Sharp estimates for variations of Coulomb and Riesz modulated energies

Matthew Rosenzweig
Based on joint work w/ Sylvia Serfaty

MIT

June 8, 2022

"Mathematical results of many-body quantum systems", Herrsching, June 6-11 2022

Modulated energies and their variations

Coulomb/Riesz modulated energies I

Let us consider the class of Riesz interactions

$$
(1.1) \qquad \mathsf{g}(x) = \begin{cases} -\log|x|, & s = 0,\ d = 1,2 \\ |x|^{-s}, & d-2 < s < d,\ d = 1,2 \\ |x|^{-s}, & d-2 \le s < d,\ d \ge 3. \end{cases}
$$

- Coulomb case $s = d-2$ well-motivated from physics (e.g., Coulomb gas/one-component plasma)
- 1D log case has connections to random matrix theory Forrester 2010
- General Riesz case of interest for approximation theory Borodachov-Hardin-Saff 2019

When studying systems of N distinct points $\underline{x}_N = (x_1, \ldots, x_N) \in (\mathbb{R}^d)^N$ with interaction energy

$$
(1.2) \qquad \sum_{1 \le i \ne j \le N} \mathsf{g}(x_i - x_j),
$$

an effective way to compare empirical measures $\mu_N := \frac{1}{N}\sum_{i=1}^N \delta_{x_i}$ to a *mean-field* density μ is by considering a *modulated energy*.[1]

Coulomb/Riesz modulated energies II

$$F_N(\underline{x}_N, \mu) := \frac{1}{2} \int_{(\mathbb{R}^d)^2 \setminus \triangle} \mathsf{g}(x - y) d(\mu_N - \mu)^{\otimes 2}(x, y), \tag{1.3}$$

- Squared Coulomb/Riesz distance
- Excision of diagonal $\triangle$ to remove infinite self-interaction of each particle
- First appeared in stat mech of Coulomb/Riesz gasses Sandier-Serfaty 2015, Rougerie-Serfaty 2016, Petrarche-Serfaty 2017; extended to derivation of mean-field dynamics Duerinckx 2016, Serfaty 2020, Q.H. Nguyen-R.-Serfaty 2021
- Think of as a "renormalization" of infinite quantity $\|\mu_N - \mu\|^2_{\dot{H}^{\frac{s-d}{2}}}$

[1] The term modulated energy goes back to at least work of Brenier 2000 on quasineutral limit of Vlasov-Poisson.

Electric reformulation I

- If $d = 1, s = 0$ or $d \neq 1, s > d-2$, the potential g is not the fundamental solution for a local operator and also fails to be superharmonic.
- Both of these properties are restored by viewing $\mathrm{g}(x) = \mathrm{G}(x, 0)$ as the restriction of a potential in extended space $\mathbb{R}^{d+k}$, i.e.
  $\mathrm{G} : \mathbb{R}^{d+k} \setminus \{0\} \to (0, \infty),\ \mathrm{G}(X) = \mathrm{g}(|X|)$.
- As popularized by Caffarelli-Silvestre 2007, the function G is a fundamental solution for a degenerate elliptic operator[2],

$$-\frac{1}{\mathsf{c}_{d,s}} \operatorname{div}(|z|^{\gamma} \nabla \mathrm{G}) = \delta_0 \tag{1.4}$$

  in the sense of distributions in $\mathbb{R}^{d+k}$, where $\gamma := s + 2 - d - k$.
- To regularize the interaction, one can introduce the truncated potential $\mathrm{G}_{\eta} := \min(\mathrm{G}, \mathrm{G}(\eta))$
- One then defines the smeared point mass/charge

$$\delta_0^{(\eta)} := -\frac{1}{\mathsf{c}_{d,s}} \operatorname{div}(|z|^{\gamma} \nabla \mathrm{G}_{\eta}) = \frac{\eta^{-s-1}}{\mathsf{c}_{d,s}} |z|^{\gamma} d\sigma_{\partial B(0,\eta)}, \tag{1.5}$$

  where $\sigma_{\partial B(0,\eta)}$ is the uniform probability measure on the sphere in $\mathbb{R}^{d+k}$.

Electric reformulation II

Introducing the "nearest-neighbor" length scale

$$\mathsf{r}_i := \frac{1}{4}\min\left(\min_{j\neq i}|x_i - x_j|, (N\|\mu\|_{L^\infty})^{-1/d}\right), \qquad 1 \le i \le N, \tag{1.6}$$

one can re-express the modulated energy, for any choice of $\eta_i \le \mathsf{r}_i$,

$$\begin{aligned} F_N(\underline{x}_N,\mu) = \frac{1}{2\mathsf{c}_{d,s}}\left(\int_{\mathbb{R}^{d+k}}|z|^\gamma|\nabla H_{N,\vec{\eta}}|^2 dX - \frac{\mathsf{c}_{d,s}}{N^2}\sum_{i=1}^N \mathsf{g}(\eta_i)\right) \\ - \frac{1}{N}\sum_{i=1}^N\int_{\mathbb{R}^d}(\mathsf{g}-\mathsf{g}_{\eta_i})(x-x_i)d\mu(x), \end{aligned} \tag{1.7}$$

where $H_{N,\vec{\eta}} := \frac{1}{N}\sum_{i=1}^N \mathsf{G}_{\eta_i}(X - X_i) - \mathsf{G}*\tilde{\mu}$, with $\tilde{\mu} := \mu\delta_{\mathbb{R}^d\times\{0\}}$.

