Brownian particle in a periodic potential

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Physical picture

Situation

1. Molecule in a periodic optical potential $\tilde{V}(x)$.
2. Molecule interacts with a sparse ideal gas of light particles.

Characteristics of the model

- Classical, stochastic, dimension one.
- Mass ratio of gas particle/molecule is $\frac{m}{M} = \lambda \ll 1$.
- Periodic potential $\tilde{V}(x) = \lambda V(\frac{x}{\lambda}) \geq 0$ has period λa.

Goal: Study behavior of the molecule in the Brownian limit.

A linear Boltzmann equation

Position-momentum coordinate vector (X_t, P_t) evolves as a Markovian process with density $\mathrm{P}_t(x,p)$ obeying

$$\frac{d}{dt}\mathrm{P}_t(x,p) = -\lambda\frac{p}{m}\,\frac{\partial \mathrm{P}_t}{\partial x}(x,p) + \frac{dV}{dx}(\frac{x}{\lambda})\,\frac{\partial \mathrm{P}_t}{\partial p}(x,p) + \int_{\mathbb{R}} dp'\,\Big(\mathcal{J}_\lambda(p,p')\,\mathrm{P}_t(x,p') - \mathcal{J}_\lambda(p',p)\,\mathrm{P}_t(x,p)\Big)$$

$\mathcal{J}_\lambda(p,p')$=Jump rate from momentum p' to momentum p.

$$\mathcal{J}_\lambda(p,p') = \frac{\eta(1+\lambda)}{2m}\big|p-p'\big|\frac{e^{-\frac{\beta}{2m}\left(\frac{\lambda-1}{2}p'+\frac{1+\lambda}{2}p\right)^2}}{(2\pi\frac{m}{\beta})^{\frac{1}{2}}}$$

β=inverse temperature,
$\lambda = \frac{m}{M}$ mass ratio,
η =density of gas

Normalizing parameters

Setting $m = \beta = a = 1$ and stretching the spatial variable $\lambda x \to x$.

$$\frac{d}{dt}\mathrm{P}_t(x,p) = -p\,\frac{\partial \mathrm{P}_t}{\partial x}(x,p) + \frac{dV}{dx}(x)\,\frac{\partial \mathrm{P}_t}{\partial p}(x,p) + \int_{\mathbb{R}} dp' \left(\mathcal{J}_\lambda(p,p')\,\mathrm{P}_t(x,p') - \mathcal{J}_\lambda(p',p)\,\mathrm{P}_t(x,p)\right)$$

$\mathcal{J}_\lambda(p,p')$=Jump rate from momentum p' to momentum p.

$$\mathcal{J}_\lambda(p,p') = \frac{\eta(1+\lambda)}{2}\left|p-p'\right|\frac{e^{-\frac{1}{2}\left(\frac{\lambda-1}{2}p'+\frac{1+\lambda}{2}p\right)^2}}{(2\pi)^{\frac{1}{2}}}.$$

Defines a λ-dependent Markovian dynamics on

$$S = \mathbb{T}\times\mathbb{R}, \qquad \mathbb{T} = [0,1).$$

The $\lambda = 0$ case is frictionless:

$$j(p-p') = \mathcal{J}_0(p,p') = \frac{\eta}{2}\left|p-p'\right|\frac{e^{-\frac{1}{8}\left(p-p'\right)^2}}{(2\pi)^{\frac{1}{2}}}.$$

Our quantities of interest

Momentum process P_t is a sum of a jump term and a force term

$$P_t = P_0 + J_t + D_t, \text{ where}$$

- J_t is the sum of momentum jumps due to collisions.
- $D_t = \int_0^t dr\, \frac{dV}{dx}(X_r)$ is the total drift in momentum due to the forcing.

We study the momentum and total drift in momentum on time scales $\propto \lambda^{-1}$:

$$P_t^{(\lambda)} = \lambda^{\frac{1}{2}} P_{\frac{t}{\lambda}} \quad \text{and} \quad D_t^{(\lambda)} = \lambda^{\kappa} D_{\frac{t}{\lambda}}, \quad \kappa = \frac{1}{4}.$$

First result: Brownian limit

Assumptions: $\sup_{x\in\mathbb{T}}\left|\frac{dV}{dx}(x)\right| < \infty$ and the distribution for (X_0, P_0) is some μ not depending on λ.

