From Microscopic Klimontovich-Maxwell (KM) to Macroscopic Vlasov-Maxwell (VM)[1]

Relativistic N-particle electron bunches in modern particle accelerator systems, N large.

Jim Ellison and Klaus Heinemann

UNM

In collaboration with
Gabriele Bassi

Brookhaven National Laboratory

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Abstract-1

We consider an N-particle electron bunch moving, at nearly the speed of light, through a particle accelerator system inside a vacuum chamber. Typically, N is of an order greater than $\approx 10^9$ and the bunch is small relative to the vacuum chamber cross-section. We model the evolution of the bunch by a random initial boundary value problem (IBVP) with random, independent identically distributed (IID) initial conditions with a given density* and where the electron evolution is given in terms of the Lorentz force and the associated microscopic Maxwell fields. The electron phase space density is Klimontovich, i.e., a sum of delta functions. Taking expected value of the associated Klimontovich evolution equation (with respect to the random initial conditions) and making reasonable assumptions, we obtain the Vlasov equation with a correction term, for the expected value of the Klimontovich density, coupled to the macroscopic Maxwell equations. With this framework we then pose the important mathematical issues: (1) How well does the Vlasov density approximate a coarse-grained Klimontovich density when N is large? We imagine that the vast literature on probabilistic limit theorems will be relevant here, e.g. the Strong-Law of-Large-Numbers (SLLN). (2) The Vlasov equation without correction terms is the starting point for many beam dynamics calculations so it is important to estimate the size of the correction term (surely related to the correction term in the BBGKY hierarchy). In addition the correction term may shed light on FEL dynamics. These mathematical issues are likely difficult analysis issues. We begin the talk with the much simpler non-collective case, assuming the electrons do not radiate and thus ignoring the Maxwell self-fields, in order to set the stage for the more complex KM $\rightarrow$ VM case.

Abstract-2

*In a physical context the N initial conditions are impossible to know. One view is to think of them as a set of scattered data from which a density can be constructed using e.g., a density estimation procedure from Mathematical Statistics. The IID random ICs are then given in terms of such a density. In our work here we simply consider the initial density as given.

Outline

Micro Klimontovich-Maxwell (KM) $\to$ Macro Vlasov-Maxwell (VM)

1. $6N$-Dimensional KM as random IBVP (ICs from scattered data (SD)) and associated 6D VM "standard" IBVP
2. Simple case: Assume electrons don't radiate, thus ignore Maxwell self-fields and thus electrons don't interact
   - Random Klimontovich density with $6N$ parameters $\to$ $6D$-Liouville density (coarse grained) approximation
3. Formulate KM to eliminate a singularity
4. Derive evolution law for Klimontovich density in KM system
5. Derive evolution law for expected value of random KM system. This leads to the VM system with a correction term (CT).
6. Open mathematical issues
   - VM with CT as a coarse-grained approximation to KM. Relevance of probabilistic limit theorems?
   - Estimates of CT. The CT must be related to the CT in the BBGKY hierarchy and may be relevant to FEL dynamics

Goal today: Relate microscopic Klimontovich-Maxwell (KM) to macroscopic Vlasov-Maxwell (VM)

First: Microscopic N-particle Klimontovich-Maxwell (KM)

The coupled KM system for $i = 1, \ldots, N$ is:

$$\dot{\mathbf{R}}_i = \mathbf{v}(\mathbf{P}_i), \quad \dot{\mathbf{P}}_i = q\big[\mathbf{E}_T(\mathbf{R}_i, t) + \mathbf{v}(\mathbf{P}_i) \times \mathbf{B}_T(\mathbf{R}_i, t)\big],$$

$$\mathbf{R}_i(0), \mathbf{P}_i(0) \text{ given}$$

$$\mathbf{E}_T = \mathbf{E} + \mathbf{E}_{ext}, \quad \mathbf{B}_T = \mathbf{B} + \mathbf{B}_{ext}, \quad \mathbf{v}(\mathbf{P}) = \mathbf{P}/m\gamma(\mathbf{P})$$

$$\partial_t \mathbf{B} = -\nabla \times \mathbf{E}, \quad \partial_t \mathbf{E} = c^2 \nabla \times \mathbf{B} - cZ_0 \mathbf{J}^K(\mathbf{R}, t),$$

$$\mathbf{J}^K(\mathbf{R}, t) = \sum_{n=1}^{N} q\mathbf{v}(\mathbf{P}_n(t))\delta(\mathbf{R} - \mathbf{R}_n(t))$$