In general, F_N is not nonnegative; but there exists a constant $C>0$ such that

$$F_N(\underline{x}_N,\mu) + \frac{\log(N\|\mu\|_{L^\infty})}{2Nd}\mathbf{1}_{s=0} + C\|\mu\|_{L^\infty}^{\frac{s}{d}}N^{\frac{s}{d}-1} \ge 0. \tag{1.8}$$

---

[2] An example of an elliptic operator with an A_2 weight, for which there is a good theory Fabes-Kenig-Serapioni 1982.

Localized modulated energies

For applications, also of interest to consider the "localized" modulated energy

$$F_N^{\Omega}(\underline{x}_N, \mu) := \frac{1}{2\mathsf{c}_{d,s}}\left(\int_{\Omega\times\mathbb{R}^k} |z|^{\gamma}|\nabla H_{N,\tilde{\mathsf{r}}}|^2 dX - \frac{\mathsf{c}_{d,s}}{N^2}\sum_{i:x_i\in\Omega} \mathsf{g}(\tilde{\mathsf{r}}_i)\right) - \frac{1}{N}\sum_{i:x_i\in\Omega}\int_{\mathbb{R}^d} (\mathsf{g}-\mathsf{g}_{\tilde{\mathsf{r}}_i})(x-x_i)d\mu(x), \tag{1.9}$$

where $\Omega \subset \mathbb{R}^d$ and $\tilde{\mathsf{r}}_i$ is a modified nearest-neighbor distance to accommodate boundaries.

Variation by transport I

In the context of mean-field limits, essential to control quantities that correspond to differentiating F_N along a transport field:

$$(1.10) \quad \frac{d^n}{dt^n|_{t=0}} F_N\Big((\mathbb{I}+tv)^{\oplus N}(\underline{x}_N), (\mathbb{I}+tv)\#\mu\Big) = \int_{(\mathbb{R}^d)^2\setminus\triangle} \nabla^{\otimes n}\mathrm{g}(x-y) : (v(x)-v(y))^{\otimes n} d(\mu_N-\mu)^{\otimes 2}(x,y),$$

where $\mathbb{I}$ is the identity on $\mathbb{R}^d$ and $(\mathbb{I}+tv)^{\oplus N}(\underline{x}_N) := \underline{x}_N + t(v(x_1),\ldots,v(x_N))$.

The important control takes the form of a *functional inequality*: for $n=1$,

$$(1.11) \qquad |\text{RHS of } (1.10)| \le C\big(F_N(\underline{x}_N,\mu) + N^{-\alpha}\big)$$

for some $\alpha > 0$.

- First proved by Leblé-Serfaty 2018 in 2D Coulomb case $s=0$; generalized to all Coulomb/super-Coulombic Riesz cases $\max\{d-2,0\} \le s < d$ and 1D log case in Serfaty 2020
- Reinterpretation as a commutator estimate R. 2020; this POV used to generalize (1.11) to all cases $0 \le s \le d$ Q.H. Nguyen-R.-Serfaty 2021 and broader class of g's that are of Riesz-type (e.g. Lennard-Jones)

Variation by transport II

- FIs crucially used to prove CLTs for fluctuations of Coulomb gasses Leblé-Serfaty 2018, Serfaty 2021; even more important for MF limits of classical particle systems Serfaty 2020, Duerinckx-Serfaty 2020, Bresch-Jabin-Wang 2019-2020, R. 2020-2022, Golse-Paul 2020, Q.H. Nguyen-R.-Serfaty 2021
- Second-order FIs (i.e. (1.11) for $n = 2$) were shown in Serfaty 2020, R. 2020 in the Coulomb case and Q.H. Nguyen-R.-Serfaty 2021 for the full Riesz case $0 \leq s < d$; important for fluctuations and MF limits with multiplicative noise
- Exponent α in error term is explicit in d, s.
  - By only counting nearest-neighbor (with typical distance of $N^{-1/d}$) interactions, one expects F_N is at least of order $N^{\frac{s}{d}-1}$
  - $F_N \geq -CN^{\frac{s}{d}-1}$, where $C = C(\|\mu\|_{L^\infty}) > 0$
  - Known that $\min |F_N|$ is of order $N^{\frac{s}{d}-1}$ Sandier-Serfaty 2015, Rougerie-Serfaty 2015, Petrarche-Serfaty 2017, Cotar-Petrarche 2019, Hardin *et al.* 2017
  - Optimal error only been shown for Coulomb case Leblé-Serfaty 2018, Serfaty 2020, R. 2021

New functional inequalities

Theorem 1 (R.-Serfaty 2022)

There exists a constant $C = C(d,s) > 0$ such that TFH. Let $\mu \in L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$ with unit mean and $v : \mathbb{R}^d \to \mathbb{R}^d$ be Lipschitz. Let Ω be a closed set containing a 2λ-neighborhood of $\operatorname{supp} v$, and assume that $\lambda < 1$. Then for any pairwise distinct $\underline{x}_N \in (\mathbb{R}^d)^N$, it holds that

$$
\begin{aligned}
(2.1)\quad & \left| \int_{(\mathbb{R}^d)^2 \setminus \triangle} (v(x) - v(y)) \cdot \nabla \mathrm{g}(x-y) d\Big(\mu_N - \mu\Big)^{\otimes 2}(x,y) \right| \\
& \leq C \|\nabla v\|_{L^\infty} \left(F_N^\Omega(\underline{x}_N, \mu) - \# I_\Omega \left(\frac{\log \lambda}{2N^2} \right) \mathbf{1}_{s=0} + C \frac{\# I_\Omega}{N} \|\mu\|_{L^\infty(\hat{\Omega})} \lambda^{d-s} \right).
\end{aligned}
$$