Theorem (Clark, Dubois)

There is convergence in law over interval $t \in [0, T]$

$$\lambda^{\frac{1}{2}} D_{\frac{t}{\lambda}} \quad \xrightarrow{\mathfrak{L}} \quad 0 \qquad \textit{and} \qquad \lambda^{\frac{1}{2}} P_{\frac{t}{\lambda}} \quad \xrightarrow{\mathfrak{L}} \quad \mathfrak{p}_t,$$

where $\mathfrak{p}_t$ is the Ornstein-Uhlenbeck process:

$$d\mathfrak{p}_t = -\gamma\mathfrak{p}_t dt + \big(\frac{2m\gamma}{\beta}\big)^{\frac{1}{2}} d\mathbf{B}_t, \qquad \mathfrak{p}_0 = 0$$

for

$$\gamma = 8\eta\big(\frac{2}{\pi m\beta}\big)^{\frac{1}{2}}, \quad \mathbf{B}_t \textit{ is a standard brownian motion.}$$

Invariant state and typical momentum

The effective Hamiltonian is

$$H(x,p) = \frac{1}{2}p^2 + V(x), \qquad (\ p \text{ is effectively a vel.}),$$

and the equilibrium state $\mathcal{P}_\infty^{(\lambda)} : \mathbb{T} \times \mathbb{R} \to \mathbb{R}^+$ is

$$\mathcal{P}_\infty^{(\lambda)}(x,p) = \frac{e^{-\lambda\, H(x,p)}}{N_\lambda}.$$

1. Typical energy $H(x,p) \sim \lambda^{-1}$
2. Typical momentum has $|p| \sim \lambda^{-\frac{1}{2}}$, since $\sup_{x\in\mathbb{T}} V(x) < \infty$.

Lesson 1: Typically, only a small fraction of the energy will be in the potential energy.
Lesson 2: Typically, the particle is passing through the period cells quickly.

Potential acts weakly–usually

Between collisions, the force $\frac{dV}{dx}(x)$ drives the momentum

$$P_{\text{fin}} - P_{\text{int}} = \int_{t_{\text{int}}}^{t_{\text{fin}}} dr\, \frac{dV}{dx}(X_r).$$

For $|P_{\text{int}}|$ large enough,

$$\big|P_{\text{fin}} - P_{\text{int}}\big| \leq \Big| |P_{\text{int}}| - \sqrt{P_{\text{int}}^2 + 2V_{\text{int}} - 2V_{\text{fin}}} \Big| \leq \frac{2\sup_x V(x)}{|P_{\text{int}}|},$$

$$|P_{\text{int}}| \sim \lambda^{-\frac{1}{2}} \implies \Big| \int_{t_{\text{int}}}^{t_{\text{fin}}} dr\, \frac{dV}{dx}(X_r) \Big| = O(\lambda^{\frac{1}{2}}).$$

Rough intuitive implication: Non-negligible contributions to

$$D_t = \int_0^t dr\, \frac{dV}{dx}(X_r), \qquad t \in [0, \frac{T}{\lambda}]$$

occur over intervals when $|P_r| \ll \lambda^{-\frac{1}{2}}$ (typical momentum) .

Returns to low momentum

If the rescaled momentum P_r for $r \in [0, \frac{T}{\lambda}]$ converges to a process of diffusion type, then that suggests...

... P_r will spend a time on the order of $\lambda^{-\frac{1}{2}}$ in a finite neighborhood $[-L, L]$ of the origin over the interval $[0, \frac{T}{\lambda}]$

Thus scale considerations alone do not motivate that $\lambda^{\frac{1}{2}} \int_0^{\frac{t}{\lambda}} dr\, \frac{dV}{dx}(X_r) \to 0$, since there may be a (mysterious) bias.

Returns to low momentum, cont.

