Markovian limits of the generalized McKean-Vlasov dynamics

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Karlstad Applied Analysis Seminar, 02 June 2021

(Weakly) interacting particle systems

- Newton's second law: $m\ddot{Q} = \mathbf{F}$.
- System of N interacting particles ($m = 1$): the underdamped McKean-Vlasov dynamics

$$\ddot{Q}_i = \underbrace{-\nabla V(Q_i)}_{\text{confining (external) force}} \underbrace{-\frac{1}{N}\sum_{j=1}^{N} \nabla_q U(Q_i - Q_j)}_{\text{interaction force}} \underbrace{-\gamma \dot{Q}_i}_{\text{friction}} + \underbrace{\sqrt{2\beta^{-1}}\dot{W}_i}_{\text{stochastic noise}},$$

for $i = 1, \ldots, N$.

- Weak interaction: interaction via the mean; e.g. $U(r) = \frac{r^2}{2}$ (Curie-Weiss models)

$$\frac{1}{N}\sum_{j=1}^{N} \nabla U(Q_i - Q_j) = Q_i - \frac{1}{N}\sum_{j=1}^{N} Q_j.$$

- Langevin dynamics: no interaction

(Weakly) interacting particle systems

1. The overdamped McKean-Vlasov dynamics (oMK-V)

$$\dot{Q}_i = -\nabla V(Q_i) - \frac{1}{N}\sum_{j=1}^{N} \nabla_q U(Q_i - Q_j) + \sqrt{2\beta^{-1}}\dot{W}_i,$$

V: confining potential, U: interaction potential

2. The underdamped McKean-Vlasov dynamics (uMK-V)

$$\ddot{Q}_i = -\nabla V(Q_i) - \frac{1}{N}\sum_{j=1}^{N} \nabla_q U(Q_i - Q_j) - \gamma \dot{Q}_i + \sqrt{2\beta^{-1}}\dot{W}_i,$$

3. The generalized McKean-Vlasov dynamics (gMK-V)

$$\ddot{Q}_i = -\nabla V(Q_i) - \frac{1}{N}\sum_{j=1}^{N} \nabla_q U(Q_i - Q_j) - \sum_{j=1}^{N}\int_0^t \gamma_{ij}(t-s)\,\dot{Q}_j(s)\,ds + F_i(t),$$

where $F(t) = (F_1(t), \dots F_N(t))$ is a mean zero, Gaussian, stationary process, and $[\gamma_{ij}(t-s)]_{i,j=1,\dots,m}$ are autocorrelation functions.

(Weakly) interacting particle systems

- Applications: statistical physics, mathematical biology, mathematical models in the social sciences (cooperative behavior, risk management and opinion formation)
- Many challenging mathematical problems:
  - Mean-field limits ($N \to \infty$)
  - Long-time behaviour ($t \to \infty$)
  - Phase transition (strength of the noise varies)
  - Model reduction (coarse-graining)
  - Hilbert's sixth problem

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Markovian approximation of the gMK-V dynamics

- Markovian approximation of the gMK-V dynamics,

$$
\begin{aligned}
dQ_i(t) &= P_i(t)\,dt \\
dP_i(t) &= -\nabla V(Q_i(t))\,dt - \frac{1}{N}\sum_{j=1}^{N}\nabla_q U(Q_i(t)-Q_j(t))\,dt + \lambda^T Z_i(t)\,dt \\
dZ_i(t) &= -\lambda P_i(t)\,dt - AZ_i(t) + \sqrt{2\beta^{-1}A}dW_i(t).
\end{aligned}
$$

- e.g., when approximating the memory kernel by a sum of exponentials

$$\gamma_m(t) = \sum_{i=1}^{m}\lambda_i^2 e^{-\alpha_i|t|},$$

one can take $\lambda = (\lambda_1, \dots, \lambda_m)$ and $A = \mathrm{diag}(\alpha_1, \dots, \alpha_m)$

[Kupferman, J. Stat. Phys, 2004.]