- $\Omega \subset \mathbb{R}^d$ is meant to represent the support of the transport field v
- $\lambda := (N\|\mu\|_{L^\infty(\Omega)})^{-\frac{1}{d}}$, which can be viewed as the typical inter-particle distance, and $\hat{\Omega}$ is the $\frac{\lambda}{4}$-neighborhood of Ω
- $I_\Omega := \{x_i\}_{i=1}^N \cap \Omega$, and let $\# I_\Omega$ denote the cardinality

Sketch of proof I

Focusing on the Coulomb case, the starting point as in past work is *electric reformulation*[3] of modulated energy as a renormalization of quantity

$$\int_{\mathbb{R}^d} |\nabla H_N|^2 dx, \qquad H_N := \mathsf{g} * (\mu_N - \mu). \tag{2.2}$$

Key observation = *stress-energy tensor* structure:

$$\begin{aligned} 2\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} v(x)\cdot\nabla\mathsf{g}(x-y)d(\mu_N-\mu)(y)d(\mu_N-\mu)(x) &= \int_{\mathbb{R}^d} v\nabla H_N \Delta H_N dx \\ &= \int_{\mathbb{R}^d} v \,\mathrm{div}\, T_{H_N} dx, \end{aligned} \tag{2.3}$$

where tensor $T_{H_N}^{ij} := 2\partial_i H_N \partial_j H_N - |\nabla H_N|^2 \delta_{ij}$.

IBP and using $\|T_{H_N}\|_{L^1} \le C\|\nabla H_N\|_{L^2}^2$ allows one to conclude

Preceding calculations formal, since we ignored excision of diagonal and $\|\nabla H_N\|_{L^2}^2$ is infinite. But computation can be properly renormalized, which is the main technical roadblock.

Sketch of proof II

Unclear how to make a pure stress-tensor approach work for higher-order estimates $n \geq 2$; delicate proofs in Leblé-Serfaty 2018, Serfaty 2020 do not seem extendable to $n \geq 3$

We exhibit a stress-tensor structure in higher-order variations, involving not only H_N but also *iterated commutators* of H_N.

Given a distribution f (e.g. $f = \mu_N - \mu$), $h^f := g * f$ its Coulomb/Riesz potential, and a vector field v, we define the first commutation of h^f as

$$k^f := \int_{\mathbb{R}^d} \nabla \mathrm{g}(x-y) \cdot (v(x) - v(y)) df(y) = h^{\mathrm{div}(vf)} - v \cdot \nabla h^f. \tag{2.4}$$

Relationship between commutator and stress-tensor through

$$\int \kappa^f df = \int v \,\mathrm{div}\, T_{h^f} = -\int Dv : T_{h^f}. \tag{2.5}$$

Polarizing (2.5) and applying it instead to f and $-\Delta \kappa^f$, Cauchy-Schwarz yields

$$\int_{\mathbb{R}^d} |\nabla \kappa^f|^2 dx \leq C \|\nabla v\|_{L^\infty} \int_{\mathrm{supp}\, v} |\nabla h^f|^2 dx. \tag{2.6}$$

Sketch of proof III

To evaluate the second variation of the energy, we thus need to compute the first variation of $\operatorname{div} T_{H_N}$ when again μ_N and μ are pushed forward by $\mathbb{I} + tv$.

It suffices to compute the derivative of H_N^t at $t = 0$, and since $H_N = \mathrm{g} * (\mu_N - \mu)$, the definition of the push-forward yields that $\frac{d}{dt|_{t=0}} H_N^t = \mathrm{g} * (\operatorname{div}(v(\mu_N - \mu))$. This involves again higher derivatives of $f = \mu_N - \mu$ and terms that we cannot directly control by the energy $\int |\nabla H_N|^2$.

But introducing the commutator κ^f, we can decompose the second order variation as

(2.7)

$$
\begin{aligned}
&-\int_{\mathbb{R}^d} Dv : \Big(\partial_i H_N \partial_j (v \cdot \nabla H_N) + \partial_i (v \cdot \nabla H_N))\partial_j H_N - \nabla H_N \cdot \nabla (v \cdot \nabla H_N)\delta_{ij}\Big) dx \\
&\qquad\qquad - \int_{\mathbb{R}^d} Dv : \Big(\partial_i H_N \partial_j \kappa^f + \partial_i \kappa^f \partial_j H_N - \nabla H_N \cdot \nabla \kappa^f \delta_{ij}\Big)\, dx.
\end{aligned}
$$

Thanks to $\dot{H}^1$ estimate for κ^f, the second line can directly be controlled by $C_v \int |\nabla H_N|^2$, while the first line can be transformed into appropriate terms with IBP of $v \cdot \nabla$.

Sketch of proof IV

Argument can be iterated at next order by introducing

$$\kappa_t^{(n),f} := \int_{\mathbb{R}^d} \nabla^{\otimes n} \mathrm{g}(x - y - tv(y)) : (v(x) - v(y))^{\otimes n} df(y), \tag{2.8}$$

which obey recursion relation (a transport equation)

$$\partial_t \kappa_t^{(n)} = -\kappa_t^{(n+1)} - v \cdot \nabla \kappa_t^{(n)}. \tag{2.9}$$

Algebra becomes increasingly more complicated, but proof is transparent in terms of using IBP and lower-order commutator estimates. Ultimately, we show, for any $n \geq 1$, the control

$$\int_{\mathbb{R}^d} |\nabla \kappa^{(n),f}|^2 dx \leq C_v \int_{\mathrm{supp}\, v} |\nabla h^f|^2 dx, \tag{2.10}$$

where the constant C is n-linear in v and involves L^∞ norms of derivatives up to order n of v.

