

Classical and quantum particles coupled to a vibrational environment

with :

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Thierry GOUDON Team COFFEE, Inria Motivation: description of dissipation in (quantum-)mechanical systems

Caldeira-Legget (Ann. Phys. 83)

Dissipation arising on a physical system might come from a coupling with a complex environment: energy is evacuated into the environment and does not come back to the system. Dissipation = transfer of energy from the single degree of freedom characterising the system to the set of degrees of freedom describing the environment.

Motivation: description of dissipation in (quantum-)mechanical systems

 $\dot{q} = -\lambda \dot{q} + F_{\text{ext}}$

Where does the friction λ come from ?

Many approaches, depending on the model of the degrees of freedom for the environment:

Komech, Spohn '90-00 Jaksic-Pillet Acta. Math. 98

A series of works by **S. De Bièvre** (Lille) with L. Bruneau (CMP'02), and P. Parris, P. Lafitte, B. Aguer, E. Soret... "Dynamical Lorentz gas": interaction of a particle with a vibrational field

"a particle in a pinball machine"

The BdB model for a single particle

A particle moving through a *transverse* continuum of vibrating membranes



$$\begin{aligned} & \mathbf{\ddot{q}}(t) = -\nabla_{\mathbf{q}} V(\mathbf{q}(t)) - \int_{\mathbb{R}^{d} \times \mathbb{R}^{n}} \sigma_{1}(\mathbf{q}(t) - \mathbf{z}) \ \sigma_{2}(\mathbf{y}) \ \nabla_{\mathbf{z}} \Psi(t, \mathbf{z}, \mathbf{y}) \, \mathrm{d}\mathbf{y} \, \mathrm{d}\mathbf{z}, \\ & \partial_{tt}^{2} \Psi(t, \mathbf{x}, \mathbf{y}) - c^{2} \Delta_{\mathbf{y}} \Psi(t, \mathbf{x}, \mathbf{y}) = -\sigma_{2}(\mathbf{y}) \sigma_{1}(\mathbf{x} - \mathbf{q}(t)) \end{aligned}$$

A particle coupled to its environment

$$\begin{aligned} & \mathbf{\ddot{q}}(t) = -\nabla_{\mathbf{q}} V(\mathbf{q}(t)) - \int_{\mathbb{R}^{d} \times \mathbb{R}^{n}} \sigma_{1}(\mathbf{q}(t) - \mathbf{z}) \ \sigma_{2}(\mathbf{y}) \ \nabla_{\mathbf{z}} \Psi(t, \mathbf{z}, \mathbf{y}) \, \mathrm{d}\mathbf{y} \, \mathrm{d}\mathbf{z}, \\ & \partial_{tt}^{2} \Psi(t, \mathbf{x}, \mathbf{y}) - c^{2} \Delta_{\mathbf{y}} \Psi(t, \mathbf{x}, \mathbf{y}) = -\sigma_{2}(\mathbf{y}) \sigma_{1}(\mathbf{x} - \mathbf{q}(t)) \end{aligned}$$

Modeling parameters: form functions σ_1, σ_2 (C_c^{∞} , non negative...), *c*: wave speed

Hamiltonian structure:

$$\begin{aligned} &\frac{1}{2} |\dot{q}(t)|^2 + V(q(t)) + \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^n} (|\partial_t \Psi|^2 + c^2 |\nabla_y \Psi|^2)(t, x, y) \, \mathrm{d}y \, \mathrm{d}x \\ &+ \int_{\mathbb{R}^d \times \mathbb{R}^n} \sigma_1(x - q(t)) \sigma_2(y) \Psi(t, x, y) \, \mathrm{d}y \, \mathrm{d}x \text{ is conserved} \end{aligned}$$

Starting point: findings of De Bièvre's group

Assume n = 3 (wave dimension) and $c \gg 1$ large enough

• If V is a confining potential, as time becomes large, q(t) converges to the potential well and the velocity $\dot{q}(t)$ tends to 0.

