Diffusion from deterministic dynamics

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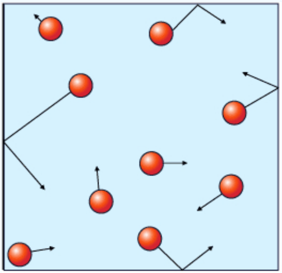
Conservative Dynamics

How to derive **dissipation** from conservative dynamics?

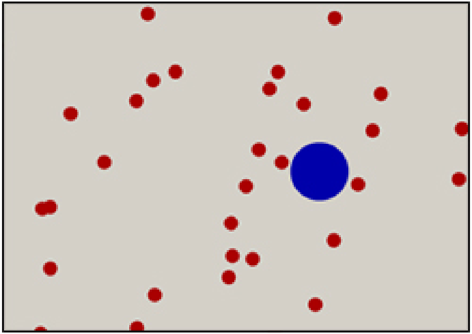
Hamiltonian system:



- Microscopic energy and momentum are **conserved**
- Microscopic dynamics invariant under time reversal
- Macroscopic equations dissipative

Brownian Motion

Particle interacting with environment:



Diffusion of particle position:

$$q(t)^2 \sim Dt \quad \text{as} \quad t \to \infty$$

Rayleigh gas

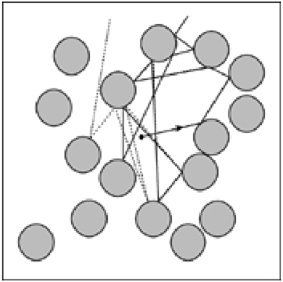
Particle (p, q), (ideal) gas $(p_i, q_i)_{i=1}^N$

$$H = \frac{p^2}{2M} + \sum_i \frac{p_i^2}{2m} + \lambda \sum_i V(q - q_i)$$

V short range

Particle+ gas = Hamiltonian dynamical system, deterministic, time reversible dynamics

Lorentz gas



Take $m \to \infty$

- Fixed scatterers at x_i
- Particle motion deterministic and time reversible

$$H = \frac{p^2}{2M} + \lambda \sum_i V(q - x_i)$$

Quantum Brownian Particle

Quantum (& lattice) version of Raleigh gas.

Particle hops on $\mathbb{Z}^d$ and interacts with a free bose field

$$\partial_t \rho = -i[H, \rho]$$

$$H = -\frac{1}{2M}\Delta + H_{field} + \lambda \sum_{x \in \mathbb{Z}^d} V(q - x)\Phi(x)$$

- ρ density matrix of particle + field
- q position of particle
- $\Phi(x) = \int dk(e^{ikx}a(k) + e^{-ikx}a^*(k))$ free field

Anderson model

Quantum (& lattice) version of Lorentz gas.

$$\partial_t \rho = -i[H, \rho]$$

$$H = -\frac{1}{2M}\Delta + \lambda V(q)$$

- ρ density matrix of particle
- $\{V(q)\}_{q \in \mathbb{Z}^d}$ i.i.d.

Diffusion

Classical

$$t^{-1}\mathbb{E}(q(t)^2) \ \rightarrow \ D \quad \text{as} \quad t \rightarrow \infty$$

(or a.s. or convergence to Brownian motion...)

$\mathbb{E}$ = expectation w.r.t.

- **initial state** at $t = 0$ of the gas (Raleigh)
- Positions of the scatterers (Lorentz)

Quantum: replace $q(t)^2$ by $\mathrm{tr}(\rho(t)q^2)$ and $\mathbb{E}$ by

- Thermal initial state at $t = 0$ for the field
- Average over random potential (Anderson)

Weak coupling limit

For **small** λ these models exhibit diffusion on time scale $1/\lambda^2$.

Equivalently, they have **Markovian** scaling limits when space and time are scaled by $1/\lambda^2$ and λ taken to zero.

Weak coupling limit

Lorentz gas

- In time t: t random scatterings with $\Delta v = \mathcal{O}(\lambda)$
- $|v(t)| = |v(0)| + \mathcal{O}(\lambda)$ (energy conservation).

$$(v(\tau/\lambda^2), \lambda^2 q(\tau/\lambda^2)) \to (V(\tau), X(\tau))$$

V Brownian motion with constant energy $V^2 = v(0)^2$.