Sketch of proof V

So far ignored the delicate question of "renormalization," which is that of dealing with the singularities in the Diracs and in H_N. But it can be handled via the point-dependent charge smearing/potential truncation mentioned at the beginning of the talk.

Writing $\mathsf{k}_v(x,y) := (v(x)-v(y))\cdot\nabla\mathsf{g}(x-y)$, we can decompose

$$\int_{(\mathbb{R}^d)^2\setminus\triangle}\mathsf{k}_v(x,y)d\left(\frac{1}{N}\sum_{i=1}^N\delta_{x_i}-\mu\right)^{\otimes 2}(x,y)=\sum_{j=1}^3\mathrm{Term}_j, \tag{2.11}$$

where...

Sketch of proof VI

$$\text{Term}_1 := \int_{(\mathbb{R}^d)^2} \mathsf{k}_v(x,y) d\left(\frac{1}{N}\sum_{j=1}^N \delta_{x_j}^{(\eta_i)} - \mu\right)^{\otimes 2}(x,y), \tag{2.12}$$

(2.13)

$$\text{Term}_2 := \frac{1}{N}\sum_{i=1}^N \int_{(\mathbb{R}^d)^2} \mathsf{k}_v(x,y) d\left(\frac{1}{N}\sum_{j=1}^N \delta_{x_j}^{(\eta_j)} - \mu\right)(x) d\left(\delta_{x_i} - \delta_{x_i}^{(\eta_i)}\right)(y),$$

(2.14)

$$\text{Term}_3 := \frac{1}{N}\sum_{i=1}^N \int_{(\mathbb{R}^d)^2\setminus\triangle} \mathsf{k}_v(x,y) d\left(\frac{1}{N}\sum_{j=1}^N \delta_{x_j} - \mu\right)(x) d\left(\delta_{x_i} - \delta_{x_i}^{(\eta_i)}\right)(y).$$

For Term_1, apply commutator estimates. For $\text{Term}_2, \text{Term}_3$, estimate directly.

---

[3] As previously mentioned, this reformulation is available for the super-Coulombic Riesz case, but not in the same way for the sub-Coulombic case $s < d-2$. This restricts us to $d-2 \le s < d$.

Higher-order functional inequalities I

By a similar, more complicated approach, in the cases $s = d - 2$, $s = d - 1$ we can obtain higher-order functional inequalities of the form

$$
\begin{aligned}
(2.15)\quad & \left| \int_{(\mathbb{R}^d)^2 \setminus \triangle} \nabla^{\otimes n} \mathrm{g}(x-y) : (v(x) - v(y))^{\otimes n} d\Big(\frac{1}{N}\sum_{i=1}^{N} \delta_{x_i} - \mu\Big)^{\otimes 2}(x,y) \right| \\
&\le C\Bigg(\Big(\|\nabla v\|_{L^\infty} + \lambda \|\nabla^{\otimes 2} v\|_{L^\infty} \Big)^n + \sum_{\substack{0 \le c_1, \dots, c_n \le n \\ c_1 + \cdots + c_n = n}} \|\nabla^{\otimes c_1} v\|_{L^\infty} \cdots \|\nabla^{\otimes c_n} v\|_{L^\infty} \Bigg) \\
&\quad \times \Bigg(F_N^{\Omega}(\underline{x}_N, \mu) - \# I_\Omega \Big(\frac{\log \lambda}{2N^2}\Big) \mathbf{1}_{s=0} + C \frac{\|\mu\|_{L^\infty(\hat{\Omega})} \# I_\Omega}{N} \Big(\lambda^{d-s} + \lambda^2 \log(\ell/\lambda) \mathbf{1}_{s=d-2}\Big) \Bigg) \\
&\quad + \frac{C\lambda^2}{\ell^{2+s}} \Bigg(\|\nabla v\|_{L^\infty}^n + \|\nabla v\|_{L^\infty}^{n-1} \|\nabla^{\otimes 2} v\|_{L^\infty} \lambda \\
&\quad + (\lambda \|\nabla^{\otimes 2} v\|_{L^\infty})^2 \Big(\|\nabla v\|_{L^\infty} + \frac{\lambda^2 \|\nabla^{\otimes 2} v\|_{L^\infty}}{\ell} \Big)^{n-2} \Bigg) \\
&\quad + C\lambda^{d-s} \|\mu\|_{L^\infty} \Big(\|\nabla v\|_{L^\infty}^{n-2} \|\nabla^{\otimes 2} v\|_{L^\infty} (\|v\|_{L^\infty} + \lambda \|\nabla v\|_{L^\infty}) + \|\nabla v\|_{L^\infty}^n \Big) \\
&\quad + C\lambda^2 \|\nabla v\|_{L^\infty}^{n-1} \Big(\|\nabla v\|_{L^\infty} + \ell \|\nabla^{\otimes 2} v\|_{L^\infty} \Big) \Big(\|\mu\|_{L^\infty} \log(\ell/\lambda) + \ell^{-d} \|\mu\|_{L^1} \Big) \mathbf{1}_{s=d-2}.
\end{aligned}
$$

Higher-order functional inequalities II

- Above, there's an additional parameter $\ell \gg \lambda$, which we think of as the typical length scale of Ω.
- If $s = d - 1$, the estimate is sharp in λ dependence, but probably room for improvement in dependence on ℓ.
- If $s = d - 2$, the λ dependence is off from the sharp λ^2 by a $\log$ factor.
- The cases $s = d - 2, d - 1$ are special because g or G is the fundamental solution of a local operator. Same argument doesn't quite work (though morally should be true) for remaining Riesz cases due to presence of weights $|z|^\gamma$. Even the proof in first-order case has to be modified somewhat to treat these Riesz cases.
- Work-in-progress on remaining cases in $(d - 2, d - 1) \cup (d - 1, d)$; difficulty in still obtaining estimates that can be localized to Ω.