• If $V(q) = \mathcal{F} \cdot q$, there exists a limiting velocity $v(\mathcal{F})$ and, for \mathcal{F} small enough, $q(t) \sim q_{\infty} + v(\mathcal{F})t$ and $\dot{q}(t) \rightarrow v(\mathcal{F})$.

It is remarkable that $v(\mathcal{F}) \sim \mu \mathcal{F}$ for small \mathcal{F} 's: linear response.

• Typical convergence rate $e^{-\gamma t/c^3}$.

These results bring out **dissipative effects** of the interaction with medium: asymptotically it acts like a friction force and energy is evacuated in the membranes.

Many particles: mean-field interpretation

Consider a set of *P* particles

$$\begin{cases} \ddot{q}_j(t) = -\nabla_q V(q_j(t)) - \nabla_q \Phi(t, q_j(t)), \\ \\ \partial_{tt}^2 \Psi(t, x, y) - c^2 \Delta_y \Psi(t, x, y) = -\sigma_2(y) \sum_{k=1}^P \sigma_1(x - q_k(t)). \end{cases}$$

Further results on the *P* particles case and the behavior as $t \to \infty$, $P \to \infty$: A. Vavasseur '20 But the large time behavior is much more complex, with several scenario, than for a single particle.

Kinetic version of the BdB model

We are finally led to

$$\begin{split} \partial_t F + \mathbf{v} \cdot \nabla_x F - \nabla_x (V + \Phi) \cdot \nabla_v F &= 0, \\ \Phi(t, x) &= \int_{\mathbb{R}^d \times \mathbb{R}^n} \sigma_1(x - z) \sigma_2(\mathbf{y}) \Psi(t, z, \mathbf{y}) \, \mathrm{d}z \, \mathrm{d}\mathbf{y}, \\ (\partial_{tt}^2 \Psi - c^2 \Delta_\mathbf{y} \Psi)(t, x, \mathbf{y}) &= -\sigma_2(\mathbf{y}) \int_{\mathbb{R}^d} \sigma_1(x - z) \rho(t, z) \, \mathrm{d}z, \\ \rho(t, x) &= \int_{\mathbb{R}^d} F(t, x, \mathbf{v}) \, \mathrm{d}\mathbf{v}. \end{split}$$

Bear in mind that $y \in \mathbb{R}^n$ is a *transverse* variable: the model differs from the coupling Vlasov-Wave (coming from Vlasov-Maxwell) dealt with e. g. by Bouchut-Golse-Pallard'04.

Overview of the results

Energy conservation

$$\frac{\mathrm{d}}{\mathrm{d}t} \left\{ \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^n} |\partial_t \Psi(t, x, y)|^2 \, \mathrm{d}x \, \mathrm{d}y + \frac{c^2}{2} \int_{\mathbb{R}^d \times \mathbb{R}^n} |\nabla_y \Psi(t, x, y)|^2 \, \mathrm{d}x \, \mathrm{d}y \right. \\ \left. + \int_{\mathbb{R}^d \times \mathbb{R}^d} F(t, x, v) \left(\frac{|v|^2}{2} + V(x) + \Phi(t, x) \right) \, \mathrm{d}v \, \mathrm{d}x \right\} = 0.$$

"Vibrational+ Kinetic & Potential particle energy + Coupling"

- Existence-uniqueness
 with general external potential x → V(x) and data
 (it slightly generalizes BdB's analysis: n ∈ N \ {0}, P > 1
 particles...)
- mean-field asymptotics
- asymptotic analysis
- equilibrium states and stability (by a variational approach)
- Landau damping

A (quite surprising) connection to the Vlasov–Poisson equation

Rescale the equation: large wave speed and strong coupling

$$\partial_{tt}^2 \Psi_\epsilon - rac{1}{\epsilon} \Delta_y \Psi_\epsilon = -rac{1}{\epsilon} \sigma_2(y) \int \sigma_1(x-z)
ho_\epsilon(t,z) \, \mathrm{d}z.$$

Formally as $\epsilon \to 0$: $-\Delta_y \Psi(t, x, y) = -\sigma_2(y) \sigma_1 * \rho(t, x)$:

