Chapter 1

Notes on Higher-order Propagation of Chaos

The following are notes based on [1].

1.1 Cluster Expansion

Recall BBGKY hierarchy: for N particles interacting via bounded force $K \in L^\infty(\mathbb{T}^{2d};\mathbb{R}^d)$, the evolution of $f_{j,N}$, j-marginal of the joint distribution, satisfies

$$\begin{cases} \partial_t f_{j,N} - \sum_{k=1}^{j} \Delta_{x_k} f_{j,N} + \frac{1}{N}\sum_{k,l=1}^{j} \nabla_{x_k}\cdot (K(x_k,x_l) f_{j,N}) = -\frac{N-j}{N}\sum_{k=1}^{j}\nabla_{x_k}\cdot \int K(x_k,x_*) f_{j+1,N}(X_j,x_*)\mathrm{d}x_* \\ f_{j,N}(0,\cdot) = f^{\otimes j} \end{cases} \tag{1.1}$$

for chaotic initial data.

For any $P \subset \mathbb{N}\cup\{*\}$ with $|P| < \infty$, and any $h : (\mathbb{T}^d)^P \mapsto \mathbb{R}$, we denote

$$\begin{aligned} &S_{k,l} h : (\mathbb{T}^d)^P \mapsto \mathbb{R} \\ &\quad S_{k,l}h(x) := \nabla_{x_k}\cdot (K(x_k,x_l)h(x)). \end{aligned} \tag{1.2}$$

Moreover, if $*, k \in P$ and $k \neq *$,

$$\begin{aligned} &H_k h : (\mathbb{T}^d)^{P-\{*\}} \mapsto \mathbb{R} \\ &\quad H_k h(x^{P-\{*\}}) := \nabla_{x_k}\cdot \int K(x_k,x_*)h(x)\mathrm{d}x_*. \end{aligned} \tag{1.3}$$

Thus the BBGKY hierarchy reads

$$\partial_t f_{j,N} - \sum_{k=1}^{j}\Delta_{x_k} f_{j,N} + \frac{1}{N}\sum_{k,l=1}^{j} S_{k,l} f_{j,N} = -\frac{N-j}{N}\sum_{k=1}^{j} H_k f_{[j]\cup\{*\},N} \tag{1.4}$$

To study the asymptotic behavior of $f_{j,N}$ as $N \to \infty$, we may write the perturbative expansion expression $f_{j,N} = \sum_{i=0}^{\infty} N^{-i} f_j^i$ due to the structure of BBGKY, where f_j^i is independent of N. Plug this ansatz into 1.4 and collect terms of the same order,

$$\partial_t f_j^i - \sum_{k=1}^{j} \Delta_{x_k} f_j^i + \sum_{k=1}^{j} H_k f_{[j]\cup\{*\}}^i = j \sum_{k=1}^{j} H_k f_{[j]\cup\{*\}}^{i-1} - \sum_{k,l=1}^{j} S_{k,l} f_j^{i-1} \tag{1.5}$$

To measure the error term, we may consider the following L^2 divergence

$$\int \left| \frac{f_{j,N} - \sum_{k=0}^{i} N^{-k} f_j^k}{\rho^{\otimes j}} \right|^2 \rho^{\otimes j} \mathrm{d}X_j \tag{1.6}$$

Now we may state the main result of this paper.

- The zeroth order term $f_j^0 = \rho^{\otimes j}$ as is expected, with ρ solution to McKean-Vlasov equation

$$\partial_t \rho - \Delta \rho = -\nabla \cdot (\rho K * \rho) \tag{1.7}$$

- For fixed time interval $[0, T]$, there exists some constant $C = C(\|K\|_{L^\infty}, i, T)$ s.t.

$$\int \left| \frac{f_{j,N} - \sum_{k=0}^{i} N^{-k} f_j^k}{\rho^{\otimes j}} \right|^2 \rho^{\otimes j} \mathrm{d}X_j \leq C \left(\frac{j}{N} \right)^{2(i+1)} \tag{1.8}$$

  for $j \leq C N^{2/3}$.

Remark 1. *For $i = 0$, we have,*

$$\int \left| \frac{f_{j,N} - \rho^{\otimes j}}{\rho^{\otimes j}} \right|^2 \rho^{\otimes j} \mathrm{d}X_j \leq C \left(\frac{j}{N} \right)^2 \tag{1.9}$$

On the other hand,

$$\int \left| \frac{f_{j,N} - \rho^{\otimes j}}{\rho^{\otimes j}} \right|^2 \rho^{\otimes j} \mathrm{d}X_j \geq \frac{1}{2} H(f_{j,N} | \rho^{\otimes j}) \geq \|f_{j,N} - \rho^{\otimes j}\|_{TV}^2, \tag{1.10}$$

so we have recovered Lacker's result [2].