We also "need a zero":

$$\int_S dxdp\,\mathcal{P}_\infty^{(\lambda)}(x,p)\frac{dV}{dx}(x) = 0.$$

If there is enough ergodicity, then we expect there to be central limit-type cancellation so that typically

$$\int_0^{\frac{t}{\lambda}} dr\,\frac{dV}{dx}(X_r) = O(\lambda^{-\frac{1}{4}}).$$

Picture: Over an interval $t \in [0, \frac{T}{\lambda}]$:

- There will be 'long' time intervals over which $|P_t| >> 1$ and $\lambda^{\frac{1}{4}} \int_0^t dr\, \frac{dV}{dx}(X_r)$ does not fluctuate much.
- The dominant contributions to $\lambda^{\frac{1}{4}} \int_0^t dr\, \frac{dV}{dx}(X_r)$ will occur at infrequent intervals of time for $|P_t| = O(1)$.

Local time process

For $\mathfrak{p}_t$, the local time $\mathfrak{l}_t^{(a)}$ is the occupation time density at $a \in \mathbb{R}$ over the interval $[0, t]$.

Formally,

$$\mathfrak{l}_t^{(a)} = \int_0^t dr\, \delta\big(\mathfrak{p}_r - a\big) \quad \text{and satisfies} \quad \int_{\mathbb{R}} da\, \mathfrak{l}_t^{(a)} = t.$$

For $a = 0$ we just write $\mathfrak{l}_t$.

The Tanaka formula gives:

$$\mathfrak{l}_t = |\mathfrak{p}_t| + \frac{1}{2}\int_0^t dr|\mathfrak{p}_r| - \tilde{\mathbf{B}}_t, \qquad \mathfrak{p}_0 = 0,$$

where $\tilde{\mathbf{B}}_t = \int_0^t S(\mathfrak{p}_r) d\mathbf{B}_r$ and $S : \mathbb{R} \to \{+, -\}$ is the sign function.

Main theorem

Let

- $\mathfrak{p}_t$ be the Ornstein-Uhlenbeck processes
- $\mathfrak{l}_t$ be the local time at zero of $\mathfrak{p}_r$ over $r \in [0, t]$.
- $\mathbf{B}'_t$ be a copy of standard Brownian motion independent of $\mathfrak{p}_t$

Theorem (Clark, Dubois)

There is convergence in law over interval $t \in [0, T]$

$$\left(\lambda^{\frac{1}{2}} P_{\frac{t}{\lambda}},\, \lambda^{\frac{1}{4}} D_{\frac{t}{\lambda}}\right) \quad \xrightarrow{\mathfrak{L}} \quad \left(\mathfrak{p}_t,\, \upsilon^{\frac{1}{2}} \mathbf{B}'_{\mathfrak{l}_t}\right),$$

for a $\upsilon > 0$.

Formal expression for the diffusion constant

Very formally, the diffusion constant is

$$\upsilon = 2 \int_{\mathbb{T}\times\mathbb{R}} dx dp\, \mathfrak{R}(\frac{dV}{dx})(x,p)\frac{dV}{dx}(x),$$

where $\mathfrak{R} = \int_0^\infty dr\, e^{r\mathcal{L}}$ is the reduced resolvent of the generator $\mathcal{L}$

$$\begin{aligned}\mathcal{L}(F)(x,p) = & \, p\,\frac{\partial F}{\partial x}(x,p) - \frac{dV}{dx}(x)\,\frac{\partial F}{\partial x}(x,p) \\ & + \int_{\mathbb{R}} dp' \Big(j(p-p')\,F(x,p') - j(p'-p)\,F(x,p) \Big).\end{aligned}$$

$$j(p-p') = \lim_{\lambda\to 0} \mathcal{J}_\lambda(p,p') = \frac{1}{2}\big|p-p'\big|\frac{e^{-\frac{1}{8}\left(p-p'\right)^2}}{(2\pi)^{\frac{1}{2}}}$$

Comparison with another class of limit theorems

There are many results on models similar to the following:

- Null-recurrent Markov process Y_t, with state space S invariant measure μ.
- Additive functional $A_t = \int_0^t dr\, f(Y_r)$ with $\int_S f\, d\mu = 0$.
- Some characterization of the recurrence, e.g. for $\epsilon \ll 1$

$$\mathfrak{R}_\epsilon(x) = \mathbb{E}_x\Big[\int_0^\infty ds\, e^{-\epsilon\, s} g(Y_s)\Big] \sim \epsilon^{-\alpha} \int_S d\mu\, g$$

  for $0 < \alpha < 1$ and $g > 0$, $g \in L^1(\mu)$.

