Longtime convergence of evolution semigroups in molecular dynamics

Gabriel STOLTZ

(CERMICS, Ecole des Ponts & MATHERIALS team, INRIA Paris)

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Outline

- **A quick introduction to molecular dynamics**
- **(Non)equilibrium Langevin dynamics**
  - Various convergence results
  - The hypocoercive approach by Dolbeault, Mouhot and Schmeiser
  - Various extensions and modifications
- **Feynmann–Kac dynamics**
  - Reformulation in terms of evolution semigroups
  - Proof for compact position spaces
  - Statement of the result in the general case
  - Elements of proof

A quick introduction to molecular dynamics

Computational statistical physics (1)

- *Predict macroscopic properties of matter from its microscopic description*

- **Microstate**
  - positions $q = (q_1, \dots, q_N)$ and momenta $p = (p_1, \dots, p_N)$
  - energy $H(q,p) = V(q) + \displaystyle\sum_{i=1}^{N} \frac{p_i^2}{2m_i}$

- **Macrostate**
  - described by a probability measure μ
  - constraints fixed exactly or in average (number of particles, volume, energy)

- **Properties :**
  - static $\langle \varphi \rangle = \displaystyle\int_{\mathcal{E}} \varphi(q,p)\,\mu(dq\,dp)$ (equation of state, heat capacity,...)
  - dynamic (transport coefficient, transition pathway, etc)

Computational statistical physics (2)

• Positions $q \in \mathcal{D} = (L\mathbb{T})^d$ or $\mathbb{R}^d$ and momenta $p \in \mathbb{R}^d$
$\to$ phase-space $\mathcal{E} = \mathcal{D} \times \mathbb{R}^d$

• The very high dimensional average $\langle \varphi \rangle$ is computed using time averages of dynamics ergodic for μ:

$$\langle \varphi \rangle = \lim_{T \to +\infty} \frac{1}{T} \int_0^T \varphi(q_t, p_t)\, dt$$

• **Examples of dynamics:**

- Deterministic dynamics (Hamiltonian, Nosé–Hoover and its variations)
- Stochastic differential equations
- Markov chains (Metropolis schemes, discretizations of SDEs)
- Piecewise deterministic Markov processes

Convergence results for evolution semigroups of Langevin dynamics

Langevin dynamics (1)

- Friction $\gamma > 0$ (could be a position-dependent matrix)

Stochastic perturbation of the Hamiltonian dynamics

$$\begin{cases} dq_t = M^{-1} p_t \, dt \\ dp_t = -\nabla V(q_t)\, dt - \gamma M^{-1} p_t \, dt + \sqrt{\dfrac{2\gamma}{\beta}}\, dW_t \end{cases}$$

- As $\gamma \to 0$, the Hamiltonian dynamics is recovered
- Overdamped limit $\gamma \to +\infty$ or $m \to 0$

$$q_{\gamma t} - q_0 = -\frac{1}{\gamma} \int_0^{\gamma t} \nabla V(q_s)\, ds + \sqrt{\frac{2}{\gamma\beta}} W_{\gamma t} - \frac{1}{\gamma}(p_{\gamma t} - p_0)$$

which converges to the solution of $dQ_t = -\nabla V(Q_t)\, dt + \sqrt{2\beta^{-1}}\, dW_t$

- In both cases, slow convergence to equilibrium

Stochastic differential equations and their generators

- General SDE $dx_t = b(x_t)\,dt + \sigma(x_t)\,dW_t$ on $\mathcal{X}$

- Generator of the dynamics $\displaystyle \frac{d}{dt}\left(\mathbb{E}\left[\varphi(x_t)\,\middle|\,x_0 = x\right]\right)\Bigg|_{t=0} = (\mathcal{L}\varphi)(x)$

- It holds $\displaystyle \mathcal{L} = b^T\nabla + \frac{1}{2}\sigma\sigma^T : \nabla^2 = \sum_{i=1}^d b_i \partial_{x_i} + \sum_{i,j=1}^d \left(\sigma\sigma^T\right)_{ij} \partial^2_{x_i,x_j}$

- Invariance of the probability measure $\pi(dx)$ characterized by

$$\forall \varphi \in C_0^\infty(\mathcal{X}), \qquad \int_{\mathcal{X}} \mathcal{L}\varphi\, d\pi = 0$$

