Quasi-stationary distributions for strongly Feller processes and application to hypoelliptic Hamiltonian systems

I will give a general framework [1] ensuring existence and uniqueness of quasi-stationary distributions (QSDs) for strongly Feller processes $(X_t, t \geq 0)$ on a set $\mathcal{D}$ in the space of measures ν such that $\nu(\mathsf{W}^{1/p}) < +\infty$, where W is a Lyapunov functional for the non-killed process $(X_t, t \geq 0)$ and $p > 1$. Exponential convergence (in this set of measures) of the law of the process (conditioned not to leave $\mathcal{D}$) towards the QSD is also derived. These results are then applied to hypoelliptic Hamiltonian systems $(X_t = (x_t, v_t), t \geq 0)$ in R^{2d} solution to

$$\begin{cases} dx_t = v_t dt, \\ dv_t = -\nabla \mathsf{V}(x_t)dt - \gamma(x_t, v_t)v_t dt + \Sigma(x_t, v_t)\, dB_t, \end{cases} \tag{1}$$

when $\mathcal{D} = \mathsf{O} \times R^d$, $\mathsf{O} \subset R^d$. Such domains are indeed those of interest to justify the use of a kinetic Monte Carlo processes to model the state-to-state dynamics of a molecular system. In some specific cases, we can also prove that the QSD of (1) inside $\mathcal{D}$ is unique in $P(\mathcal{D})$. The approach also applies to singular potentials V such as the Lennard-Jones potential and the Coulomb potential [2].

-[1] *Quasi-stationary distribution for strongly Feller Markov processes by Lyapunov functions and applications to hypoelliptic Hamiltonian systems.* A. Guillin, B. Nectoux, L. Wu. 2020. Submitted.
-[2] *Quasi-stationary distribution for Hamiltonian dynamics with singular potentials.* A. Guillin, B. Nectoux, L. Wu. 2021. Submitted.