Classical applications

Optimal rate of convergence for MF limits I

With new functional inequalities, we can obtain optimal rate of convergence for the mean-field limit of first-order systems

$$(3.1) \qquad \begin{cases} \dot{x}_i^t = \dfrac{1}{N} \displaystyle\sum_{1 \le j \le N : j \ne i} \mathbb{M} \nabla \mathsf{g}(x_i^t - x_j^t) + \mathsf{V}(x_i^t) \\ x_i^t|_{t=0} = x_i^0 \end{cases} \qquad i \in \{1, \ldots, N\}.$$

- $\mathbb{M}$ is a real $d \times d$ matrix. $\mathbb{M} = -\mathbb{I}$ corresponds to gradient flow/dissipative dynamics; $\mathbb{M}$ antisymmetric corresponds to Hamiltonian/conservative dynamics.
- V is some external force (e.g. $-\nabla V_{\text{ext}}$)
- Summation over $j = i$ excluded because no self-interaction

Optimal rate of convergence for MF limits II

Limiting equation for empirical measure $\frac{1}{N}\sum_{i=1}^{N}\delta_{x_i^t}$ is

$$
\begin{cases} \partial_t \mu = -\operatorname{div}((\mathsf{V} + \mathbb{M}\nabla \mathsf{g} * \mu)\mu) \\ \mu|_{t=0} = \mu^0, \end{cases} \qquad (t,x) \in \mathbb{R}_+ \times \mathbb{R}^d. \tag{3.2}
$$

From our $n = 1$ functional inequality, we obtain

$$
\begin{aligned}
F_N(\underline{x}_N^t, \mu^t) + \frac{\log\left(N\|\mu^t\|_{L^\infty}\right)}{2Nd}\mathbf{1}_{s=0} &\leq e^{C_1\int_0^t (\|\nabla^{\otimes 2}\mathsf{g}*\mu^\tau\|_{L^\infty} + \|\nabla \mathsf{V}\|_{L^\infty})d\tau} \\
&\quad \times \Bigg(F_N(\underline{x}_N^0, \mu^0) + \frac{\log\left(N\|\mu^0\|_{L^\infty}\right)}{2Nd}\mathbf{1}_{s=0} \\
&\qquad + C_2 N^{\frac{s}{d}-1}\int_0^t (\|\nabla u^\tau\|_{L^\infty} + \|\nabla \mathsf{V}\|_{L^\infty})\|\mu^\tau\|_{L^\infty}^{\frac{s}{d}} d\tau \Bigg).
\end{aligned} \tag{3.3}
$$

Optimal rate of convergence for MF limits III

Much work over the years on MF limits:

- $W^{2,\infty}$ potentials Dobrushin 1979, Sznitman 1991
- sub-Coulombic $s < d - 2$ Hauray 2009, Carrillo-Choi-Hauray 2014
- Coulomb/super-Coulombic $d - 2 \leq s < d$ Duerinckx 2016, Carrillo-Ferreira-Precioso 2012, Berman-Önnheim 2019, Serfaty 2020
- all cases $0 \leq s < d$ Bresch-Jabin-Wang 2019, Q.H. Nguyen-Rosenzweig-Serfaty 2021

Previously, only in the Coulomb case $s = d - 2$ has the sharp error been obtained. With our result, question of sharp error only remains for sub-Coulombic case $0 \leq s < d - 2$

Effective equations for large Newtonian systems

Consider Newtonian dynamics for N indistinguishable particles:

(3.4)

$$\begin{cases} \dot{x}_i = v_i \\ \dot{v}_i = -\frac{1}{\varepsilon^2 N} \sum_{1 \le j \le N : j \ne i} \nabla \mathrm{g}(x_i - x_j) - \frac{1}{\varepsilon^2} \nabla V_{\mathrm{ext}}(x_i^t), \end{cases} \qquad i \in \{1, \dots, N\}$$

- $(x_i, v_i) \in \mathbb{R}^d \times \mathbb{R}^d$ are position/velocity of i-th particle
- ε is a parameter which encodes physical information about the system
- g is an interaction potential (e.g. Coulomb $-\Delta \mathrm{g} = \mathrm{c}_{d,s}\delta_0$); V_{ext} is an external, confining potential

Question: What is the *effective* behavior of the system when N is very large and ε somehow varies with N?

To answer this question, we consider possible convergence as $N \to \infty$ of the *empirical measure*

$$f_N^t(x, v) := \frac{1}{N} \sum_{j=1}^{N} \delta_{(x_j^t, v_j^t)}(x, v). \tag{3.5}$$

Why do we care?

In theory, one can solve the system of ODEs (3.4) given initial data $(x_i^0, v_i^0)_{i=1}^N$.

But in practice, the number of particles N is very large (e.g. 10^{23}); computationally expensive or unfeasible to directly study N-body dynamics

Goal: Obtain a reduction in complexity by showing that *typical* solutions to the system (3.4) are "close" to a solution of a *nonlinear PDE* when $N \gg 1$: if $f_N^0 \xrightharpoonup[N\to\infty]{} f^0$, then

$$f_N^t \xrightharpoonup[N\to\infty]{} f^t, \qquad t > 0, \tag{3.6}$$

where f^t is a solution to a certain nonlinear PDE to be determined.

To have any hope of achieving this goal, we need to impose some assumptions on the relationship between ε and N.