- Evolution semigroup $\left(\mathrm{e}^{t\mathcal{L}}\varphi\right)(x) = \mathbb{E}\left[\varphi(x_t)\,\middle|\,x_0 = x\right]$

- The latter quantity is expected to converge to $\displaystyle \int_{\mathcal{X}} \varphi\, d\pi$

Fokker–Planck equations

• Dual viewpoint: convergence of the distribution rather than convergence of observables (Schrödinger vs. Heisenberg)

• Evolution of the law $\psi(t,x)$ of the process at time $t \geqslant 0$

$$\frac{d}{dt}\left(\int_{\mathcal{X}} \varphi\, \psi(t)\right) = \int_{\mathcal{X}} (\mathcal{L}\varphi)\, \psi(t)$$

• Fokker–Planck equation (with $\mathcal{L}^\dagger$ adjoint of $\mathcal{L}$ on $L^2(\mathcal{X})$)

$$\partial_t \psi = \mathcal{L}^\dagger \psi$$

• It is expected that $\psi(t,x)\, dx$ converges to $\pi(dx)$

Langevin dynamics (2)

Generator of the Langevin dynamics $\mathcal{L} = \mathcal{L}_{\mathrm{ham}} + \gamma \mathcal{L}_{\mathrm{FD}}$

$$\mathcal{L}_{\mathrm{ham}} = p^T M^{-1} \nabla_q - \nabla V^T \nabla_p, \qquad \mathcal{L}_{\mathrm{FD}} = -p^T M^{-1} \nabla_p + \frac{1}{\beta} \Delta_p$$

- Preserves the canonical measure

$$\mu(dq\,dp) = Z^{-1} \mathrm{e}^{-\beta H(q,p)}\, dq\, dp = \nu(dq)\, \kappa(dp)$$

- It is convenient to work in $L^2(\mu)$ with $f(t) = \psi(t)/\mu$
  - denote the adjoint of $\mathcal{L}$ on $L^2(\mu)$ by $\mathcal{L}^*$

$$\mathcal{L}^* = -\mathcal{L}_{\mathrm{ham}} + \gamma \mathcal{L}_{\mathrm{FD}}$$

  - Fokker–Planck equation $\partial_t f = \mathcal{L}^* f$
- Convergence results for $\mathrm{e}^{t\mathcal{L}}$ on $L^2(\mu)$ are very similar to the ones for $\mathrm{e}^{t\mathcal{L}^*}$

Ergodicity results (1)

- Almost-sure convergence[1] of ergodic averages $\widehat{\varphi}_t = \frac{1}{t}\int_0^t \varphi(q_s, p_s)\, ds$

- Asymptotic variance of ergodic averages

$$\sigma_\varphi^2 = \lim_{t\to+\infty} t\mathbb{E}\left[\widehat{\varphi}_t^2\right] = 2\int_{\mathcal{E}} \left(-\mathcal{L}^{-1}\Pi_0\varphi\right)\Pi_0\varphi\, d\mu$$

where $\Pi_0\varphi = \varphi - \mathbb{E}_\mu(\varphi)$

- A central limit theorem holds[2] when the equation has a solution in $L^2(\mu)$

Poisson equation in $L^2(\mu)$

$$-\mathcal{L}\Phi = \Pi_0\varphi$$

- Well-posedness of such equations? Hypoelliptic operator

[1] Kliemann, *Ann. Probab.* **15**(2), 690-707 (1987)

[2] Bhattacharya, *Z. Wahrsch. Verw. Gebiete* **60**, 185–201 (1982)

Ergodicity results (2)

- Invertibility of $\mathcal{L}$ on subsets of $L^2_0(\mu) = \left\{ \varphi \in L^2(\mu) \,\middle|\, \int_{\mathcal{E}} \varphi \, d\mu = 0 \right\}$?

$$-\mathcal{L}^{-1} = \int_0^{+\infty} \mathrm{e}^{t\mathcal{L}} \, dt$$

- Prove exponential convergence of the semigroup $\mathrm{e}^{t\mathcal{L}}$
  - various Banach spaces $E \cap L^2_0(\mu)$
  - Lyapunov techniques[3,4,5] $L^\infty_W(\mathcal{E}) = \left\{ \varphi \, \text{measurable}, \left\| \frac{\varphi}{W} \right\|_{L^\infty} < +\infty \right\}$
  - standard hypocoercive[6] setup $H^1(\mu)$
  - $E = L^2(\mu)$ after hypoelliptic regularization[7] from $H^1(\mu)$
  - coupling arguments[8]