Mean-field limits ($N \to +\infty$)

- Each particle convergence to the following SDE (propagation of chaos)

$$
\begin{aligned}
dQ(t) &= P(t)\,dt,\\
dP(t) &= -\nabla V(Q(t))\,dt - \nabla_q U * \rho_t(Q_t)\,dt + \lambda^T Z(t)\,dt,\\
dZ(t) &= -P(t)\lambda\,dt - AZ(t) + \sqrt{2\beta^{-1}A}dW(t).
\end{aligned}
$$

- The empirical measure converges to the solution of

$$
\partial_t \rho = -\operatorname{div}_q(p\rho) + \operatorname{div}_p\Big[(\nabla_q V(q) + \nabla_q U * \rho(q) - \lambda^T z)\rho\Big] + \operatorname{div}_z\Big[(p\lambda + Az)\rho\Big] + \beta^{-1}\operatorname{div}_z(A\nabla_z \rho),
$$

  which is the forward Kolmogorov equation associated to the SDE, $\rho_t = \mathrm{Law}(Q_t, P_t, Z_t)$.

[**D.**, Nonlinear Analysis, 2015] using the coupling method. See [Golse, Lecture Notes in Applied Mathematics and Mechanics (Editors: Muntean, Rademacher & Zagaris), 2016] for a survey of the topics.

Stationary solution (and phase-transition)

Proposition (D.-Pavliotis, 2018; D.-Tugaut 2016, 2018)

If there exists a solution $\rho_\infty \in L^1(\mathbf{X}) \cap L^\infty(\mathbf{X})$ to the mean-field (PDE) equation, then

$$\rho_\infty(q,p,z) = \frac{1}{Z}\exp\left[-\beta\left(\frac{|p|^2}{2} + \frac{\|z\|^2}{2} + V(q) + (U * \rho_\infty)(q)\right)\right],$$

where Z is the normalization constant

$$Z = \int_{\mathbf{X}} \exp\left[-\beta\left(\frac{|p|^2}{2} + \frac{\|z\|^2}{2} + V(q) + (U * \rho_\infty)(q)\right)\right] d\mathbf{x}.$$

Conversely, any probability measure whose density satisfies the above equation is a stationary solution to the mean-field PDE.

Corollary: for nonconvex confining potentials, and for the Curie-Weiss quadratic interaction potential, the bifurcation diagrams and even the critical temperature are the same for the three models.

From the uMK-V dynamics to the oMK-V dynamics

Classical result: the oMK-V dynamics can be obtained from the uMK-V dynamics under the high-friction limit ($\gamma \to +\infty$) or the zero-mass limit ($m \to 0$).
Heuristic idea: the underdamped Langevin dynamics

$$m\ddot{Q} = -\nabla V(Q) - \gamma \dot{Q} + \sqrt{2\beta^{-1}}\dot{W}.$$

Sending $m \to 0$ yields the overdamped Langevin dynamics

$$\gamma \dot{Q} = -\nabla V(Q) + \sqrt{2\beta^{-1}}\dot{W}$$

Many different approaches, [D.-Lamacz-Peletier-Sharma, CVPDEs 2017] and [D.-Lamacz-Peletier-Schlichting-Sharma, Nonlinearity 2018]: variational approach and quantification of errors.

From the gMK-V dynamics to the uMK-V dynamics

- White noise (Markovian) limits: $\lambda \mapsto \lambda/\varepsilon$ and $A \mapsto A/\varepsilon^2$.
- At the particle-system level

$$
\begin{aligned}
dQ_i^\varepsilon &= P_i^\varepsilon\, dt, \\
dP_i^\varepsilon &= -\nabla V(Q_i^\varepsilon)\, dt - \frac{1}{N}\sum_{j=1}^{N} \nabla U(Q_i^\varepsilon - Q_j^\varepsilon)\, dt + \frac{1}{\varepsilon}\lambda^T Z_i^\varepsilon\, dt, \\
dZ_i^\varepsilon &= -\frac{1}{\varepsilon} P_i^\varepsilon \lambda\, dt - \frac{1}{\varepsilon^2} A Z_i\, dt + \frac{1}{\varepsilon}\sqrt{2\beta^{-1}A}\, dW_i.
\end{aligned}
$$

- At the mean-field level

$$
\begin{aligned}
dQ^\varepsilon(t) &= P^\varepsilon(t)\, dt, \\
dP^\varepsilon(t) &= -\nabla V(Q^\varepsilon(t))\, dt - \nabla_q U * \rho_t^\varepsilon(Q_t^\varepsilon)\, dt + \frac{1}{\varepsilon}\lambda^T Z^\varepsilon(t)\, dt, \\
dZ^\varepsilon(t) &= -\frac{1}{\varepsilon} P^\varepsilon(t)\lambda\, dt - \frac{1}{\varepsilon^2} A Z^\varepsilon(t) + \frac{1}{\varepsilon}\sqrt{2\beta^{-1}A}\, dW(t).
\end{aligned}
$$

