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 \(D\) in the space of measures \(\nu\) such that \(\nu(W^{1/p}) < +\infty\), 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 \(D\)) 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

\[
\begin{align*}
\frac{dx_t}{dt} &= v_t dt, \\
\frac{dv_t}{dt} &= -\nabla V(x_t) dt - \gamma(x_t, v_t)v_t dt + \Sigma(x_t, v_t) dB_t,
\end{align*}
\]

when \(D = O \times R^d\), \(O \subset R^d\). 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 \(D\) is unique in \(P(D)\). The approach also applies to singular potentials \(V\) such as the Lennard-Jones potential and the Coulomb potential [2].