(Kesten and Papanicolau, Durr, Goldstein and Lebowitz)

Anderson model: scaling limit for density matrix $\rho_t(q, q')$

$$\lim_{\lambda \to 0} \lambda^{-2d} \rho_{\tau/\lambda^2}(\frac{x}{\lambda^2} + y, \frac{x}{\lambda^2} - y) := f(x, y)$$

f satisfies a linear Boltzman equation (Erdös and Yau)

Limit motion diffusive: $\tau^{-1}\mathbb{E}X(\tau)^2 \to D$ as $\tau \to \infty$.

Beyond the weak coupling limit

Other Markovian limits: small density, large mass......

However we want λ **fixed** and $t \to \infty$.

Limits might not commute. E.g. in 2d Anderson localization sets in time scale e^{c/λ^2}

Very few results for fixed system

- Periodic Lorentz gas (Bunimovich and Sinai)
- 1d Rayleigh gas (Sinai and Soloveichik, Szasz and Toth)
- Markovian in time random potential (Kang and Schenker)
- 3d Anderson: diffusion $t \sim \lambda^{-2-\delta}$ (Erdös, Salmhofer, Yau)
- 3d σ model (Disertori, Spencer, Zirnbauer)
- De Roeck and Fröhlich, De Roeck and A.K.

Annealed dynamics

Consider for simplicity Anderson model $H = -\Delta + \lambda V$

$$\rho_t = e^{-itH} \rho_0 e^{itH} := e^{-itL} \rho_0$$

with $L = [H, \cdot]$. Go to kinetic scale

$$U_\tau^{(\lambda)} := \mathcal{S}_{\lambda^{-2}} \circ e^{-i\tau/\lambda^2 L} \circ \mathcal{S}_{\lambda^{-2}}^{-1}$$

where $\mathcal{S}_{\lambda^{-2}}$ is spatial scaling. Set

$$T_\tau^{(\lambda)} = \mathbb{E} U_\tau^{(\lambda)}$$

Weak coupling limit states that for **fixed** τ

$$\lim_{\lambda \to 0} T_\tau^{(\lambda)} = e^{\tau M}$$

M is generator of a q-Markov process which diffuses:

$$\mathcal{S}_{\tau^{\frac{1}{2}}} \circ e^{\tau M} \circ \mathcal{S}_{\tau^{\frac{1}{2}}}^{-1} \to T_0^* \quad as \quad \tau \to \infty$$

Diffusive limit

However, we are interested in $\tau \to \infty$ with **fixed λ**. E.g. diffusion constant is given by

$$D = \lambda^{-2} \lim_{\tau \to \infty} \tau^{-1} \mathrm{tr}\, q^2 T_\tau^{(\lambda)}$$

More generally, under **diffusive scaling** want to show

$$\mathcal{S}_{\tau^{\frac{1}{2}}} \circ T_\tau^{(\lambda)} \circ \mathcal{S}^{-1}_{\tau^{\frac{1}{2}}} \to T^* \quad as \quad \tau \to \infty$$

where $T^* \sim e^{-(x-x')^2/\kappa}$ on diagonal $\rho(x,x)$.

Erdös, Salmhofer and Yau proved

$$\mathcal{S}_{\lambda^{-\kappa/2}} \circ T^{(\lambda)}_{\lambda^{-\kappa}} \circ \mathcal{S}^{-1}_{\lambda^{-\kappa/2}} \to T_0^* \quad as \quad \lambda \to 0$$

Random walk in random environment

Fix λ. Then Markov property fails:

$$T^{(\lambda)}_{\tau+\tau'} = \mathbb{E} U^{(\lambda)}_{\tau+\tau'} \neq \mathbb{E} U^{(\lambda)}_{\tau} \mathbb{E} U^{(\lambda)}_{\tau'} = T^{(\lambda)}_{\tau} T^{(\lambda)}_{\tau'}$$

Let $U := U^{(\lambda)}_1$ be the time 1 dynamics in kinetic time scale. Set

$$T := \mathbb{E} U, \quad b := U - \mathbb{E} U$$

so $U = T + b$ and we have for $\tau \in \mathbb{N}$

$$U^{(\lambda)}_{\tau} = (T + b)^{\tau}$$

Think of U as a **random transition kernel** with T its average and b fluctuation with $\mathbb{E} b = 0$.

Renormalization

Since $T = T_1^{(\lambda)} \to e^M$ as $\lambda \to 0$ we expect

$$T = e^{M+o(\lambda)}$$

and T^τ, $\tau = 1, 2, \ldots$ should be a a diffusive Markov chain.

b provides a **random** environment for it.