It is hard to get the bound directly due to the hierarchical structure, and we shall study f_j^i through the lens of cluster expansion.
For P a collection of indices, we denote $h_{|P|,N}$ with domain $(\mathbb{T}^d)^P$ by $h_{P,N}$. Now we introduce the cluster expansion, i.e., we express $f_{j,N}$'s in terms of a family of exchangeable functions $g_{1,N}, \ldots, g_{N,N}$, namely

$$f_{j,N} = \sum_{\pi \vdash [j]} \prod_{P \in \pi} g_{P,N}. \tag{1.11}$$

From the combinatorial identity

$$\sum_{\sigma\le\pi}(-1)^{|\sigma|-1}(|\sigma|-1)! = \begin{cases} 1, & |\pi|=1, \\ 0, & |\pi|\ge 2, \end{cases} \tag{1.12}$$

we may inverse the expression into

$$g_{j,N} = \sum_{\pi\vdash[j]}(-1)^{|\pi|-1}(|\pi|-1)!\prod_{P\in\pi} f_{P,N}. \tag{1.13}$$

From 1.4, 1.13 and 1.11 we may get the evolution of $g_{j,N}$

$$\begin{aligned}
\partial_t g_j - \sum_{k=1}^{j}\Delta_{x_k} g_j = &-\frac{N-j}{N}\sum_{k=1}^{j} H_k g_{[j]\cup\{*\}} + \sum_{k=1}^{j}\sum_{W\subset[j]-\{k\}}\frac{j-1-|W|}{N} H_k g_{W\cup\{k,*\}} g_{[j]-\{k\}-W} \\
&-\frac{N-j}{N}\sum_{k=1}^{j}\sum_{W\subset[j]-\{k\}} H_k g_{W\cup\{k\}} g_{[j]\cup\{*\}-W-\{k\}} \\
&+\sum_{k=1}^{j}\sum_{W\subset[j]-\{k\}}\sum_{R\subset[j]-\{k\}-W}\frac{j-1-|W|-|R|}{N} H_k g_{W\cup\{k\}} g_{R\cup\{*\}} g_{[j]-R-W-\{k\}} \\
&-\frac{1}{N}\sum_{k,l=1}^{j} S_{k,l} g_j - \frac{1}{N}\sum_{k,l=1,k\neq l}^{j}\sum_{W\subset[j]-\{k,l\}} S_{k,l} g_{W\cup\{k\}} g_{[j]-\{k\}-W}.
\end{aligned} \tag{1.14}$$

Now we shall expand $g_{j,N} = \sum_{i=0}^{\infty} N^{-i} g_j^i$ with g_j^i independent of N. And we may collect terms of the same order to get

$$\begin{aligned}
\partial_t g_j^i - \sum_{k=1}^{j}\Delta_{x_k} g_j^i = &-\sum_{k=1}^{j} H_k g^i_{[j]\cup\{*\}} - \sum_{k=1}^{j}\sum_{W\subset[j]-\{k\}}\sum_{m=0}^{i} H_k g^m_{W\cup\{k\}} g^{i-m}_{[j]\cup\{*\}-W-\{k\}} \\
&+ j\sum_{k=1}^{j} H_k g^{i-1}_{[j]\cup\{*\}} + \sum_{k=1}^{j}\sum_{W\subset[j]-\{k\}}(j-1-|W|)\sum_{m=0}^{i-1} H_k g^m_{W\cup\{k,*\}} g^{i-1-m}_{[j]-\{k\}-W} \\
&+ j\sum_{k=1}^{j}\sum_{W\subset[j]-\{k\}}\sum_{m=0}^{i-1} H_k g^m_{W\cup\{k\}} g^{i-1-m}_{[j]\cup\{*\}-W-\{k\}} \\
&+\sum_{k=1}^{j}\sum_{W\subset[j]-\{k\}}\sum_{R\subset[j]-\{k\}-W}(j-1-|W|-|R|)\sum_{m=0}^{i-1}\sum_{n=0}^{i-1-m} H_k g^m_{W\cup\{k\}} g^n_{R\cup\{*\}} g^{i-1-m-n}_{[j]-R-W-\{k\}} \\
&-\sum_{k,l=1}^{j} S_{k,l} g_j^{i-1} - \sum_{k,l=1,k\neq l}^{j}\sum_{W\subset[j]-\{k,l\}}\sum_{m=0}^{i-1} S_{k,l} g^m_{W\cup\{k\}} g^{i-1-m}_{[j]-\{k\}-W}.
\end{aligned} \tag{1.15}$$

For chaotic initial data, we may assume that $g_1^0 \equiv \rho$ and that $g_j^0 \equiv 0$ for $j \ge 2$. Let

$$T := \{(i,j)\in\mathbb{N}^2 : 1 \le j \le i+1\} \tag{1.16}$$

Then we have the following proposition

Proposition 2.