Primary interest: 6D Klimontovich phase space density

$$f^K(\mathbf{R}, \mathbf{P}, t) = \frac{1}{N} \sum_{n=1}^{N} \delta(\mathbf{R} - \mathbf{R}_n(t))\delta(\mathbf{P} - \mathbf{P}_n(t))$$

ODEs do not make sense since fields are infinite at particles, we revise later

Second: Macroscopic Vlasov-Maxwell (VM)

The coupled VM system for $f^V(\mathbf{R},\mathbf{P},t),\mathbf{E}(\mathbf{R},t)),\mathbf{B}(\mathbf{R},t)$ is

$$\{\partial_t + \mathbf{v}(\mathbf{P})\cdot\nabla_{\mathbf{R}} + q[\mathbf{E}_T(\mathbf{R},t) + \mathbf{v}(\mathbf{P})\times(\mathbf{B}_T(\mathbf{R},t)]\cdot\nabla_{\mathbf{P}}\}f^V = 0$$

$f^V(\mathbf{R},\mathbf{P},0)$ smooth

$$\mathbf{E}_T = \mathbf{E} + \mathbf{E}_{ext},\ \ \mathbf{B}_T = \mathbf{B} + \mathbf{B}_{ext},\ \ \mathbf{v}(\mathbf{P}) = \mathbf{P}/m\gamma(\mathbf{P})$$

$$\partial_t\mathbf{B} = -\nabla\times\mathbf{E},\ \ \partial_t\mathbf{E} = c^2\nabla\times\mathbf{B} - cZ_0\mathbf{J}^V(\mathbf{R},t)$$

$$\mathbf{J}^V(\mathbf{R},t) = Nq\int_{\mathbb{R}^3} d\mathbf{P}\mathbf{v}(\mathbf{P})f^V(\mathbf{R},\mathbf{P},t),$$

Goal: Relate the Klimontovich and Vlasov phase space densities

Note: $\int_A f^{K,V}$ = fraction of electron bunch in A

Remark on Newton vs. Einstein

$$\mathbf{F} = m\mathbf{a} = \frac{d}{dt} m\mathbf{v} \rightarrow \mathbf{F} = \frac{d}{dt} m\gamma\mathbf{v},\ \gamma = (1 - \frac{v^2}{c^2})^{-1/2}, \text{thus } |\mathbf{v}| < c$$

Consider single particle dynamics where self fields $\mathbf{E}, \mathbf{B}$ are zero
Uncoupled EOM for the N-electrons are

$$\dot{\mathbf{R}}_i = \mathbf{v}(\mathbf{P}_i),$$
$$\dot{\mathbf{P}}_i = q\left[\mathbf{E}_{ext}(\mathbf{R}_i, t) + \mathbf{v}(\mathbf{P}_i) \times \mathbf{B}_{ext}(\mathbf{R}_i, t)\right] =: \mathbf{F}(\mathbf{R}_i, \mathbf{P}_i, t),$$
$$\mathbf{v}(\mathbf{P}) = \mathbf{P}/m\gamma(\mathbf{P}),\ \ \gamma^2 = 1 + \frac{\mathbf{P}\cdot\mathbf{P}}{m^2c^2}$$

$\mathbf{F} = q(\mathbf{E}_{ext} + \mathbf{v} \times \mathbf{B}_{ext})$ is called the Lorentz force
More compactly we write

$$\dot{\mathbf{u}}_i = \mathbf{G}(\mathbf{u}_i, t),\ \ \nabla_{\mathbf{u}}\mathbf{G}(\mathbf{u}, t) = 0,\ \ \mathbf{u}_i = (\mathbf{R}_i, \mathbf{P}_i)^T,\ \ \mathbf{G} = (\mathbf{v}, \mathbf{F})^T$$