[3] L. Rey-Bellet, *Lecture Notes in Mathematics* (2006)
[4] Hairer and Mattingly, *Progr. Probab.* **63** (2011)
[5] Mattingly, Stuart and Higham, *Stoch. Proc. Appl.* (2002)
[6] Villani (2009) and before Talay (2002), Eckmann/Hairer (2003), Hérau/Nier (2004)
[7] F. Hérau, *J. Funct. Anal.* **244**(1), 95-118 (2007)
[8] A. Eberle, A. Guillin and R. Zimmer, *arXiv preprint* **1703.01617** (2017)

Direct $L^2(\mu)$ approach

- Assume that the potential V is smooth and[9,10]
  - the marginal measure ν satisfies a Poincaré inequality
$$\|\Pi_0\varphi\|_{L^2(\nu)}^2 \leqslant \frac{1}{C_\nu}\|\nabla_q\varphi\|_{L^2(\nu)}^2.$$
  - there exist $c_1 > 0$, $c_2 \in [0,1)$ and $c_3 > 0$ such that V satisfies
$$\Delta V \leqslant c_1 + \frac{c_2}{2}|\nabla V|^2, \quad |\nabla^2 V| \leqslant c_3\left(1 + |\nabla V|\right).$$

There exist $C > 0$ and $\lambda_\gamma > 0$ such that, for any $\varphi \in L_0^2(\mu)$,
$$\forall t \geqslant 0, \qquad \left\|\mathrm{e}^{t\mathcal{L}}\varphi\right\|_{L^2(\mu)} \leqslant C\mathrm{e}^{-\lambda_\gamma t}\|\varphi\|_{L^2(\mu)}.$$

with convergence rate of order $\min(\gamma,\gamma^{-1})$: there exists $\overline{\lambda} > 0$ such that
$$\lambda_\gamma \geqslant \overline{\lambda}\min(\gamma,\gamma^{-1}).$$

[9] Dolbeault, Mouhot and Schmeiser, *C. R. Math. Acad. Sci. Paris* (2009)
[10] Dolbeault, Mouhot and Schmeiser, *Trans. AMS*, **367**, 3807–3828 (2015)

Sketch of proof

- Modified square norm $\mathcal{H}[\varphi] = \frac{1}{2}\|\varphi\|^2 - \varepsilon \langle A\varphi, \varphi \rangle$ for $\varepsilon \in (-1,1)$ and

$$A = \Big(1 + (\mathcal{L}_{\mathrm{ham}}\Pi_p)^*(\mathcal{L}_{\mathrm{ham}}\Pi_p)\Big)^{-1}(\mathcal{L}_{\mathrm{ham}}\Pi_p)^*, \qquad \Pi_p\varphi = \int_{\mathbb{R}^D} \varphi \, d\kappa$$

- $A = \Pi_p A(1-\Pi_p)$ and $\mathcal{L}_{\mathrm{ham}}A$ are bounded so that $\mathcal{H} \sim \|\cdot\|^2_{L^2(\mu)}$

Coercivity in the scalar product $\langle\langle \cdot, \cdot \rangle\rangle$ induced by $\mathcal{H}$

$$\mathscr{D}[\varphi] := \langle\langle -\mathcal{L}\varphi, \varphi \rangle\rangle \geqslant \widetilde{\lambda}_\gamma \|\varphi\|^2,$$

- Idea: control of $\|(1-\Pi_p)\varphi\|^2$ by $\langle -\mathcal{L}_{\mathrm{FD}}\varphi, \varphi\rangle$ (Poincaré); for $\|\Pi_p\varphi\|^2$,

$$\|\mathcal{L}_{\mathrm{ham}}\Pi_p\varphi\|^2 \geqslant \frac{DC_\nu}{\beta m}\|\Pi_p\varphi\|^2, \qquad \text{hence } A\mathcal{L}_{\mathrm{ham}}\Pi_p \geqslant \lambda_{\mathrm{ham}}\Pi_p$$

- Gronwall inequality $\frac{d}{dt}\left(\mathcal{H}\left[\mathrm{e}^{t\mathcal{L}}\varphi\right]\right) = -\mathscr{D}\left[\mathrm{e}^{t\mathcal{L}}\varphi\right] \leqslant -\frac{2\widetilde{\lambda}_\gamma}{1+\varepsilon}\mathcal{H}\left[\mathrm{e}^{t\mathcal{L}}\varphi\right]$