1) *For* $(i,j)\notin T$, *we have* $g_j^i\equiv 0$;
2) *For* $(i,j)\in T$,*the equation for* g_j^i *depends only in the* g_l^k*'s with* $k\leq i$;
3) *The equation is linear in* $(g_j^i)_{j=1}^\infty$ *for* $(i,j)>(0,1)$.
4) *If the solution to McKean-Vlasov equation is unique, the* g_j^i*'s are unique.*

Proof.

- If we take $g_j^i=0$ for all $(i,j)\notin T$, there is no contradiction in 1.15. To see this, we only need to verify that if $(i,j)\notin T$, then all terms in RHS of 1.15 involve g_l^k for some $(k,l)\notin T$. We may verify, e.g., the term

$$H_k g^m_{W\cup\{k\}} g^{i-m}_{[j]\cup\{*\}-W-\{k\}} \tag{1.17}$$

does. Otherwise, we have $(m,|W|+1),(i-m,j-|W|)\in T$, then

$$|W|+1\leq m+1, j-|W|\leq i-m+1\Rightarrow j\leq i+1\Rightarrow (i,j)\in T, \tag{1.18}$$

which is a contradiction.

- Since our initial data guarantees $g_j^i(0,\cdot)=0$ for $(i,j)\neq(0,1)$, we only need to prove uniqueness of solution to 1.15. Consider energy of the form

$$\sum_{j=1}^\infty e^{-8jCt}\int_{\mathbb{T}^{jd}}|f_j(t,\cdot)|^2\mathrm{d}X_j, \tag{1.19}$$

where $C=\|K\|_{L^\infty}^2\|\rho\|_{L^2}^2+1$. Now we prove uniqueness by induction on i. In fact, if we have proven uniqueness of $(g_l^k)_{l=1}^\infty$ for $k<i$, and there are two solutions (g_j^i) and $(\bar g_j^i)$. Let $G_j^i=g_j^i-\bar g_j^i$, then

$$\partial_t G_j^i-\sum_{k=1}^j\Delta_{x_k}G_j^i=-\sum_{k=1}^j H_k\rho(x_k)G^i_{[j]\cup\{*\}-\{k\}}-\sum_{k=1}^j H_k\rho(x_*)G^i_{[j]}-\sum_{k=1}^j H_k G^i_{[j]\cup\{*\}}+0. \tag{1.20}$$

Thus

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\left(e^{-8jCt}\int|G_j^i|^2\mathrm{d}X_j\right)\\
=&-8jCe^{-8jCt}\int|G_j^i|^2\mathrm{d}X_j+e^{-8jCt}2\int\partial_tG_j^iG_j^i\mathrm{d}X_j\\
=&-8jCe^{-8jCt}\int|G_j^i|^2\mathrm{d}X_j+\\
&+2e^{-8jCt}\sum_{k=1}^j\Big\{\int\Delta_{x_k}G_j^iG_j^i\mathrm{d}X_j-\int G_j^i\nabla_{x_k}\cdot\int K(x_k,x_*)G^i_{[j]\cup\{*\}-\{k\}}\mathrm{d}x_*\mathrm{d}X_j\\
&-\int G_j^i\nabla_{x_k}\cdot(\int K(x_k,x_*)\rho(x_*)\mathrm{d}x_*G^i_{[j]})\mathrm{d}X_j-\int G_j^i\nabla_{x_k}\cdot(\int K(x_k,x_*)G^i_{[j]\cup\{*\}}\mathrm{d}x_*)\mathrm{d}X_j\Big\}\\
\leq&-8jCe^{-8jCt}\int|G_j^i|^2\mathrm{d}X_j+2jCe^{-8jCt}\left(2\int|G_j^i|^2\mathrm{d}X_j+\int|G_{j+1}^i|^2\mathrm{d}X_{j+1}\right)
\end{aligned}\tag{1.21}$$

For $t \in [0, \frac{\log 2}{8C}]$, we have $e^{8Ct} \leq 2$, then summing over all the terms and we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\sum_{j=1}^{\infty} e^{-8jCt}\int |G_j^i|^2 \mathrm{d}X_j \leq \sum_{j=1}^{\infty}\left\{\left[(j-1)e^{8Ct}-4j\right]C\int |G_j^i|^2\mathrm{d}X_j\right\} \leq 0 \tag{1.22}$$

Then we may find $G_j^i \equiv 0$ for all j at any time interval. □

Proposition 3. *For any i, j and any $1 \leq l \leq j$*

$$\int g_j^i \mathrm{d}x_l = \begin{cases} 1 & i=0, j=1, \\ 0 & \textit{otherwise}. \end{cases} \tag{1.23}$$

Thus $\int f_{j+1}^i \mathrm{d}x_{j+1} = f_j^i$.