Non-collective case II

General Solution

Consider the IVP with general solution φ,

$$\dot{\mathbf{u}} = \mathbf{G}(\mathbf{u}, t), \;\; \mathbf{u}(t_0) = \mathbf{u}_0,$$
$$\mathbf{u}(t) = \varphi(t, t_0, \mathbf{u}_0), \;\; \varphi(t_0, t_0, \mathbf{u}_0) = \mathbf{u}_0$$

1. Divergence free $\implies$ measure preserving flow.
2. The system can be transformed into a Hamiltonian system.
3. General Solution satisfies (No-Name in standard ODE books)

$$\varphi(t_2, t_0, \mathbf{u}_0) = \varphi(t_2, t_1, \varphi(t_1, t_0, \mathbf{u}_0))$$

It is a Markov Property: Future depends on the past only through the present. Some call it a co-cycle condition.

Main quantity: N-particle phase space (Klimontovich) density

$$\psi_N(\mathbf{u},t) := \frac{1}{N}\sum_{n=1}^{N}\delta(\mathbf{u}-\varphi(t,t_0,\mathbf{u}_{0n})),$$

Differentiating gives

$$\partial_t\psi_N(\mathbf{u},t) := -\frac{1}{N}\sum_{n=1}^{N}D\delta(\mathbf{u}-\varphi(t,t_0,\mathbf{u}_{0n}))\mathbf{G}(\varphi(t,t_0,\mathbf{u}_{0n}),t),$$

$$= -\frac{1}{N}\sum_{n=1}^{N}D\delta(\mathbf{u}-\varphi(t,t_0,\mathbf{u}_{0n}))\mathbf{G}(\mathbf{u},t)$$

Thus ψ_N is the unique solution of the IVP

$$\partial_t\psi_N + \mathbf{G}(\mathbf{u},t)\cdot\nabla_{\mathbf{u}}\psi_N = 0,$$
$$\psi_N(\mathbf{u},t_0) = \tfrac{1}{N}\textstyle\sum_{n=1}^{N}\delta(\mathbf{u}-\mathbf{u}_{0n}),$$

Physical issue on ICs: How to view the ICs? My current view: $\{\mathbf{u}_{0n}\}_1^N$ is a given set of "scattered data" from which a density can be constructed via density estimation from Statistics. I then consider the Random IVP where the $\{\mathbf{u}_{0n}\}_1^N$ are replaced by IID RVs $\{\mathbf{U}_n\}_1^N$ from the constructed density. But, is this the right physics?

Let $\{\mathbf{U}_n\}_1^N$ be a sequence of IID random vectors with density $\psi_0(\mathbf{u})$, i.e., $Prob(\mathbf{U}_n \in A) = \int_A \psi_0(\mathbf{u}) d\mathbf{u}$ then

$$E\psi_N(\mathbf{u}, t; \mathbf{U}_1, \ldots, \mathbf{U}_N) = \psi_0(\varphi(t_0, t, \mathbf{u})).$$

SLLN Conjecture: $\psi_N(\mathbf{u}, t) \to \psi_0(\varphi(t_0, t, \mathbf{u}))$ a.s. in coarse grain sense, i.e. $\int_A d\mathbf{u}\psi_N(\mathbf{u}, t) \to \int_A d\mathbf{u}\psi_0(\varphi(t_0, t, \mathbf{u}))$ for rich class of sets A

Fact: $\psi(\mathbf{u}, t) = \psi_0(\varphi(t_0, t, \mathbf{u}))$ is the unique solution of the IVP for the $6D$ Liouville equation:

$$\mathcal{L}\psi = \partial_t \psi + \mathbf{G}(\mathbf{u}, t) \cdot \nabla_{\mathbf{u}} \psi = 0,$$
$$\psi(\mathbf{u}, t_0) = \psi_0(\mathbf{u}).$$

Summary of Non-collective case

The microscopic evolution of the N-particle electron bunch is governed by the Klimontovich IVP