Extensions/modifications/variations

- General kinetic energy function $U(p)$ in the Langevin dynamics[11]
  - heavy/light tails
  - ∇U vanishes on open sets (generator not hypoelliptic)

- Galerkin discretization and variance reduction[12]

- Convergence of certain nonequilibrium methods for computing free energy differences[13]

- **One more precise result:** nonequilibrium Langevin dynamics with external forcing

[11] G. Stoltz and Z. Trstanova, accepted in *Multiscale Model. Sim.* (2018)
[12] J. Roussel and G. Stoltz, *M2AN*, 2018
[13] G. Stoltz and E. Vanden-Eijnden, *Nonlinearity*, 2018

Rates of convergence for nonequilibrium Langevin dynamics

- Compact position space $\mathcal{D} = (2\pi\mathbb{T})^d$, constant force $|F| = 1$

Langevin dynamics perturbed by a constant force term

$$\begin{cases} dq_t = \dfrac{p_t}{m} dt, \\ dp_t = (-\nabla V(q_t) + \tau F) dt - \gamma \dfrac{p_t}{m} dt + \sqrt{\dfrac{2\gamma}{\beta}} dW_t, \end{cases}$$

- Non-zero velocity in the direction F is expected in the steady-state
- F **does not derive from the gradient of a periodic function**
  - of course, $F = -\nabla W_F(q)$ with $W_F(q) = -F^T q$
  - ...but W_F is not periodic!

Rates of convergence for nonequilibrium Langevin dynamics

- Lyapunov approaches are non-perturbative but also non-quantitative
- Suboptimal results by the standard hypocoercive approach in $H^1(\mu)$
$\to$ nonequilibrium perturbation[14] of direct $L^2(\mu)$ strategy
- Invariant measure $\psi_\eta = h_\tau \mu$ with $h_\tau \in L^2(\mu)$ for $|\tau|$ small

Uniform rates for nonequilibrium perturbations

There exist $C, \delta_* > 0$ such that, for any $\delta \in [0, \delta^*]$, there is $\overline{\lambda}_\delta > 0$ for which, for all $\gamma \in (0, +\infty)$ and all $\tau \in [-\delta \min(\gamma, 1), \delta \min(\gamma, 1)]$,

$$\left\| \mathrm{e}^{t\mathcal{L}^*_{\gamma,\tau}} f - h_\tau \right\|_{L^2(\mu)} \leqslant C \mathrm{e}^{-\overline{\lambda}_\delta \min(\gamma,\gamma^{-1})t} \|f - h_\tau\|_{L^2(\mu)}.$$

- As a corollary: lower bounds on the spectral gap of order $\min(\gamma, \gamma^{-1})$
$\to$ can be checked numerically [15]

[14] E. Bouin, F. Hoffmann, and C. Mouhot, *arXiv preprint* **1605.04121**

[15] A. Iacobucci, S. Olla and G. Stoltz, to appear in *Ann. Math. Quebec* (2017)

Convergence of Feynmann–Kac dynamics

Feynmann–Kac averages

- Diffusion process X_t, weighted with an exponential factor $\displaystyle\int_0^t f(X_s)\,ds$
- Evolution of probability measures as

$$\Theta_t(\mu)(\varphi) = \frac{\mathbb{E}\left[\varphi(X_t)\,\mathrm{e}^{\int_0^t f(X_s)\,ds} \,\middle|\, x_0 \sim \mu\right]}{\mathbb{E}\left[\mathrm{e}^{\int_0^t f(X_s)\,ds} \,\middle|\, x_0 \sim \mu\right]},$$

Convergence of $\Theta_t(\mu)$?

Show that there exists a unique probability measure μ_f^* such that $\Theta_t(\mu)(\varphi) \to \mu_f^*(\varphi)$ as $t \to +\infty$, and quantify the rate of convergence.