 $\Psi(t, x, y) = \Upsilon(y)\sigma_1 * \rho(t, x) \text{ with } \Delta_y \Upsilon(y) = \sigma_2(y).$

Therefore, we get $\Phi(t, x) = -\Lambda \sigma_1 * \sigma_1 * \rho(t, x)$, with $\Lambda = -\int \Upsilon \sigma_2(y) \, dy \Big(= \int |\nabla_y \Upsilon(y)|^2 \, dy > 0 \Big).$

• We can rescale as well $\sigma_1 \to \sigma_{1,\epsilon}$ so that $|\widehat{\sigma_{1,\epsilon}}(\xi)|^2 \sim \frac{1}{|\xi|^2}$. It yields the *ATTRACTIVE* Vlasov–Poisson system.

From VW to attractive VP

$$\begin{aligned} & \partial_t F_\epsilon + \mathbf{v} \cdot \nabla_x F_\epsilon - \nabla_x \Phi_\epsilon \cdot \nabla_\mathbf{v} F_\epsilon = \mathbf{0} \\ & \mathbf{\Phi}_\epsilon = \sigma_{\mathbf{1},\epsilon} * \int \sigma_2 \Psi_\epsilon \, \mathrm{d}y \\ & \mathbf{\Psi}_\epsilon(t, x, y) \simeq \Upsilon(y) \sigma_{\mathbf{1},\epsilon} * \rho_\epsilon(t, x) \text{ with } \Delta_y \Upsilon = \sigma_2 \\ & \mathbf{\Phi}_\epsilon \simeq -\Lambda \sigma_{\mathbf{1},\epsilon} * \sigma_{\mathbf{1},\epsilon} * \rho_\epsilon \text{ with } \Lambda = -\int \Upsilon \sigma_2 \, \mathrm{d}y > \mathbf{0}, \\ & \mathbf{\Phi}_\epsilon \to -\frac{\Lambda}{\xi^2} \widehat{\rho} \end{aligned}$$

It yields the ATTRACTIVE Vlasov-Poisson system:

$$\begin{aligned} \partial_t F + \mathbf{v} \cdot \nabla_x F - \nabla_x \Phi \cdot \nabla_v F &= \mathbf{0}, \\ \Delta \Phi &= \Lambda \rho, \qquad \Lambda > \mathbf{0}. \end{aligned}$$

Intuition that VW inherits some features of the attractive VP system

A modified formulation

We rewrite the pb. as

$$\partial_t F + \mathbf{v} \cdot \nabla_x F = \nabla_\mathbf{v} F \cdot \nabla_x \left(\Phi_\mathbf{I} + \Phi_\mathbf{S} \right)$$

where we set

$$\Phi_{I}(t,x) = \frac{1}{(2\pi)^{n}} \int_{\mathbb{R}^{n}} \int_{\mathbb{R}^{d}} \sigma_{1}(x-z) \\ \times \left(\widehat{\Psi_{0}}(z,\xi) \cos(c|\xi|t) + \widehat{\Psi_{1}}(z,\xi) \frac{\sin(c|\xi|t)}{c|\xi|}\right) \widehat{\sigma_{2}}(\xi) \, \mathrm{d}z \, \mathrm{d}\xi$$

and

$$\Phi_{S}(t,x) = -\int_{\mathbb{R}^{d}} \Sigma(x-z) \left(\int_{0}^{t} p_{c}(t-s)\rho(s,z) \, \mathrm{d}s \right) \, \mathrm{d}z$$

with $\rho(t,x) = \int F(t,x,v) \, \mathrm{d}v, \quad \Sigma = \sigma_{1} * \sigma_{1},$
and $t \mapsto p_{c}(t) = \frac{1}{(2\pi)^{n}} \int_{\mathbb{R}^{n}} \frac{\sin(c|\xi|t)}{c|\xi|} |\widehat{\sigma_{2}}(\xi)|^{2} \, \mathrm{d}\xi.$

The kernel p_c drives the dissipation mechanism (σ_2 , c and n)

Landau Damping

Given $M: v \mapsto M(v) > 0$, with $\int M dv = 1$, $\rho_0 M(v)$ defines a homogeneous solution, with mass ρ_0 of the VW system.