We want to study $(T + b)^\tau$ as $\tau \to \infty$.
Pick an integer L. Take time $\tau = L^{2n}$ and rescale diffusively:

$$U_n := \mathcal{S}_{L^n} \circ (T + b)^{L^{2n}} \circ \mathcal{S}_{L^n}^{-1}$$

Want to show

$$T_n := \mathbb{E} U_n \to T^* \quad as \quad n \to \infty$$

Renormalization

Do this step by step:

$$U_n = T_n + b_n, \quad T_n := \mathbb{E} U_n$$

$$T_{n+1} = \mathbb{E}\left(\mathcal{S}_L \circ (T_n + b_n)^{L^2} \circ \mathcal{S}_L^{-1}\right)$$

This is a perturbative **finite time** problem:

$$T_{n+1} = \mathcal{S}_L \circ T_n^{L^2} \circ \mathcal{S}_L^{-1} + \mathbb{E}(\text{polynomial in } b_n)$$

$$b_{n+1} = \mathcal{S}_L \circ \left(\sum_i T_n^{L^2-i} b_n T_n^i\right) \circ \mathcal{S}_L^{-1} + \mathcal{O}(b_n^2)$$

Renormalization

If we could show that moments of b_n tend to zero as $n \to \infty$ i.e. that the noise is **irrelevant** then

$$T_n \to T^* \ \ as \ \ n \to \infty$$

In Anderson model this is hard but in a modification of the Rayleigh gas introduced by De Roeck and Fröhlich it can be done.

Rayleigh with spin

Interaction of spinning particle with free field environment.

Particle state space $l^2(\mathbb{Z}^d) \otimes \mathbb{C}^2$

$$
\begin{aligned}
H &= -\frac{1}{2M}\Delta + H_{spin} + H_E + \lambda \sum_x V(q-x)\Phi(x) \\
H_E &= \int \omega(k) a^*(k) a(k)
\end{aligned}
$$

- q: position of particle
- $\Phi(x) = \int dk(e^{ikx}a(k) + e^{-ikx}a^*(k))$ Free field
- $V \in \mathbb{C}^{2\times 2}$ supported near $x = 0$ couples particle position and spin to field near particle
- **Heavy** particle: we take **mass** $M \propto \lambda^{-2}$

States

- Initial state (density matrix)

$$\rho_0 = \rho_{P,0} \otimes \rho_{E,0}$$

- Particle initial state localized near origin

$$\langle q', e' | \rho_{P,0} | q, e \rangle \sim \delta_{q,0} \delta_{q',0}$$

with $q, q' \in \mathbb{Z}^d$ and e, e' energy levels of H_{spin}.

- Environment initial state equilibrium Gibbs state

$$\rho_{E,0} = \frac{e^{-\beta H_E}}{\mathrm{Tr}\ e^{-\beta H_E}}$$

Dynamics

- **Dynamics of full system**

$$\rho_t = e^{-itH}\rho_0 e^{itH} := e^{-itL}\rho_0$$

  with $L = [H, \cdot]$.
- **Reduced dynamics** for the particle: trace over environment

$$\rho_{P,t} = \mathrm{Tr}_E \rho_t = \mathrm{Tr}_E e^{-itL}(\rho_P \otimes \rho_E) := (\mathbb{E}e^{-itL})\rho_P$$

- Tr_E plays the role of $\mathbb{E}$ in Anderson model
- For $M = \mathcal{O}(1)$ weak coupling limit

$$\lim_{\lambda \to 0} \mathcal{S}_{\lambda^{-2}} \circ (\mathbb{E}e^{-i\tau/\lambda^2 L}) \circ \mathcal{S}^{-1}_{\lambda^{-2}}$$

  is a diffusive Markov semigroup (Erdös)
- For $M = \mathcal{O}(1)$, $\lambda \neq 0$ similar difficulties as in Anderson model

Markovian limit

For $M = \mathcal{O}(\lambda^{-2})$ things are simpler. During time $1/\lambda^2$

- Particle moves distance $\mathcal{O}(1)$
- Spin and particle momentum thermalize

Weak coupling limit is obtained with **no scaling of space**. Let

$$T_\tau^{(\lambda)} = \mathbb{E} e^{-i\frac{\tau}{\lambda^2}L}.$$

Then

$$\lim_{\lambda \to 0} T_\tau^{(\lambda)} = e^{\tau M}$$

M is generator of a (quantum) Markov process where particle moves ballistically between random jumps in spin and direction of velocity.