Scaling choices

There are many scaling regimes of potential interest for the system (3.4), but let us consider the following scenario.

Suppose that each pairwise interaction $\nabla \mathrm{g}(x_i^t - x_j^t) = O(1)$. What is the size of the force term

$$\frac{1}{\varepsilon^2 N} \sum_{1 \leq j \leq N: j \neq i} \nabla \mathrm{g}(x_i^t - x_j^t)? \tag{3.7}$$

$\varepsilon \gg 1$ In the *subcritical* regime, force term formally vanishes as $N \to \infty$ and expect f to solve free transport equation

$\varepsilon \sim 1$ In the *critical* regime, called *mean-field*, the force term is $O(1)$ as $N \to \infty$ and expect f to solve *Vlasov equation*

$\varepsilon \ll 1$ In the *supercritical* regime, force term formally diverges as $N \to \infty$ and expect singular behavior; *a priori* unclear whether there is a limiting equation

Formal derivation of supercritical effective equation I

Suppose $\varepsilon > 0$ is fixed. Then a formal calculation shows that the empirical measure $f_N^t := \frac{1}{N}\sum_{i=1}^N \delta_{(x_i^t, v_i^t)}$ converges as $N \to \infty$ to a solution of Vlasov equation

$$\begin{cases} \partial_t f_\varepsilon + v \cdot \nabla_x f_\varepsilon - \frac{1}{\varepsilon^2}\nabla(V_{\text{ext}} + \mathrm{g} * \mu_\varepsilon) \cdot \nabla_v f_\varepsilon = 0, \\ \mu_\varepsilon = \int_{\mathbb{R}^d} df_\varepsilon(\cdot, v), \\ f_\varepsilon|_{t=0} = f_\varepsilon^0. \end{cases} \tag{3.8}$$

Suppose that $f_\varepsilon \to f$ and $\mu_\varepsilon \to \bar{\mu}$, where $\bar{\mu}$ minimizes the potential energy

$$\frac{1}{2}\int_{(\mathbb{R}^d)^2} \mathrm{g}(x-d)d\mu^{\otimes 2}(x,y) + \int_{\mathbb{R}^d} V_{ext}(x)d\mu(x) \tag{3.9}$$

(i.e., $\bar{\mu}$ is the equilibrium measure).

Formal derivation of supercritical effective equation II

Then writing

$$\varepsilon^{-2}\nabla(V_{\mathrm{ext}} + \mathrm{g} * \mu_\varepsilon) = \varepsilon^{-2}\nabla(V_{\mathrm{ext}} + \mathrm{g} * \bar{\mu}) + \varepsilon^{-2}\nabla \mathrm{g} * (\mu_\varepsilon - \bar{\mu}), \tag{3.10}$$

the first term vanishes on $\mathrm{supp}(\bar{\mu})$ since $\bar{\mu}$ is the minimizer. Now if $\varepsilon^{-2}\mathrm{g} * (\mu_\varepsilon - \bar{\mu}) \to p$, then f should satisfy

$$\begin{cases} \partial_t f + v \cdot \nabla_x f - \nabla p \cdot \nabla_v f = 0, \\ \bar{\mu} = \int_{\mathbb{R}^d} df(\cdot, v), \\ f|_{t=0} = f^0. \end{cases} \tag{3.11}$$

In the case where $\bar{\mu} \equiv 1$, (3.11) is known as the *kinetic incompressible Euler equation (KIE)* Brenier 1989

Introduce the *current* $J(x) := \int_{\mathbb{R}^d} v df(x, v)$. Since $\int_{\mathbb{R}^d} df(x, \cdot) = \bar{\mu}$ (i.e. constant in time), follows from KIE that $\operatorname{div} J = 0$. Through some calculus, one finds

$$\partial_t J + \operatorname{div} \int_{\mathbb{R}^d} v^{\otimes 2} df(\cdot, v) + \bar{\mu}\nabla p = 0. \tag{3.12}$$

Formal derivation of supercritical effective equation III

Making the monokinetic/cold ansatz $f(x, v) = \bar{\mu}(x)\delta(v - u(x))$, follows that $J = \bar{\mu}u$ and

$$\begin{cases} \partial_t u + u \cdot \nabla u = -\nabla p \\ \mathrm{div}(\bar{\mu}u) = 0. \end{cases} \tag{3.13}$$

(3.13) known as Lake/Anelastic equation and appears in modeling of atmospheric flows Ogura-Phillips 1962, Masmoudi 2007, superconductivity Chapman-Richards 1997, Duerinckx-Serfaty 2018, shallow water Levermore-Oliver-Titi 1996. “Pressure” p is a Lagrange multiplier:

$$-\mathrm{div}(\bar{\mu}\nabla p) = \mathrm{div}(\bar{\mu}u \cdot \nabla u). \tag{3.14}$$

- Nowhere above did we assume specific form of potential g
- Suggests that the Lake/KIE equations should be “universal” effective equation for empirical measure f_N^t in limit as $\varepsilon + N^{-1} \to 0$

Interpretations of the supercritical mean-field regime

Non-neutral plasmas

- System (3.4) describes evolution of trapped system of ions (e.g. Paul, Penning traps) Dubin-O'neil 1999; also applications to trapped systems of neutral atoms Wineland-Bollinger-Itano-Prestage 1985, Mendonca-Kaiser-Tercas-Loureiro 2008
- ε has interpretation of *Debye (screening) length* - scale below which charge separation in plasma occurs
- If $\varepsilon \ll 1$, Debye length is below length scale of an observer and plasma appears neutral; $\varepsilon \to 0$ is called quasineutral limit Brenier-Grenier 1994, Grenier 1995-1999, Brenier 2000, Masmoudi 2001, Barré-Chrion-Goudon-Masmoudi 2015, Han Kwan-Hauray 2015, Han Kwan-Rousset 2016, Han Kwan-Iacobelli 2017, Griffin Pickering-Iacobelli 2018-2020, Iacobelli 2021
- $\varepsilon + N^{-1} \to 0$ is then a combined mean-field and quasineutral limit