- Applications in Diffusion Monte Carlo and computation of large deviations estimates

Analytical reformulation

- Evolution semigroup $\left(P_t^f \varphi\right)(x) = \mathbb{E}^x \left(\varphi(X_t) \, \mathrm{e}^{\int_0^t f(X_s)\,ds} \right)$

- In fact, $P_t^f = \mathrm{e}^{t(\mathcal{L}+f)}$ where $\mathcal{L}$ is the generator of X_t, so that

$$\Theta_t(\mu)(\varphi) = \frac{\displaystyle\int_{\mathcal{X}} \mathrm{e}^{t(\mathcal{L}+f)} \varphi \, d\mu}{\displaystyle\int_{\mathcal{X}} \mathrm{e}^{t(\mathcal{L}+f)} \mathbf{1} \, d\mu}.$$

- One expects that $\Theta_t(\mu)$ converges to some probability measure

- Convergence rate related to some spectral gap

- Simple analysis for compact spaces $\mathcal{X} = \mathbb{T}^d$ or for self-adjoint generators

A simple case: additive noise, compact space $\mathcal{D}$ (1)

- Dynamics $dX_t = b(X_t)\,dt + \sqrt{2}\,dW_t$
  - Invariant probability measure $\nu(dx)$ (unknown expression)
  - Generator $\mathcal{L} = b^T\nabla + \Delta$, considered on $L^2(\nu)$, discrete spectrum
  - First eigenvectors of $\mathcal{L}$ and $\mathcal{L}^*$: positive, unique up to normalization

$$(\mathcal{L}+f)\widehat{h}_f = \lambda_f \widehat{h}_f, \quad (\mathcal{L}^*+f)h_f = \lambda_f h_f, \quad \int_{\mathcal{D}} h_f\,d\nu = \int_{\mathcal{D}} \widehat{h}_f\,d\nu = 1$$

- Then $\mathrm{e}^{t(\mathcal{L}+f-\lambda_f)}g$ converges exponentially fast to $\dfrac{\langle g, h_f\rangle_{L^2(\nu)}}{\langle h_f, \widehat{h}_f\rangle_{L^2(\nu)}} h_f$

- This allows to identify the limiting probability measure $\mu_f^* \propto h_f\,d\nu$

Convergence in the general case (1)

- Unstructured dynamics: Lyapunov approach

Assumption 1 (Lyapunov conditions)

There is a $C^2(\mathcal{X})$ function $W : \mathcal{X} \to [1, +\infty)$ going to infinity at infinity such that

$$W^{-1}(\mathcal{L} + f)W \xrightarrow[|x|\to+\infty]{} -\infty.$$

In addition, there exist a $C^2(\mathcal{X})$ function $\mathscr{W} : \mathcal{X} \to [1, +\infty)$ and a constant $c \geqslant 0$ such that

$$\varepsilon(x) := \frac{\mathscr{W}(x)}{W(x)} \xrightarrow[|x|\to+\infty]{} 0, \qquad \mathscr{W}^{-1}(\mathcal{L} + f)\mathscr{W} \leqslant c.$$

- Typical choice: $W(x) = \mathrm{e}^{\alpha V(x)}$ and $\mathscr{W}(x) = \mathrm{e}^{\alpha' V(x)}$ with $\alpha' \leqslant \alpha$
- Example: $\sigma(x) = \sqrt{2}$, $b(x) = -\nabla V(x)$, with, for some $a \in (1/2, 1)$,

$$\lim_{|x|\to+\infty} \Big(-\beta(1-a)|\nabla V|^2 + a\Delta V + f \Big) = -\infty$$

Convergence in the general case (2)

Assumption 2 (Regularity and positivity of the transition kernel)

The functions f and σ are continuous and, for any $t > 0$, the transition kernel P_t^f has a continuous positive density with respect to the Lebesgue measure: $P_t^f(x, dy) = p_t^f(x, y)\, dy$ with $p_t^f(x, y) > 0$ for all $x, y \in \mathcal{X}$.

- Introduce $B_W^\infty(\mathcal{X}) = \left\{ \varphi \text{ measurable}, \quad \sup_{x \in \mathcal{X}} \left| \dfrac{\varphi(x)}{W(x)} \right| < +\infty \right\}$

Theorem (Ferré/Rousset/Stoltz, 2018)

There exist a unique invariant measure μ_f^* and $\kappa > 0$ such that, for any initial measure $\mu \in \mathcal{P}(\mathcal{X})$ with $\mu(W) < +\infty$, there is $C_\mu > 0$ for which

$$\forall\, \varphi \in B_W^\infty(\mathcal{X}), \quad \forall\, t > 0, \quad \left| \Theta_t(\mu)(\varphi) - \mu_f^*(\varphi) \right| \leqslant C_\mu \, \mathrm{e}^{-\kappa t} \|\varphi\|_{B_W^\infty}.$$

Moreover, the invariant measure satisfies $\mu_f^*(W) < +\infty$.