Proof. We may integrate both sides of 1.15 by x_l to get the first claim. And by comparing terms of the same order in 1.11

$$f_j^i = \sum_{\pi \vdash [j]} \sum_{\substack{(i_P)_{P\in\pi} \\ \sum i_P = i}} \prod_{P\in\pi} g_P^{i_P}. \tag{1.24}$$

Thus the second claim follows. □

1.2 Hierarchy Bounds

Proposition 4. *Let $\tilde{g}_j^i := \frac{g_j^i}{\rho^{\otimes j}}$, there is a constant $C(\|K\|_{L^\infty}, i)$ s.t.*

$$\int |\tilde{g}_j^i|^2 \rho^{\otimes j}\mathrm{d}X_j \leq Ce^{Ct}. \tag{1.25}$$

Proof. We may prove it by induction on i. Suppose the claim is true for g_l^k's with $k < i$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int |\tilde{g}_j^i|^2\rho^{\otimes j}\mathrm{d}X_j \leq 3j\int |\tilde{g}_j^i|^2\rho^{\otimes j}\mathrm{d}X_j + Ce^{Ct}\left(\sup_{k<i}\int |\tilde{g}_l^k|^2\rho^{\otimes l}\mathrm{d}X_j\right)^3, \tag{1.26}$$

and since $\tilde{g}_j^i = 0$ for $j > i+1$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int |\tilde{g}_j^i|^2\rho^{\otimes j}\mathrm{d}X_j \leq C\int |\tilde{g}_j^i|^2\rho^{\otimes j}\mathrm{d}X_j + Ce^{Ct}\left(\sum_{k=0}^{i-1}\|(\tilde{g}_l^k)\|^2_{l_l^2(L^2_{X_l}(\rho^{\otimes l}))}\right)^3 \tag{1.27}$$

Summing over j and applying Gronwall we may conclude. □

If we let

$$\varphi_j^i := \sum_{k=0}^{i} N^{-k} f_j^k \tag{1.28}$$

and

$$R_j^i := N^{-i-1} \sum_{k=1}^{j} e_k \otimes \sum_{l=1}^{j} \left(\int K(x_k, x_*) f_{[j]\cup\{*\}}^i \mathrm{d}x_* - K(x_k, x_l) f_j^i \right) \tag{1.29}$$

Then

$$\partial_t \varphi_j^i - \sum_{k=1}^{j} \Delta_{x_k} \varphi_j^i + \frac{N-j}{N} \sum_{k=1}^{j} \nabla_{x_k} \cdot \int K(x_k, x_*) \varphi_{j+1}^i (X_{[j]\cup\{*\}}) \mathrm{d}x_* + \frac{1}{N} \sum_{k,l=1}^{j} \nabla_{x_k} \cdot (K(x_k, x_l)\varphi_j) = \nabla \cdot R_j^i. \tag{1.30}$$

Proposition 5. *For* $\gamma_j^i := \varphi_j^i - f_j$,

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} \int \left| \frac{\gamma_j^i}{\rho^{\otimes j}} \right|^2 \rho^{\otimes j} \mathrm{d}X_j \leq & 2j \|K\|_{L^\infty}^2 \left(\int \left| \frac{\gamma_{j+1}^i}{\rho^{\otimes (j+1)}} \right|^2 \rho^{\otimes (j+1)} \mathrm{d}x_* \mathrm{d}X_j - \int \left| \frac{\gamma_j^i}{\rho^{\otimes j}} \right|^2 \rho^{\otimes j} \mathrm{d}X_j \right) \\ & + 4 \frac{j^3}{N^2} \|K\|_{L^\infty}^2 \int \left| \frac{\gamma_j^i}{\rho^{\otimes j}} \right|^2 \rho^{\otimes j} \mathrm{d}X_j + 2 \int \left| \frac{R_j^i}{\rho^{\otimes j}} \right|^2 \rho^{\otimes j} \mathrm{d}X_j. \end{aligned} \tag{1.31}$$

Proof. Direct computation. □

Proposition 6. *There exist* $C = C(\|K\|_{L^\infty}, i) < +\infty$, *s.t.*

$$\int \left| \frac{R_j^i}{\rho^{\otimes j}} \right|^2 \rho^{\otimes j} \mathrm{d}X_j \leq C e^{Ct} \left(\frac{j}{N} \right)^{2(i+1)} \tag{1.32}$$

By the two proposition above, the main result follows from a slight adjustment of Lacker's hierarchical inequality [2].

Bibliography

[1] Elias Hess-Childs and Keefer Rowan. Higher-order Propagation of Chaos in L^2 for Interacting Diffusions. *arXiv preprint arXiv:2310.09654*, 2023.

[2] Daniel Lacker. Hierarchies, Entropy, and Quantitative Propagation of Chaos for Mean Field Diffusions. *arXiv preprint arXiv:2105.02983*, 2021.