"Theorem". Initial data $F_0(x, v) = \rho_0 M(v) + f_0(x, v)$. Assume

- smooth data $\sigma_1, \sigma_2, M, f_0$,
- ▶ n ≥ 3 odd
- the (L) stability criterion

There exists $\epsilon_0>0$ such that if $\|\mathit{f}_0\|\leq\epsilon_0,$ then

 $\rho - \int F_0 \, \mathrm{d} v \, \mathrm{d} x$ and $\nabla_x \Phi$ tend to 0 as $t \to \infty$.

Landau '46 (linearized pb.) Mouhot-Villani '11 (torus) Faou-Rousset '16 (finite regularity) Bedrossian-Masmoudi-Mouhot '16-'18 (torus, whole space) Han-Kwan-Nguyen-Rousset '19 (whole space)

Quantum version: Schrödinger-Wave

$$\begin{split} i\partial_t u &+ \frac{1}{2} \Delta_x u = \left(\sigma_1 \star \int_{\mathbb{R}^n} \sigma_2(\mathbf{y}) \psi(t, \mathbf{x}, \mathbf{y}) \, \mathrm{d}\mathbf{y} \right) \ u, \\ \partial_{tt}^2 \psi &- \mathbf{c}^2 \Delta_y \psi = -\mathbf{c}^2 \sigma_2(\mathbf{y}) \sigma_1 \star |\mathbf{u}|^2 \end{split}$$

Energy conservation

$$\begin{aligned} \frac{1}{2} \int |\nabla_x u|^2 \, \mathrm{d}x &+ \frac{1}{2} \int \left(\frac{|\partial_t \psi|^2}{c^2} + |\nabla_y \psi|^2 \right) \mathrm{d}y \, \mathrm{d}x \\ &+ \int \sigma_1 (x - x') \sigma_2 (y) \psi(x', y) |u(x)|^2 \, \mathrm{d}y \, \mathrm{d}x' \, \mathrm{d}x. \end{aligned}$$

- Well-posedness in the energy space
- Semi-classical analysis à la Lions-Paul makes the connection with the kinetic model.

Connection to other models: preliminary observations

• The limit $c \rightarrow \infty$ leads to the Hartree model

$$i\partial_t u + \frac{1}{2}\Delta_x u = -(\Lambda\Sigma\star|u|^2)u.$$

Many results known when Σ is replaced by δ_0 (focusing NLS) and in dimension 3 when Σ is replaced by $\frac{1}{|x|}$ (Newton-Hartree: Lieb, Lenzmann...)

Intuition that the space dimension d might be important...

- But SW has no scale invariance, and it does not satisfy Galilean invariance.
- Both systems admit **Solitary Wave** solutions: $(u, \psi) = (e^{i\omega t}Q(x), \Psi(x, y))$

$$-\frac{1}{2}\Delta_{x}Q + \omega Q + \Lambda \Sigma \star |Q|^{2}Q = 0, \qquad -\Delta_{y}\Psi = -\sigma_{2}(y)\sigma_{1} \star |Q|^{2}$$

Choquard's equation... which has infinitely many solutions.

Ground states

Minimization of the energy

$$\begin{aligned} \frac{1}{2} \int |\nabla_x u|^2 \, \mathrm{d}x &+ \frac{1}{2} \int \left(\frac{|\chi|^2}{c^2} + |\nabla_y \psi|^2 \right) \mathrm{d}y \, \mathrm{d}x \\ &+ \int \sigma_1 (x - x') \sigma_2 (y) \psi(x', y) |u(x)|^2 \, \mathrm{d}y \, \mathrm{d}x' \, \mathrm{d}x, \end{aligned}$$

with a mass constraint $||u||_{L^2}^2 = M$.

Mass threshold:

the minimal energy is 0 for $M < M_0$; it is negative when $M > M_0$ and it is reached at $(Q, \Psi, 0)$, solution of Choquard's equation for a certain ω .