Hydrodynamic limit Rescale time and velocity by setting $(y_i^t, w_i^t) := (x_i^{\varepsilon t}, \varepsilon v_i^{\varepsilon t})$,

$$
\begin{cases} \dot{y}_i^t = w_i^t \\ \dot{w}_i^t = -\dfrac{1}{N} \displaystyle\sum_{1 \le j \le N : j \ne i} \nabla \mathsf{g}(y_i^t - y_j^t). \end{cases} \tag{3.15}
$$

What's known?

Mean-field

- Case where g is regular (e.g., ∇g is Lipschitz) is classical Neunzert-Wick 1974, Braun-Hepp 1977, Dobrushin 1979
- Convergence to Vlasov-Poisson known if $d = 1$ Trocheris 1982, Hauray 2014
- For $d \geq 2$, only partial results: $|\nabla g| \lesssim |x|^{-1+}$ Hauray-Jabin 2007-2015, regularized Coulomb g at small length scale vanishing as $N \to \infty$ Boers-Pickl 2016, Lazarovici 2016, Lazarovici-Pickl 2017, Graß 2021
- $d \geq 1$ monokinetic case $f^t(x, v) = \mu^t \delta(v - u^t(x))$ Duerinckx-Serfaty 2020, for which (μ^t, u^t) solve *pressureless Euler-Poisson system*

Supercritical mean-field Suppose the density of f_N^t is uniform as $N \to \infty$

- In analogy with quasineutral limit Grenier 1996-1999, Han Kwan-Hauray 2015, Han Kwan-Iacobelli 2016, supercritical MF limit should be false in general. Only work is by Griffin-Pickering-Iacobelli 2018 starting from a regularized version of (3.4).
- Monokinetic/cold electrons - Han Kwan-Iacobelli 2021,[4] R. 2021

[4] This work introduced in the terminology supercritical mean-field limit.

Returning to supercritical MF limit I

Let's return to question of limiting equation for $f_N^t := \frac{1}{N}\sum_{i=1}^N \delta_{z_i^t}$ as $\varepsilon + N^{-1} \to 0$, where $z_i^t := (x_i^t, v_i^t)$ solve

$$\begin{cases} \dot{x}_i = v_i \\ \dot{v}_i = -\dfrac{1}{\varepsilon^2 N} \displaystyle\sum_{1 \le j \le N : j \ne i} \nabla \mathrm{g}(x_i - x_j) - \dfrac{1}{\varepsilon^2} \nabla V_{\mathrm{ext}}(x_i). \end{cases} \tag{3.16}$$

Want to rigorously derive Lake equation

$$\begin{cases} \partial_t u + u \cdot \nabla u = -\nabla p \\ \mathrm{div}(\bar{\mu} u) = 0. \end{cases} \tag{3.17}$$

from system (3.16) under optimal assumptions on size of ε relative to N.

Second-order modulated energy

Introduce second-order modulated energy

$$H_{N,\varepsilon}(\underline{z}_N^t, u^t) := \frac{1}{N}\sum_{i=1}^N |v_i^t - u^t(x_i^t)|^2 + \frac{1}{\varepsilon^2} F_N(\underline{x}_N^t, \bar{\mu} + \varepsilon^2 \mathfrak{U}^t) + \frac{2}{\varepsilon^2 N}\sum_{i=1}^N \zeta(x_i^t). \tag{3.18}$$

- Here, u^t is an extension of the solution of Lake equation to all of $\mathbb{R}^d$ and $\mathfrak{U}^t$ is a certain "corrector" obtained from u^t. "Morally," $\mathfrak{U}^t = (-\Delta)^{\frac{d-s}{2}} p$
- Function $\zeta := \mathsf{g} * \bar{\mu} + V_{\mathrm{ext}} - c$, where c is the modified Robin constant. Uniquely characterizes minimizer $\bar{\mu}$.
- Functionals of form $H_{N,\varepsilon}$ with general μ^t (but without $\zeta, \mathfrak{U}^t$) introduced by Duerinckx-Serfaty 2020 in derivation of pressureless Euler-Poisson/Euler-Riesz
- Idea to add corrector $\mathfrak{U}^t$ originates in Han Kwan-Iacobelli 2021; motivation comes from earlier work of Brenier 2000 on quasineutral limit of Vlasov-Poisson
- Addition of ζ term new to trapped setting; motivated by work of Barré *et al.* 2015 on quasineutral limit of VP with confinement

Past work

On $\mathbb{T}^d$ and with $V_{\text{ext}} = 0$, $\bar{\mu} \equiv 1$, and g Coulomb Han Kwan-Iacobelli 2021 proved a Gronwall relation of form

$$|H_{N,\varepsilon}(\underline{z}_N^t, u^t)| \leq e^{-Ct}\Big(|H_{N,\varepsilon}(\underline{z}_N^0, u^0)| + \varepsilon^{-2} N^{-\frac{2}{d(d+1)}}\Big). \tag{3.19}$$

For “well-prepared” initial data, RHS vanishes provided error term vanishes as $\varepsilon + N^{-1} \to 0$.

Since $\bar{\mu} \equiv 1$, Lake equation is nothing but *incompressible Euler equation*! So their result provides a rigorous derivation of Euler's equation from Newton's second law in this scaling regime.