Then prove limit laws

$$\lambda^{\frac{\alpha}{2}} A_{\frac{t}{\lambda}} \quad \xrightarrow{\mathfrak{L}} \quad D^{\frac{1}{2}} \mathbf{B}_{\tau_t},$$

where τ_t is a Mittag-Leffler process of exponent α and $\mathbf{B}$ is an independent Brownian motion.

Note: When $\alpha = \frac{1}{2}$, then τ_t has the same distribution as the local time ℓ_t at zero for a standard Brownian motion.

Comparison with other limit theorems, cont.

These limit laws satisfy a scale invariance

$$\mathbf{B}_{\tau_{at}} \quad \overset{d}{=} \quad a^{\frac{\alpha}{2}} \mathbf{B}_{\tau_t} \quad \text{since} \quad \tau_{at} \quad \overset{d}{=} \quad a^{\alpha} \tau_t,$$

whereas our limiting law has no scale invariance

$$\mathbf{B}_{\mathfrak{l}_{at}} \quad \overset{d}{\neq} \quad a^{\beta} \mathbf{B}_{\mathfrak{l}_t}, \qquad \text{for any } \beta,$$

since the process $\mathfrak{l}_t$ comes from an Ornstein-Uhlenbeck process.

Most related articles:

1. A. Touati: *Théorèmes limites...* , (Unpublished), (1988).
2. R. Höpfner, E. Löcherbach: *Limit Theorems*... (2003).
3. E. Löcherbach, D. Loukianova: *On Nummelin split...*, (2007).

Some comments on approach

One of the fundamental ideas comes from (A. Touati, 88').

Construct a martingale close to $\int_0^t dr\, \frac{dV}{dx}(X_r)$ by adding some artificial structure to the process $\mathbf{s}_t = (X_t, P_t)$.

Construct a process $\tilde{\mathbf{s}}_t = (\mathbf{s}_t, \epsilon_t) \in \mathbb{T} \times \mathbb{R} \times \{0, 1\}$.

1. Let $\tau_n = e_1 + \cdots e_n$ for a sequence e_m of independent exponential random variables with mean 1. Construct chain $s_n = \mathbf{s}_{\tau_n}$.
2. Extend the state space of chain (s_n) to $\mathbb{T} \times \mathbb{R} \times \{0, 1\}$ via Nummelin splitting. This requires picking function $0 \leq h(s) < 1$, and probability measure ν on $\mathbb{T} \times \mathbb{R}$

$$\mathcal{T}_\lambda(ds, s') \geq d\nu(s) h(s'), \qquad s, s' \in \mathbb{T} \times \mathbb{R}.$$

   The set $\mathbb{T} \times \mathbb{R} \times 1$ is identified as the atom.
3. Use the chain $\tilde{s}_n$ to construct a split (non-Markovian) process $\tilde{\mathbf{s}}_t \in \mathbb{T} \times \mathbb{R} \times \{0, 1\}$.

Some comments, cont.

The recipe for constructing the extended transition rates $\tilde{\mathcal{T}}_\lambda$ in terms of the transition rates $\mathcal{T}_\lambda$ for the orignal chain $s_n = \mathbf{s}_{\tau_n}$

$$\tilde{\mathcal{T}}_\lambda(ds_2, \epsilon_2; s_1, \epsilon_1) = \begin{cases} \frac{1-h(s_2)}{1-h(s_1)}\big(\mathcal{T}_\lambda - \nu \times h\big)(ds_2, s_1) & \epsilon_1 = \epsilon_2 = 0, \\ \frac{h(s_2)}{1-h(s_1)}\big(\mathcal{T}_\lambda - \nu \times h\big)(ds_2, s_1) & \epsilon_1 = 1 - \epsilon_2 = 0, \\ \big(1 - h(s_2)\big)\nu(ds_2) & \epsilon_1 = 1 - \epsilon_2 = 1, \\ h(s_2)\nu(ds_2) & \epsilon_1 = \epsilon_2 = 1. \end{cases}$$

The component $\epsilon_t \in \{0, 1\}$ in the slit process $\tilde{\mathbf{s}}_t = (X_t, P_t, \epsilon_t)$ does not change between times τ_n and τ_{n+1}.