Weak coupling limit dynamics is **diffusive**. Diffusion constant is $\mathcal{O}(\lambda^2)$ instead of $\mathcal{O}(\lambda^{-2})$ due to lack of spatial scaling.

Renormalization

Now **fix** λ and study large time asymptotics with RG.

To recall: write the full dynamics in time $1/\lambda^2$ as

$$e^{-i\lambda^{-2}L} = \mathbb{E}e^{-i\lambda^{-2}L} + b := T + b, \quad \mathbb{E}b = 0.$$

Look then at times L^{2n}/λ^2, $n = 1, 2, \ldots$, rescale diffusively

$$U_n := \mathcal{S}_{L^n} \circ (T + b)^{L^{2n}} \circ \mathcal{S}_{L^n}^{-1}$$

and show

$$T_n := \mathbb{E}U_n \to T^* \quad as \quad n \to \infty.$$

Study U_n iteratively: $U_n = T_n + b_n$, with

$$U_{n+1} = \mathcal{S}_L \circ (T_n + b_n)^{L^2} \circ \mathcal{S}_L^{-1}$$

Need to show the noise b_n vanishes as $n \to \infty$.

RWRE

Diffusive behavior of random walk in a random environment depends on the environment correlations.

Our environment is produced by the interaction of the particle with the field.

The field has dynamical correlations in the Gibbs state

$$\mathbb{E}(\Phi(t,x)\Phi(0,0)) = \int e^{i\omega(k)t+ikx}(e^{-\beta\omega(k)} - 1)^{-1} dk$$

The correlation function has long memory

$$\sup_x |\mathbb{E}(\Phi(t,x)\Phi(0,0))| = O(|t|^{-a})$$

a depends on type of phonons: $\omega(k) \sim \sqrt{k^2 + m^2}$ as $k \to 0$

- Acoustic phonons ($m = 0$), $a = (d-1)/2$
- Optical phonons ($m \neq 0$), $a = d/2$

Result

Let V be such that the weak coupling limit is diffusive (this is generic) and $a > 1$ (optical phonons in $d = 3$)

Theorem (W. De Roeck, A.K.)

Then, for $\lambda \neq 0$ small enough, the particle motion is diffusive:

$$\lim_{t\to\infty} t^{-1} \mathrm{tr}\, q^2 \rho_t = D_\lambda$$

with $D_\lambda = \lambda^2(D_0 + o(|\lambda|^0))$.

- D_0 is the diffusion constant of the Markov semigroup $e^{\tau M}$
- Earlier work by De Roeck and Fröhlich, $d \geq 4$

Dyson expansion

The dynamics up to time scale $1/\lambda^2$ is controlled by Dyson expansion i.e. we expand in powers of λ:

$$
\begin{aligned}
e^{-itL} &= e^{-it(L_P+L_E+\lambda L_I)} \\
T_\tau^{(\lambda)}\rho_P &= \mathrm{Tr}_E e^{-itL}(\rho_P\otimes\rho_E) = \sum_{m=0}^{\infty}(-\lambda^2)^m \int_{0<t_1<\ldots<t_{2m}<t} dt_1\ldots t_{2m} \\
&\quad \mathrm{Tr}_E\Big[V_{t-t_{2m}}L_I(t_{2m})\ldots V_{t_2-t_1}L_I(t_1)V_{t_1}(\rho_P\otimes\rho_E)\Big]
\end{aligned}
$$

with $t=\tau/\lambda^2$ and $V_s=e^{-isL_P}$ and $L_I(t)=e^{itL_E}L_I$. L_I is **linear** in the field $\implies$ pairings of t_i with field correlation function

$$\|\mathbb{E}L_I(t_i)L_I(t_j)\| \leq (1+|t_i-t_j|)^{-a}$$

Dyson expansion

Dyson expansion **converges** for all τ but it yields useful bounds only for $\tau < \mathcal{O}(1)$:

- Ladder diagrams give Markovian semigroup:

$$T_\tau^{(\lambda)} = e^{\tau M} + o(\lambda) \;\text{ if }\; \tau < \mathcal{O}(1)$$

- Correlation functions of the random environment have similar expansion yielding for $t_1 < t_2 < \cdots < t_m$

$$\|(\mathbb{E}\,(b(t_1)b(t_2)\ldots b(t_m))_{connected}\| \sim \delta^m \prod_{j=2}^{m} |t_j - t_{j-1}|^{-a}$$

with $\delta = o(\lambda)$.

RG flow

To go to longer time scales we need to do the RG iteration with the input given by the T-operator and noise b-correlation functions obtained from the Dyson expansion.