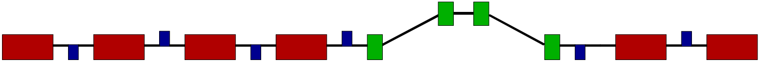
$$\mathcal{L}\psi = \partial_t \psi_N + \mathbf{G}(\mathbf{u}, t) \cdot \nabla_{\mathbf{u}} \psi_N = 0,$$
$$\psi_N(\mathbf{u}, t_0) = \frac{1}{N} \sum_{n=1}^{N} \delta(\mathbf{u} - \mathbf{U}_n),$$

The macroscopic evolution of the (smooth) electron bunch is governed by Liouville IVP

$$\mathcal{L}\psi^L = \partial_t \psi^L + \mathbf{G}(\mathbf{u}, t) \cdot \nabla_{\mathbf{u}} \psi^L = 0,$$
$$\psi(\mathbf{u}, t_0) = \psi_0(\mathbf{u}).$$

Remark: This is a **Huge** simplification (going from $6N$ to 6 dimensions) assuming the coarse graining and Strong-Law-of-Large-Numbers (SLLN) can be justified.

In a typical situation $\mathbf{E}_{ext} = 0$ and $\mathbf{B}_{ext} = \mathbf{B}(\mathbf{R})$ is determined by dipole and quadrupole magnets.



Proposed layout of FERMI@Elettra first bunch compressor system. Accelerating rf cavities in red, quadrupole magnets in blue, drift sections in black and dipoles in green.

The coupled macro VM system for $f^V(\mathbf{R},\mathbf{P},t),\mathbf{E}(\mathbf{R},t),\mathbf{B}(\mathbf{R},t)$ is

$$\{\partial_t + \mathbf{v}(\mathbf{P})\cdot\nabla_{\mathbf{R}} + q[\mathbf{E}_T(\mathbf{R},t) + \mathbf{v}(\mathbf{P})\times(\mathbf{B}_T(\mathbf{R},t)]\cdot\nabla_{\mathbf{P}}\}f^V = 0$$

$$\mathbf{E}_T = \mathbf{E} + \mathbf{E}_{ext}, \quad \mathbf{B}_T = \mathbf{B} + \mathbf{B}_{ext}$$

$$\partial_t\mathbf{B} = -\nabla\times\mathbf{E}, \quad \partial_t\mathbf{E} = c^2\nabla\times\mathbf{B} - cZ_0\mathbf{J}(\mathbf{R},t)$$

$$\mathbf{J}^V(\mathbf{R},t) = Q\int_{\mathbb{R}^3} d\mathbf{P}\mathbf{v}(\mathbf{P})f^V(\mathbf{R},\mathbf{P},t), \quad f^V(\mathbf{R},\mathbf{P},0)\text{ smooth}$$

The coupled micro KM system for $f^K(\mathbf{R},\mathbf{P},t),\mathbf{E}(\mathbf{R},t)),\mathbf{B}(\mathbf{R},t)$ is

$$f^K(\mathbf{R},\mathbf{P},t) = \frac{1}{N}\sum_{n=1}^{N}\delta(\mathbf{R}-\mathbf{R}_n(t))\delta(\mathbf{P}-\mathbf{P}_n(t))$$

$$\dot{\mathbf{R}}_i = \mathbf{v}(\mathbf{P}_i), \quad \dot{\mathbf{P}}_i = q\left[\mathbf{E}_T(\mathbf{R}_i,t) + \mathbf{v}(\mathbf{P}_i)\times\mathbf{B}_T(\mathbf{R}_i,t)\right],$$

$$\partial_t\mathbf{B} = -\nabla\times\mathbf{E}, \quad \partial_t\mathbf{E} = c^2\nabla\times\mathbf{B} - cZ_0\mathbf{J}^K(\mathbf{R},t),$$

$$\mathbf{J}^K(\mathbf{R},t) = \sum_{n=1}^{N} q\mathbf{v}(\mathbf{P}_n(t))\delta(\mathbf{R}-\mathbf{R}_n(t)), \quad \mathbf{R}_i(0),\mathbf{P}_i(0)\text{ Random IID}$$