Regularity and radial symmetry... but uniqueness is open !

Orbital stability

- P-L. Lions' concentration-compactness approach leads to a weak stability statement: starting close to a ground state, the solutions remains close to the manifold on all ground states.
- Strengthened results can be obtained by linearization and spectral analysis:

$$\|u(t)-e^{i\gamma(t)}Q(\cdot-x(t))\|_{H^{1}}^{2}+\|\nabla_{y}\psi(t)-\nabla_{y}\Psi(\cdot-x(t))\|_{L^{2}}^{2}+\frac{1}{c^{2}}\|\partial_{t}\psi\|_{L^{2}}^{2}\leq\epsilon.$$

The proof relies on a perturbation argument from Lenzmann's analysis of the case where d = 3 and $\Sigma \rightarrow \frac{1}{|x|}$. Critical step: coercivity estimate.

The stability is shown for an admissible class of relevant form functions σ₁ such that by rescaling σ₁ ★ σ₁ approaches ¹/_{|x|}.

Surprising fact: the convolution with the smooth kernel Σ is much harder than the case with $\frac{1}{|x|}$!

Numerical experiments

Initial data $u_0(x) = Q(x)e^{ip_0/M^2}$ with $|p_0| \ll 1$. Simplified dynamics:

$$\begin{split} M\dot{q} &= p, \\ \dot{p} &= -\nabla_x \int_{\mathbb{R}^d} \left(\int_{\mathbb{R}^d} \sigma_1(x - x') \int_{\mathbb{R}^d} \sigma_2(y) \psi(t, x', y) \, \mathrm{d}y \, \mathrm{d}x' \right) Q^2(x - q(t)) \, \mathrm{d}x \\ \partial_{tt}^2 \psi - c^2 \Delta_y \psi &= -c^2 \sigma_2(y) \int_{\mathbb{R}^d} \sigma_1 \star (x - x') Q^2(x' - q) \, \mathrm{d}x'. \end{split}$$

- *p*, *q* close to the center of mass and the impulsion defined from the SW system
- analogy with the classical dynamics

$$\blacktriangleright |q(t)-q_{\infty}|+|p(t)| \leq C e^{-\lambda t/c}$$



A modified formulation

We rewrite the pb. as

$$\partial_t F + \mathbf{v} \cdot \nabla_x F = \nabla_\mathbf{v} F \cdot \nabla_\mathbf{x} \left(\Phi_\mathbf{l} + \Phi_\mathbf{s} \right)$$

where we set **Del**

$$\Phi_{I}(t,x) = \frac{1}{(2\pi)^{n}} \int_{\mathbb{R}^{n}} \int_{\mathbb{R}^{d}} \sigma_{1}(x-z) \\ \times \left(\widehat{\Psi_{0}}(z,\xi) \cos(c|\xi|t) + \widehat{\Psi_{1}}(z,\xi) \frac{\sin(c|\xi|t)}{c|\xi|}\right) \widehat{\sigma_{2}}(\xi) \, \mathrm{d}z \, \mathrm{d}\xi$$

and

$$\begin{split} \Phi_{\mathcal{S}}(t,x) &= -\int_{\mathbb{R}^d} \Sigma(x-z) \left(\int_0^t p_c(t-s) \rho(s,z) \, \mathrm{d}s \right) \, \mathrm{d}z \\ \text{with } \rho(t,x) &= \int F(t,x,v) \, \mathrm{d}v, \quad \Sigma = \sigma_1 * \sigma_1, \\ \text{and } t \mapsto p_c(t) &= \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \frac{\sin(c|\xi|t)}{c|\xi|} \, |\widehat{\sigma_2}(\xi)|^2 \, \mathrm{d}\xi. \end{split}$$

VP vs VW

Vlasov eq.

$$\partial_t F + \mathbf{v} \cdot \nabla_x F - \nabla_x \Phi \cdot \nabla_v F = 0.$$

with either

V

$$\begin{aligned} & \text{VP case: } \Phi(t,x) = \Sigma \star \rho(t,x) \\ & \text{W case: } \Phi(t,x) = \Phi_I(t,x) + \int_0^t p_c(t-s)\Sigma \star \rho(s,x)\,\mathrm{d}s \end{aligned}$$