Upshot: the noise is **irrelevant** under RG if $a > 1$.

We prove for the noise b_n at scale L^n

$$\|(\mathbb{E}(b_n(t_1)b_n(t_2)\ldots b_n(t_m)_{connected}\| \sim \delta_n^m \prod_{j=2}^{m} |t_j - t_{j-1}|^{-a}$$

with $\delta_n \to 0$ as $n \to \infty$.

Confined particle

When $M = \infty$ we have a confined system interacting with radiation field. Two cases:

• $\beta < \infty$: **return to (non) equilibrium**

$$\rho_{P,t} \to \rho^* \text{ as } t \to \infty$$

(W. De Roeck, A.K.)

• $\beta = \infty$: return to ground state and **asymptotic completeness**: every excited state relaxes to the ground state by emission of photons whose dynamics is asymptotically free (M. Griesemer, W. De Roeck and A.K., Faupin and Sigal)

Proof by high temperature expansion, no RG needed.

Markovian limits for extended systems

Weakly anharmonic coupled oscillators $(p_x, q_x)_{x\in\mathbb{Z}^d}$

$$H = \sum_{x\in\mathbb{Z}^d} (\tfrac{1}{2}p_x^2 + \lambda q_x^4) + \sum_{|x-y|=1} (q_x - q_y)^2$$

Time evolution has formally a Markovian limit as $\lambda \to 0$ and time and space are scaled as $t \to t/\lambda^2$, $x \to x/\lambda^2$:

- Let μ_0 be a gaussian measure on $(p_x, q_x)_{x\in\mathbb{Z}^d}$ with covariance G_0
- Let $\mu_\tau^\lambda = \mathcal{S}_{1/\lambda^2}\phi_{\tau/\lambda^2}\mu_0$ where ϕ_t is Hamiltonian evolution
- Then $\lim_{\lambda\to 0}\mu_\tau^\lambda$ is a Gaussian measure with covariance G_τ.
- G_τ satisfies a closed equation which is diffusive with diffusion constant $\mathcal{O}(1/\lambda^2)$. (Spohn, Bricmont and A.K.)

Analogous to Rayleigh and Anderson models.

Markovian limits for extended systems

Coupled chaotic flows: $(p_x, q_x)_{x \in \mathbb{Z}^d}$, $H_0(q_x, p_x)$ chaotic systems (Anosov, billiard)

$$H = \sum_x H_0(q_x, p_x) + \lambda \sum_{|x-y|=1} H_1(q_x, p_x, q_y, p_y)$$

Markovian limit $t \to t/\lambda^2$: local energy

$$E_x(q(\tau/\lambda^2), p(\tau/\lambda^2)) \to e_x(\tau) \text{ as } \lambda \to 0$$

with $e_x(t)$ a diffusion process. (Dolgopyat, Liverani)

The fast dynamics of H_0 randomizes p_x, q_x which act as a noise to the slow variables E_x.

This model is suitable for the RG in the manner of the heavy particle with spin. For **coupled chaotic maps** see (J. Bricmont, A.K.)

Conclusions

Our proof can be viewed as a scale by scale resummation of the Dyson expansion.

It is not excluded that one could proceed along these lines also in the case of Anderson model, band matrices or Quantum Rayleigh gas.

Scaling1

Continuum version:

$$\dot{U}(t,x) = \kappa \Delta U(t,x) + \nabla \cdot (b(t,x)U(t,x))$$

with

$$\mathbb{E}(b(t,x)b(0,0)) = C(t,x).$$

Scale:

$$U_L(t,x) := L^d U(L^2 t, Lx)$$

Get

$$\dot{U}_L(t,x) = \kappa \Delta U_L(t,x) + \nabla \cdot (b_L(t,x)U_L(t,x))$$

with

$$b_L(t,x) = Lb(L^2 t, Lx)$$

Scaling 2

Hence renormalized noise correlation is

$$\mathbb{E}(b_L(t,x)b_L(0,0) = L^2 C(L^2 t, Lx) := C_L(t,x).$$

Examples:

1.Time independent space decorrelated environment

$$C(t,x) = \delta(x) \implies C_L(t,x) = L^{2-d} C(x).$$

Noise irrelevant $d > 2$.

2. No spatial decay, $\sup_x C(t,x) \sim t^{-a} \implies$

$$\sup_x C_L(t,x) \sim L^{2(1-a)} t^{-a}.$$

Noise irrelevant $a > 1 \implies$ **optical** phonons in $d = 3$.