Sketch of proof (1)

- Reduction to time-discrete case: $Q^f = \mathrm{e}^{t_0(\mathcal{L}+f)}$ for some fixed $t_0 > 0$

Key result

The operator Q^f considered on $B^\infty_W(\mathcal{X})$ has a zero essential spectral radius, admits its spectral radius $\Lambda > 0$ as a largest eigenvalue (in modulus), and has an associated eigenfunction $h \in B^\infty_W(\mathcal{X})$, normalized so that $\|h\|_{B^\infty_W} = 1$, and which satisfies $0 < h(x) < +\infty$ for all $x \in \mathcal{X}$.

- It is then possible to consider the Markov kernel $Q_h\phi = \Lambda^{-1}h^{-1}Q^f(h\phi)$
- It suffices to understand the convergence of Q_h since

$$\Theta_{kt_0}(\mu)(\varphi) = \frac{\mu\left(h(Q_h)^k(h^{-1}\varphi)\right)}{\mu\left(h(Q_h)^k h^{-1}\right)}$$

- Denoting by μ_h the invariant measure for Q_h,

$$\mu_f^*(\varphi) = \frac{\mu_h\left(h^{-1}\varphi\right)}{\mu_h\left(h^{-1}\right)}$$

Sketch of proof (2)

- Convergence of Q_h: standard convergence results for Markov operators[16]

Lyapunov condition

There exist a function $\mathcal{K} : \mathcal{X} \to [1, +\infty)$ and constants $C \geqslant 0$, $\gamma \in (0,1)$ such that $Q\mathcal{K} \leqslant \gamma \mathcal{K} + C$.

The Lyapunov function for Q_h is $Wh^{-1} : \mathcal{X} \to [1, +\infty)$.

Minorization

There exist $\alpha \in (0,1)$ and $\eta \in \mathcal{P}(\mathcal{X})$ such that $\inf_{x \in \mathcal{C}} Q(x, \cdot) \geqslant \alpha \eta(\cdot)$, where $\mathcal{C} = \{x \in \mathcal{X} \,|\, \mathcal{W}(x) \leqslant R + 1\}$ for some $R > 2C/(1-\gamma)$.

Then, Q has a unique invariant measure μ_*, which is such that $\mu_*(\mathcal{W}) < +\infty$. Moreover, there exist $K > 0$ and $\bar{\alpha} \in (0,1)$ such that,

$$\forall \varphi \in B^\infty_{\mathcal{W}}(\mathcal{X}), \quad \forall\, k \geqslant 0, \quad \|Q^k \varphi - \mu_*(\varphi)\|_{B^\infty_{\mathcal{W}}} \leqslant K \bar{\alpha}^k \|\varphi - \mu_*(\varphi)\|_{B^\infty_{\mathcal{W}}}.$$

[16] Hairer and Mattingly, *Progr. Probab.* **63** (2011)

Elements of proof of the key result

- The essential spectral radius θ of Q^f is zero: rely on the decomposition

$$(Q^f)^3 = (\mathbf{1}_K Q^f \mathbf{1}_K)^2 Q^f + \mathbf{1}_{K^c} Q^f (\mathbf{1}_K Q^f)^2 + Q^f \mathbf{1}_{K^c} (Q^f)^2 + Q^f \mathbf{1}_K Q^f \mathbf{1}_{K^c} Q^f$$

with $(\mathbf{1}_K Q^f \mathbf{1}_K)^2$ compact (using some continuity property and Ascoli) while $\mathbf{1}_{K^c} Q^f$ tends to 0 as K increases

- The spectral radius Λ of Q^f (considered as an operator on $B^\infty_W(\mathcal{X})$) is positive [rely on minorization conditions]

- **Krein–Rutman theorem** on the cone $\mathbb{K}_W = \left\{ u \in B^\infty_W(\mathcal{X}) \;\middle|\; u \geqslant 0 \right\}$:
  - the cone is total (the norm closure of $\mathbb{K}_W - \mathbb{K}_W$ is $B^\infty_W(\mathcal{X})$)
  - The positiveness of $Q^f \in B^\infty_W(\mathcal{X})$ shows that $Q^f \mathbb{K}_W \subset \mathbb{K}_W$.
  - $\theta < \Lambda$

This shows that Λ is an eigenvalue of Q^f with an eigenvector in $\mathbb{K}_W$.