- Effect of the initial data for the vibrational field: decay related to the dispersion of the wave eq.
- "Memory effect" through *p_c* interplay between dispersion (depends on *n* and *c*) and regularity of the coefficients σ₁, σ₂

The kernel p_c

Let W solution of $\Box_{t,z}W = 0$, $(W, \partial_t W)|_{t=0} = (0, \sigma_2)$

$$p_c(t) = \frac{1}{c} \int_{\mathbb{R}^n} \sigma_2(z) W(ct,z) \, \mathrm{d}z = \int_{\mathbb{R}^n} \frac{\sin(c|\zeta|t)}{c|\zeta|} |\widehat{\sigma}_2(\zeta)|^2 \frac{\mathrm{d}\zeta}{(2\pi)^n}.$$

Energy dissipation mechanisms \longleftrightarrow decay of p_c .

When $n \ge 3$, p_c is integrable and satisfies

$$\int_0^\infty p_c(t) \, \mathrm{d}t = \frac{\Lambda}{c^2}, \qquad \text{with} \qquad \Lambda = \int_{\mathbb{R}^n} \frac{|\widehat{\sigma}_2(\zeta)|^2}{|\zeta|^2} \, \mathrm{d}\zeta < \infty,$$

In dimension n = 1, a direct computation by means of D'Alembert formula shows that

$$p_c(t) = \frac{1}{2c} \int_{-\infty}^{+\infty} \sigma_2(z) \left(\int_{z-ct}^{z+ct} \sigma_2(s) \, \mathrm{d}s \right) \, \mathrm{d}z \xrightarrow[t \to \infty]{} \frac{1}{2c} \|\sigma_2\|_{L^1_z}^2 > 0.$$

The kernel p_c , ctn'd

$$p_{c}(t) = \frac{1}{c} \int_{\mathbb{R}^{n}} \sigma_{2}(z) W(ct, z) \, \mathrm{d}z, \quad \Box_{t,z} W = 0 \quad (W, \partial_{t} W) \big|_{t=0} = (0, \sigma_{2})$$

If $n \ge 3$ odd, $\sigma_2 \in C_c^0(\mathbb{R}^n)$ with $\operatorname{supp}(\sigma_2) \subset B(0, R_2)$, then p_c has a compact support included in $[0, \frac{2R_2}{c}]$ and $|p_c(t)| \le 1/c$.



Assumptions on σ_2 can be relaxed, and including for even dimension $n \ge 4$ we can obtain algebraic decay of p_c

A modified formulation **FRD** The splitting of $\Phi(t, x) = \left(\sigma_1 * \int_{\mathbb{R}^n} \sigma_2(y)\Psi(t, \cdot, y) \, dy\right)(x)$ with $(\partial_{tt}^2 - c^2 \Delta_y)\Psi(t, x, y) = -\sigma_2(y) \, \sigma_1 * \rho(t, x), \qquad (\Psi, \partial_t \Psi)\Big|_{t=0} = (\Psi_0, \Psi_1)$

relies on the *linearity* of the wave eq.:

$$\Phi = \Phi_I + \Phi_S$$

with Φ_I associated to the **free** wave equation

 $(\partial_{tt}^2 - c^2 \Delta_y) \Upsilon(t, x, y) = 0, \qquad (\Upsilon, \partial_t \Upsilon)\Big|_{t=0} = (\Psi_0, \Psi_1)$

(or with data $\sigma_1 * (\Psi_0, \Psi_1)$), and Φ_S associated to the sol. of

$$\left(\partial_{tt}^2 - c^2 \Delta_y\right) \widetilde{\Psi}(t, x, y) = -\sigma_2(y) \sigma_1 * \rho(t, x), \qquad \left(\widetilde{\Psi}, \partial_t \widetilde{\Psi}\right)\Big|_{t=0} = 0$$

Proceeding this way, we distinguish the influence of the initial data and the influence of the coupling.