Using sharp $n = 1$ FI for Coulomb g, R. 2021 improved the error term to $\varepsilon^{-2} N^{-\frac{2}{d}}$; Argued that this is the optimal error size

New result

Theorem 2 (R.-Serfaty 2022)

Let $\underline{z}_N^t = (\underline{x}_N^t, \underline{v}_N^t)$ be a solution to Newtonian system. Let $\bar{\mu}$ be the equilibrium measure for

$$\frac{1}{2}\int_{(\mathbb{R}^d)^2} \mathrm{g}(x-d)d\mu^{\otimes 2}(x,y) + \int_{\mathbb{R}^d} V_{ext}(x)d\mu(x), \tag{3.20}$$

and suppose that on the interior of its support Σ, $\bar{\mu}$ is sufficiently regular. Let u be an extension from Σ° to $\mathbb{R}^d$ of a solution of the Lake equation, such that $u \in L^\infty([0,T], H^\sigma(\mathbb{R}^d))$ for $\sigma > \frac{d+2}{2}$. Then there exist continuous functions $C_1, \ldots, C_4 : [0,T] \to \mathbb{R}_+$, which depend on d, s, and norms of u, and an exponent $\beta \in (0,1)$, such that

$$\begin{aligned} \left| H_{N,\varepsilon}(\underline{z}_N^t, u^t) + \frac{\log N}{2dN\varepsilon^2}\mathbf{1}_{s=0} \right| \leq e^{C_1^t}\Big(H_{N,\varepsilon}(\underline{z}_N^0, u^0) + \frac{\log N}{2dN\varepsilon^2}\mathbf{1}_{s=0} \\ + \frac{C_2^t N^{\frac{s}{d}-1}}{\varepsilon^2} + C_3^t N^{-\beta} + C_4^t \varepsilon^2 \Big). \end{aligned} \tag{3.21}$$

Comments on theorem I

In particular, if

$$\lim_{\varepsilon+N^{-1}\to 0}\left(H_{N,\varepsilon}(\underline{z}_N^0,u^0)+\frac{\log N}{2dN\varepsilon^2}\mathbf{1}_{s=0}+\frac{N^{\frac{s}{d}-1}}{\varepsilon^2}\right)=0, \tag{3.22}$$

then

$$\forall t\in[0,T],\qquad f_N^t \xrightarrow[\varepsilon+N^{-1}\to 0]{} d\delta_{u^t(x)}(v)d\bar{\mu}(x) \tag{3.23}$$

in the weak-* topology for measures.

The error size $\varepsilon^{-2}N^{\frac{s}{d}-1}$ is optimal in the sense that there exists a solution $\underline{z}_N^t$ to Newtonian system (3.16) such that $f_N^t \rightharpoonup \bar{\mu}\delta(v-u^t(x))$, but $H_N(\underline{z}_N^t,u^t)$ does not vanish as $N\to\infty$.

- If $\underline{x}_N^0$ minimizes the microscopic energy $\sum_{i\neq j} g(x_i-x_j)+\sum_i V_{\text{ext}}(x_i)$, then $\underline{z}_N^t := (\underline{x}_N^0,0)$ is a stationary solution of (3.16)
- Since $\frac{1}{N}\sum_{i=1}^N \delta_{x_i^0} \rightharpoonup \bar{\mu}$, follows $f_N^t \rightharpoonup \bar{\mu}\delta(v)$, but
  (3.24)
  $$H_{N,\varepsilon}(\underline{z}_N^t,0)+\frac{\log N}{2dN\varepsilon^2}\mathbf{1}_{s=0}=\frac{1}{\varepsilon^2}\left(F_N(\underline{x}_N^0,\bar{\mu})+\frac{\log N}{2dN}\mathbf{1}_{s=0}\right)=C_{d,s,V_{ext}}\frac{N^{\frac{s}{d}-1}}{\varepsilon^2}$$

Comments on theorem II

- Proof is by a Gronwall argument for modulated energy $H_{N,\varepsilon}(\underline{z}_N^t, u^t)$
- Main ingredient is the sharp $n = 1$ FI for all super-Coulombic Riesz cases
- Need estimates for how fast $\zeta(x)$ and its derivatives grow as x detaches from the support of $\bar{\mu}$. For this, use connection between minimizers $\bar{\mu}$ of interaction energies and solutions of fractional obstacle problem Silvestre 2007, Caffarelli-Silvestre-Salsa 2008, regularity of the free boundary for the latter Jhaveri-Neumayer 2017.
- The corrector

$$\mathfrak{U}^t := (-\Delta)^{\frac{d-2-s}{2}} \operatorname{div}(\partial_t u + u \cdot \nabla u). \tag{3.25}$$

Needed to cancel out term of form

$$\frac{1}{N}\sum_{i=1}^{N}(v_i - u(x_i)) \cdot (\partial_t u(x_i) + u(x_i) \cdot \nabla u(x_i)) \tag{3.26}$$

appearing after computing time derivative of modulated energy.

Last words

Last words

- Didn't discuss sub-Coulombic case $0 \leq s < d - 2$. Have estimates for variations of modulated energies Q.H. Nguyen-R. Serfaty 2021, but a ways off from being sharp.
- These modulated energies have quantum analogues Golse-Paul 2020, R. 2021, which are useful for obtaining uniform-in-$\hbar$ rates of (supercritical) mean-field convergence for many-body Bose systems with Coulomb/Riesz interactions
- Would be interesting to develop a theory for energies with interactions beyond binary; seem very far away from that

The End

Thank you for your attention!