From the gMK-V dynamics to the uMK-V dynamics

Theorem (D.-Pavliotis, 2018)

Let $(Q^\varepsilon, P^\varepsilon, Z^\varepsilon)$ be the solution of the gMK-V dynamics, and assume that the matrix A is invertible. Then $(Q^\varepsilon, P^\varepsilon)$ converges weakly to the solution of the uMK-V dynamics

$$dQ(t) = P(t)\,dt,$$
$$dP(t) = -\nabla V(Q(t))\,dt - \nabla_q U * \rho_t(Q(t))\,dt - \gamma P(t)\,dt + \sqrt{2\gamma\beta^{-1}}dW(t),$$

where the friction coefficient is given by

$$\gamma = \langle \lambda, A^{-1}\lambda \rangle.$$

(Similar results hold at the particle-system level) Method of proof: perturbation expansions method. The key is the Fredholm alternative (solvability) theorem.

[Ottobre-Pavliotis, Nonlinearity 2011: without the interaction term]

Main steps of the proof

Step 1. The forward Kolmogorov (Fokker-Planck) equation

$$\begin{aligned}\frac{\partial\rho^\varepsilon}{\partial t} &= \mathcal{L}^*\rho^\varepsilon\\ &= -p\cdot\nabla_q\rho^\varepsilon + (\nabla V(q) + \nabla_q U(q) * \rho_t^\varepsilon)\cdot\nabla_p\rho^\varepsilon\\ &\qquad + \frac{1}{\varepsilon}\Big(-\lambda^T z\cdot\nabla_p\rho^\varepsilon + p\lambda\cdot\nabla_z\rho^\varepsilon\Big)\\ &\qquad\qquad + \frac{1}{\varepsilon^2}\Big(\mathrm{div}_p(Az\rho^\varepsilon) + \beta^{-1}\,\mathrm{div}(A\nabla_p\rho^\varepsilon)\Big)\\ &:= \Big(\mathcal{L}_2^* + \frac{1}{\varepsilon}\mathcal{L}_1^* + \frac{1}{\varepsilon^2}\mathcal{L}_0^*\Big)\rho^\varepsilon.\end{aligned}$$

- Invariant measure ρ_∞:

$$\rho_\infty(q,p,z) = \frac{\exp\Big[-\beta\Big(\frac{|p|^2}{2} + \frac{\|z\|^2}{2} + V(q) + U*\rho_\infty(q)\Big)\Big]}{\int\exp\Big[-\beta\Big(\frac{|p|^2}{2} + \frac{\|z\|^2}{2} + V(q) + U*\rho_\infty(q)\Big)\Big]\,dqdpdz}.$$

Main steps of the proof (cont.)

Step 2: We define the function $f^\varepsilon(q,p,z,t)$ through

$$\rho^\varepsilon(q,p,z,t) = \rho_\infty(q,p,z) f^\varepsilon(q,p,z,t).$$

• The function $f^\varepsilon(q,p,z,t)$ satisfies the equation

$$\begin{aligned}\frac{\partial f^\varepsilon}{\partial t} &= -p\cdot\nabla_q f^\varepsilon + (\nabla V(q) + \nabla_q U(q) * (f^\varepsilon \rho_\infty))\cdot\nabla_p f^\varepsilon \\ &\quad + \beta f^\varepsilon p\cdot\nabla U(q) * \rho_\infty (1 - f^\varepsilon) + \frac{1}{\varepsilon}\Big(-\lambda^T z\cdot\nabla_p f^\varepsilon + p\lambda\cdot\nabla_z f^\varepsilon\Big) \\ &\quad + \frac{1}{\varepsilon^2}\Big(-Az\cdot\nabla_z f^\varepsilon + \beta^{-1}\mathrm{div}_z(A\nabla_z f^\varepsilon)\Big) \\ &=: \Big(\hat{\mathcal{L}}_2 + \frac{1}{\varepsilon}\hat{\mathcal{L}}_1 + \frac{1}{\varepsilon^2}\hat{\mathcal{L}}_0\Big) f^\varepsilon.\end{aligned}$$