The statistics for $\tilde{s}_t$ for $t \in (\tau_n, \tau_{n+1})$ agrees with the original processes conditioned on s_{τ_n} and $s_{\tau_{n+1}}$.

The marginal for the first component of $\tilde{\mathbf{s}}_t = (\mathbf{s}_t, \epsilon_t)$ has the same law as the original process.

Some comments, cont.

Let R_n be the sequence of return times to the atom $\mathbf{a}$ for the split process $\tilde{\mathbf{s}}_t$.

Let $\mathbf{N}_t$ be the number of returns up to time t.

$$\int_0^t dr\, \frac{dV}{dx}(X_r) = \sum_{n=1}^{\mathbf{N}_t - 1} \int_{R_n}^{R_{n+1}} dr\, \frac{dV}{dx}(X_r) + (\text{ Boundary terms }).$$

$$\int_{\mathbb{T}\times\mathbb{R}} dxdp\, \mathcal{P}_\infty^{(\lambda)}(x,p) \frac{dV}{dx}(x) = 0 \implies \tilde{\mathbb{E}}_{\mathbf{a}}^{(\lambda)}\Big[\int_{R_n}^{R_{n+1}} dr\, \frac{dV}{dx}(X_r) \Big] = 0.$$

The predictable quadratic variation for the martingale $\sum_{n=1}^{\mathbf{N}_t-1} \int_{R_n}^{R_{n+1}} dr\, \frac{dV}{dx}(X_r)$ is $\sigma_\lambda \int_0^t dr\, h(\mathbf{s}_r)$ for

$$\sigma_\lambda := \mathbb{E}_{\mathbf{a}}^{(\lambda)}\Big[\Big(\int_{R_n}^{R_{n+1}} dr\, \frac{dV}{dx}(X_r) \Big)^2 \Big] \longrightarrow \frac{\upsilon}{\int_{\mathbb{T}\times\mathbb{R}} ds\, h(s)}.$$

Some comments, cont.

Touati's idea has been applied in a limit theorem recently in Löcherbach, Loukianova: (2007).

A different process splitting argument was developed in Höpfner, Löcherbach (2003).

Another part of the argument involves showing that as $\lambda \to 0$, then

$$\frac{\lambda^{\frac{1}{2}} \int_0^{\frac{t}{\lambda}} dr\, h(\mathbf{s}_r)}{\int_{\mathbb{T}\times\mathbb{R}} ds\, h(s)} \quad \xrightarrow{\mathfrak{L}} \quad \mathfrak{l}_t.$$

To prove

$$\Big(\lambda^{\frac{1}{4}} \int_0^{\frac{t}{\lambda}} dr\, \frac{dV}{dx}(X_r),\ \frac{\lambda^{\frac{1}{2}} \int_0^{\frac{t}{\lambda}} dr\, h(\mathbf{s}_r)}{\int_{\mathbb{T}\times\mathbb{R}} ds\, h(s)}\Big) \quad \xrightarrow{\mathfrak{L}} \quad \big(\mathbf{B}'_{\mathfrak{l}_t}, \mathfrak{l}_t\big)$$

involves showing an asymptotic independence seen in the limiting quantities $\mathbf{B}'$ and $\mathfrak{l}_t$. We adopt arguments from Höpfner, Löcherbach (2003).

Last remark

Current techniques improves some of those in

J. Clark, C. Maes: *Diffusive behavior for randomly kicked...*, Comm. Math. Phys. (2011),

where a similar model (degenerate $\lambda = 0$) was studied, but an extra torus-reflection symmetry $V(x) = V(Rx)$ was assumed in order to use a time-reversal symmetry argument to show that the forcing is negligible.