m) (\rho(n, m)\delta(n, m) - \rho(n, m))$$

$$[H_0, \rho] = -\omega(n, m)\rho(n, m)$$

Set  $Z(n, m) = \gamma(n, m) + i\omega(n, m)$ :

$Z(n, m) = 0$  for  $n = m$ , and  $\overline{Z(n, m)} = Z(m, n)$ .

$$\begin{aligned} \partial_t \rho(t; n, m) + \frac{1}{\epsilon^2} Z(n, m) \rho(n, m) &= \frac{1}{\epsilon} \Theta_\epsilon[\rho](t; n, m) \\ &= -\frac{i}{\epsilon} \sum_{k \in \mathbb{N}} \left[ V_\epsilon(n, k) \rho(t; k, m) - V_\epsilon(k, m) \rho(t; n, k) \right]. \end{aligned}$$

$\Theta_\epsilon$  is a (uniformly) bounded operator on  $\ell^2$

The problem is well-posed in  $C^0([0, \infty); \ell^2) +$  (uniform) estimates.



Eq. for the populations:

$$\partial_t \rho(t; n, n) = -\frac{i}{\epsilon} \sum_{k \in \mathbb{N}} \left[ V_\epsilon(n, k) \rho(t; k, n) - V_\epsilon(k, n) \rho(t; n, k) \right].$$

depends only on the coherences

Eq. for the quantum coherences: ( $n \neq m$ )

$$\begin{aligned} \partial_t \rho(t; n, m) = & -\frac{1}{\epsilon^2} Z(n, m) \rho(n, m) \\ & -\frac{i}{\epsilon} \sum_{k \in \mathbb{N}} \left[ V_\epsilon(n, k) \rho(t; k, m) - V_\epsilon(k, m) \rho(t; n, k) \right]. \end{aligned}$$

Quantum Coherences are **Damped** when  $\text{Re}Z(n, m) = \gamma(n, m) \neq 0$ ,

Hence the solution **relaxes** to  $\rho(t; n, m) \delta(n, m)$ .

## The Two-level Model

“1”=Ground state, “2”=Excited state

$$\frac{d}{dt}\rho_{11}^\epsilon = -\frac{2}{\epsilon}\text{Im}(V_{12}^\epsilon\rho_{21}^\epsilon), \quad \frac{d}{dt}\rho_{21}^\epsilon = -\frac{1}{\epsilon^2}(i\omega+\gamma)\rho_{21}^\epsilon + \frac{i}{\epsilon}V_{21}^\epsilon(2\rho_{11}^\epsilon-1).$$

Perturbation  $V_{12}^\epsilon(t) = \exp(i(\Delta + \omega)t/\epsilon^2)$ .

Set  $\rho_{21}^\epsilon(0) = 0$ , then as  $\epsilon \rightarrow 0$

$$\frac{d}{dt}\rho_{11} = \frac{2\gamma}{\gamma^2 + \Delta^2}(\rho_{22} - \rho_{11}), \quad \frac{d}{dt}(\rho_{11} + \rho_{22}) = 0$$

( $\Delta = 0$  as well.)

However, when  $\gamma = 0$ , we have

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

Rabi's oscillations

## Quantum Model: (Quasi-)Periodic oscillations

$V_\epsilon(t; n, m) = \mathcal{V}(t, \Omega t/\epsilon^2; n, m)$  with  $\Omega \in \mathbb{R}^d \setminus \{0\}$ , rationally independent components and  $\gamma(n, m) \geq \gamma_* > 0$  for  $n \neq m$ .

Multiscale Ansatz:  $\rho_\epsilon(t; n, m) = \sum_j \epsilon^j \rho^{(j)}(t, \Omega t/\epsilon^2; n, m)$ .