Step 3: We look for a solution of the form

$$f^{\varepsilon} = f_0 + \varepsilon f_1 + \varepsilon^2 f_2 + \dots.$$

We obtain the following sequence of equations

$$\begin{aligned} \hat{\mathcal{L}}_0 f_0 &= 0, \\ -\hat{\mathcal{L}}_0 f_1 &= \hat{\mathcal{L}}_1 f_0, \\ -\hat{\mathcal{L}}_0 f_2 &= \hat{\mathcal{L}}_2 f_0 + \hat{\mathcal{L}}_1 f_1 - \frac{\partial f_0}{\partial t} \end{aligned}$$

Step 4:

- f_0 is independent of z:

$$f_0 = f(q,p,t).$$

- The second equation becomes

$$\hat{\mathcal{L}}_0 f_1 = \lambda^T z \cdot \nabla_p f.$$

- The solvability condition is satisfied [since $\lambda^T z \cdot \nabla_p f$ is orthogonal to the null space of $\hat{\mathcal{L}}_0^*$ which consists of functions of the form $e^{-\beta\frac{\|z\|^2}{2}} u(q,p)$]. Therefore, it has a unique solution, up to a term in the null space of $\hat{\mathcal{L}}_0^*$,

$$f_1 = -zA^{-1}\lambda \cdot \nabla_p f \quad \Big(\text{thus } \hat{\mathcal{L}}_1 f_1 = \lambda^T A^{-1}\lambda\Big(\|z\|^2 \Delta_p f - p\cdot\nabla_p f\Big)\Big).$$

- The solvability condition for the last equation:

$$\int \Big(\hat{\mathcal{L}}_2 f + \hat{\mathcal{L}}_1 f_1 - \frac{\partial f}{\partial t}\Big) Z^{-1} e^{-\beta\frac{\|z\|^2}{2}}\, dz = 0.$$

Since $\hat{\mathcal{L}}_2 f - \frac{\partial f}{\partial t}$ does not depends on z,

$$\frac{\partial f}{\partial t} = \hat{\mathcal{L}}_2 f + \int (\hat{\mathcal{L}}_1 f_1) Z^{-1} e^{-\beta\frac{\|z\|^2}{2}}\, dz.$$

- Direct computations give

$$\hat{\mathcal{L}}_2 f = -p\cdot\nabla_q f + (\nabla V(q) + \nabla_q U(q) * (f\hat{\rho}_\infty))\cdot\nabla_p f + \beta f p\cdot\nabla U(q) * \hat{\rho}_\infty (1-f),$$

where $\hat{\rho}_\infty$ satisfies

$$\hat{\rho}_\infty(q,p) = \frac{\exp\Big[-\beta\Big(\frac{|p|^2}{2} + V(q) + U * \hat{\rho}_\infty(q)\Big)\Big]}{\int \exp\Big[-\beta\Big(\frac{|p|^2}{2} + V(q) + U * \hat{\rho}_\infty(q)\Big)\Big]\,dqdp}.$$

and

$$\int (\hat{\mathcal{L}}_1 f_1) Z^{-1} e^{-\beta\frac{\|z\|^2}{2}}\,dz = \lambda^T A^{-1}\lambda\Big(\beta^{-1}\Delta_p f - p\cdot\nabla_p f\Big).$$

- We obtain the limiting equation for f

$$\frac{\partial f}{\partial t} = -p\cdot\nabla_q f + (\nabla V(q) + \nabla_q U(q) * (f\hat{\rho}_\infty))\cdot\nabla_p f + \beta f p\cdot\nabla U(q) * \hat{\rho}_\infty (1-f) + \lambda^T A^{-1}\lambda\Big(\beta^{-1}\Delta_p f - p\cdot\nabla_p f\Big).$$

Thus $\hat{\rho}(q,p,t) = f(q,p,t)\hat{\rho}_\infty(q,p)$ satisfies the uMK-V dynamics, with $\gamma = \lambda^T A^{-1}\lambda$.

Summary

Interacting particle systems:

- mean-field limit
- phase-transition
- model reduction

Future work

- singular interactions
- non-Markovian systems

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THANK YOU FOR YOUR ATTENTION!