$\partial_t \rightarrow \partial_t + \frac{1}{\epsilon^2} \Omega \cdot \nabla_{\vartheta}$  yields

$$1/\epsilon^2 \text{ terms: } \Omega \cdot \nabla_{\vartheta} \rho^{(0)} + Z(n, m) \rho^{(0)} = 0,$$

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

$$1/\epsilon^0 \text{ terms: } \Omega \cdot \nabla_{\vartheta} \rho^{(2)} + Z(n, m) \rho^{(2)} = -\partial_t \rho^{(0)} + \Theta(t, \vartheta) [\rho^{(1)}], \dots$$

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

$$\rho^{(1)}(t, \vartheta; n, m) = i\chi(t, \vartheta; n, m) (\rho^{(0)}(t; m, m) - \rho^{(0)}(t; n, n)),$$

$$\chi(t, \vartheta; n, m) = - \int_0^{+\infty} e^{-Z(n, m)\sigma} \mathcal{V}(t, \vartheta - \Omega\sigma; n, m) d\sigma, \quad n \neq m$$

## Statement for the Quantum Model: (Quasi-)Periodic oscillations

**Theorem.**  $\rho_\epsilon$  converges to  $\rho(t; n, n)\delta(n, m)$  weakly in  $L^2(\mathbb{R}^+; \ell^2)$ ; the diagonal part  $\rho_\epsilon(t; n, n)$  converges to  $\rho(t; n, n)$  in  $C^0([0, T]; \ell^2 - \text{weak})$  and the limit satisfies the Einstein rate equation

$$\partial_t \rho(t; n, n) = \sum_{k \in \mathbb{N}} A(t; n, k) (\rho(t; k, k) - \rho(t; n, n)),$$

$$\rho(0; n, n) = \lim_{\epsilon \rightarrow 0} \rho_\epsilon^0(n, n) \quad \text{weakly in } \ell^2,$$

$$A(t; n, k) = 2\text{Re}(Z(n, k)) \int_{\Theta} |\chi(t, \vartheta; n, k)|^2 d\vartheta > 0, \text{ for } n \neq k.$$

## Method of proof

- Uniform estimates
- Use Double-scale convergence [Nguetseng 89, Allaire 92] (to be adapted to the quasi-periodic framework):

Let  $u_\epsilon$  be a bounded sequence in  $L^2(\mathbb{R})$ . Then, there exists a subsequence and  $U \in L^2_{\#}(\mathbb{R} \times \Theta)$  such that for any trial function

$$\lim_{\epsilon \rightarrow 0} \int_{\mathbb{R}} u_\epsilon(t) \psi(t, \Omega t / \epsilon^2) dt = \int_{\mathbb{R}} \int_{\Theta} U(t, \vartheta) \psi(t, \vartheta) d\vartheta dt.$$

- Multiply the equation by “oscillating test functions” [Evans 89-92, Tartar 86-89]

## Quantum Model: Random Framework

$V_\epsilon(t; n, m) = \mathcal{V}(t/\epsilon^2; n, m)$  with  $\mathcal{V}$  bounded random variable such that

- i)  $\mathbb{E}(\mathcal{V}(\tau; n, m)) = 0,$
- ii)  $E(\mathcal{V}(\tau; k, l) \mathcal{V}(\sigma; m, n)) = \mathcal{R}(\tau - \sigma; k, l, m, n)$
- iii) If  $|\tau - \sigma| \geq \mathcal{T}$  then  $\mathcal{V}(\tau)$  and  $\mathcal{V}(\sigma)$  are independent.

**Theorem.** Let  $\rho_\epsilon^0$  be **deterministic**. Suppose

$Z(n, m) = \gamma(n, m) + i\omega(n, m)$  **vanishes iff  $n = m$** . Then,

$\mathbb{E}\rho_\epsilon(t; n, m)$  converges weakly to  $\rho(t; n, n)\delta(n, m)$  and  $\mathbb{E}\rho_\epsilon(t; n, n)$  converges in  $C^0([0, T]; \ell^2 - weak)$  to  $\rho \in L^\infty(\mathbb{R}^+; \ell^2)$  sol. of the Einstein eq. with

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

## Comments

- If all  $\gamma(n, m) = 0$  it means that  $\omega(n, m) = H_0(m, m) - H_0(n, n) \neq 0$  where  $H_0(n, n)$  = eigenvalues of a differential operator: **non-degeneracy assumption**.

Need relaxation for energy levels corresponding to multidimensional eigenspaces.

- Alternative: Same statement with possibly vanishing damping coefficients

$$\gamma_\epsilon(n, m) \geq \underline{\gamma}_\epsilon > 0, \quad \gamma_\epsilon(n, m) \xrightarrow{\epsilon \rightarrow 0} \gamma(n, m) \geq 0, \quad \frac{\epsilon^2}{\underline{\gamma}_\epsilon} \xrightarrow{\epsilon \rightarrow 0} 0.$$

Trick: use the “Entropy Estimate”

$$\rho_\epsilon(t; n, m) = \rho_\epsilon(t; n, n)\delta(n, m) + \frac{\epsilon}{\sqrt{\underline{\gamma}_\epsilon}} r_\epsilon(t; n, m)$$

with  $r_\epsilon(t; n, m)$  bounded.

## A New Classical Model

Goal: Mimic the quantum relaxation operator

Populations  $\simeq$  # of particles on a energy shell  $\Sigma_E = \{H_0(x, p) = E\}$ .

Hypothesis (think of  $H_0(x, p) = x^2 + p^2$ )

•  $H_0 \in C^\infty(\mathbb{R}^{2D})$ ,  $\lim_{|(x,p)| \rightarrow \infty} H_0(x, p) = +\infty$  (Confining).

• For a.a.  $E \in \mathbb{R}$ ,  $\Sigma_E$  is a smooth orientable  $(2D - 1)$  submanifold

of  $\mathbb{R}^{2D}$ . We set  $\delta(H_0(x, p) - E) := \frac{d\Sigma_E(x, p)}{|\nabla_{x,p} H_0(x, p)|}$  (Liouville's

measure) and suppose  $h_0(E) := \int_{\Sigma_E} \delta(H_0(x, p) - E) < +\infty$ .

Define  $Pf(x, p) = \frac{1}{h_0(E)} \int_{\Sigma_E} f(y, q) \delta(H_0(y, q) - E) \Big|_{E=H_0(x,p)}$



## Classical Model

Fundamental properties follow from the coarea formula

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

which yields

$$\begin{cases} P \text{ is a bounded operator on } L^r, & P(Pf) = Pf, \\ \int Pf \, dp \, dx = \int f \, dp \, dx, & P\{H_0, f\} = 0 \end{cases}$$

$$\underbrace{\partial_t f_\epsilon + \frac{1}{\epsilon^2} \{H_0, f_\epsilon\}}_{\text{Transport along}} + \underbrace{\frac{1}{\epsilon} \{V_\epsilon, f_\epsilon\}}_{\text{Fast Varying}} = \underbrace{\frac{\gamma}{\epsilon^2} (Pf_\epsilon - f_\epsilon)}_{\text{Resonant Interaction}}$$

Transport along      Fast Varying      Resonant Interaction

$X_\epsilon(t), P_\epsilon(t)$       Perturbation

where  $\frac{d}{dt}(X_\epsilon, P_\epsilon) = \frac{1}{\epsilon^2} (\nabla_p H_0, -\nabla_x H_0)(X_\epsilon, P_\epsilon)$

“H-Theorem”:  $\|f_\epsilon(t)\|_{L^2(\mathbb{R}^{2N})}^2 + \frac{\gamma}{\epsilon^2} \|f_\epsilon - Pf_\epsilon\|_{L^2((0, \infty) \times \mathbb{R}^{2N})}^2 \leq \|f_0\|_{L^2(\mathbb{R}^{2N})}^2$

Write  $f_\epsilon = Pf_\epsilon + \epsilon g_\epsilon$  where

$$\partial_t Pf_\epsilon = -P\{V_\epsilon, g_\epsilon\}$$

$$\partial_t g_\epsilon = -\frac{\gamma}{\epsilon^2}g_\epsilon - \frac{1}{\epsilon^2}\{H_0, g_\epsilon\} - \frac{1}{\epsilon^2}\{V_\epsilon, Pf_\epsilon\} - \frac{1}{\epsilon}(I - P)\{V_\epsilon, g_\epsilon\}$$

The remainder is **damped** for  $\gamma > 0$

and the solution **relaxes** to  $Pf(t, H_0(x, p))$ .

## Quasi-periodic Framework

**Theorem.** Suppose  $V_\epsilon(t; x, p) = V(t, \Omega t/\epsilon^2; x, p)$  with  $\Omega$  having rationally indep. components. Then,  $f_\epsilon = P f_\epsilon + \epsilon g_\epsilon$  where  $g_\epsilon$  is bounded in  $L^2((0, T) \times \mathbb{R}^{2D})$  and, up to a subsequence,  $P f_\epsilon(t; x, p)$  converges to  $F(t; H_0(x, p))$  in  $C^0([0, T]; L^2(\mathbb{R}^{2D}) - weak)$ , with

$$\partial_t(h_0 F) = \partial_E(h_0 d \partial_E F)$$

$$d(t; E) = \Pi \left( \int_{\Theta} \{ \mathcal{V}, H_0 \} \chi \, d\vartheta \right) (E) \geq 0,$$

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

### Crucial Assumptions

- Damping  $\gamma > 0$
- **Stability Property** (or increase  $\gamma$ )

$$\sup_{|(x,p)| \leq R} \left| \nabla_{x,p} (\mathcal{X}(t; x, p), \mathcal{P}(t; x, p)) \right| \leq C_R (1 + |t|)^{q_R}$$

## A Simple Example

$$H_0(x, p) = \frac{x^2 + p^2}{2}, \quad V(t/\epsilon^2, x) = x \cos(\omega t/\epsilon^2)$$

$$\Pi f(E) = \frac{1}{2\pi} \int_0^{2\pi} f\left(\sqrt{2E} \cos(\sigma), \sqrt{2E} \sin(\sigma)\right) d\sigma$$

$$d(E) = \frac{\pi E}{2} \left( \frac{\gamma}{(\omega + 1)^2 + \gamma^2} + \frac{\gamma}{(\omega - 1)^2 + \gamma^2} \right)$$

If  $\omega = \pm 1$ , the coefficient blows up as  $\gamma \rightarrow 0$ : resonance phenomena

## Random Framework

**Theorem.** Let  $\gamma = 0$ . Suppose that  $\{H_0, f\} = 0$  iff  $f(y) = F(H_0(y))$ . Then,  $\mathbb{E}P f_\epsilon \rightarrow F(t; H_0(y))$  in  $C^0([0, T]; L^2(\mathbb{R}^{2D}) - weak)$ , sol. of a diffusion eq. with

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

- Is it interesting ? Not so much!

$H_0(x, p) = (x^2 + p^2)/2$ , works in 1D but fails for  $D \geq 2$  (since  $\{H_0, x \wedge p\} = 0$ ). Related to ergodicity of  $H_0$  [Knauf 87, Donnay-Liverani 91]

- But we can deal with **vanishing** damping coefficients

$$\gamma_\epsilon \rightarrow \gamma_0 \geq 0, \quad \gamma_\epsilon > 0, \quad \epsilon^2/\gamma_\epsilon \xrightarrow{\epsilon \rightarrow 0} 0$$

- Relaxed Assumptions on  $H_0$ : bounded derivatives of order 2, 3.

## Comments

- More general oscillating potentials can be dealt with **KBM**= Krylov-Bogolioubov-Mitropolski type (long time average assumption)

Difficulty: the action of  $P$  on Sobolev spaces is unclear.

- Solutions of  $\{H_0, f\} = 0: H_0, I_1, \dots, I_K$ , then defines  $P$  to be a projection onto given involution quantities. This would lead a  $K + 1$ -dimensional diffusion equation.
- Establish relation between the quantum and the classical models through Semi-Classical Limit.