But the KM system has singularities. To remove the infinities we rewrite as follows for $i = 1, \ldots, N$:

$$f^K(\mathbf{R}, \mathbf{P}, t) = \frac{1}{N} \sum_{n=1}^{N} \delta(\mathbf{R} - \mathbf{R}_n(t))\delta(\mathbf{P} - \mathbf{P}_n(t))$$

$$\dot{\mathbf{R}}_i = \mathbf{v}(\mathbf{P}_i) \quad \dot{\mathbf{P}}_i = q\left[\mathbf{E}_{Ti}(\mathbf{R}_i, t) + \mathbf{v}(\mathbf{P}_i) \times \mathbf{B}_{Ti}(\mathbf{R}_i, t)\right] =: \mathbf{F}_i(\mathbf{R}_i, \mathbf{P}_i, t)$$

$$\partial_t \mathbf{B}_i = -\nabla \times \mathbf{E}_i, \quad \partial_t \mathbf{E}_i = c^2 \nabla \times \mathbf{B}_i - cZ_0 \mathbf{J}_i^K(\mathbf{R}, t),$$

$$\mathbf{J}_i^K(\mathbf{R}, t) = \sum_{\substack{n=1 \\ n \neq i}}^{N} q\mathbf{v}(\mathbf{P}_n(t))\delta(\mathbf{R} - \mathbf{R}_n(t)), \quad (\mathbf{R}_i(0), \mathbf{P}_i(0)) \text{ Random ICs}$$

Note: $\mathbf{E}_i(\mathbf{R}_i, t)$ is not singular even though $\mathbf{E}_i(\mathbf{R}_n, t)$ is for $n \neq i$ (same for $\mathbf{B}_i$). Thus the ODEs are well defined, assuming no two particles occupy the same position.

$$f^K(\mathbf{R},\mathbf{P},t)=\frac{1}{N}\sum_{n=1}^{N}\delta(\mathbf{R}-\mathbf{R}_n(t))\delta(\mathbf{P}-\mathbf{P}_n(t))$$

We emphasize that f^K is random through the electron ICs, i.e.,

$$f^K(\mathbf{R},\mathbf{P},t)=f^K(\mathbf{R},\mathbf{P},t;\Theta) \text{ where}$$
$$\Theta=(\mathbf{R}_1(0),\mathbf{P}_1(0),\ldots,\mathbf{R}_N(0),\mathbf{P}_N(0))$$

$$\partial_t f^K(\mathbf{R},\mathbf{P},t)=-\frac{1}{N}\sum_{n=1}^{N}D\delta(\mathbf{R}-\mathbf{R}_n(t))\mathbf{v}(\mathbf{P}_n(t))\delta(\mathbf{P}-\mathbf{P}_n(t))$$
$$+\delta(\mathbf{R}-\mathbf{R}_n(t))D\delta(\mathbf{P}-\mathbf{P}_n(t)\mathbf{F}_n(\mathbf{R}_n(t),\mathbf{P}_n(t),t)$$
$$=-\frac{1}{N}\sum_{n=1}^{N}D\delta(\mathbf{R}-\mathbf{R}_n(t))\delta(\mathbf{P}-\mathbf{P}_n(t))\mathbf{v}(\mathbf{P})$$
$$+\delta(\mathbf{R}-\mathbf{R}_n(t))D\delta(\mathbf{P}-\mathbf{P}_n(t))\mathbf{F}_n(\mathbf{R},\mathbf{P},t)$$

Convention: For $f:\mathbb{R}^n\to\mathbb{R}^m$, $Df:=[\partial_1 f,\ldots,\partial_n f]=[m\times n]$

Taking Expected Value with Respect to ICs - 1

Taking expected value we obtain

$$\partial_t \bar{f}^K(\mathbf{R},\mathbf{P},t) = -D_{\mathbf{R}}\bar{f}^K(\mathbf{R},\mathbf{P},t)\mathbf{v}(\mathbf{P})$$
$$-\frac{1}{N}\sum_{n=1}^{N} \overline{\delta(\mathbf{R}-\mathbf{R}_n(t))D\delta(\mathbf{P}-\mathbf{P}_n(t))}\ \ \overline{\mathbf{F}_n(\mathbf{R},\mathbf{P},t)}$$
$$+\text{Correction Term}.$$

Here Correction Term $= -\frac{1}{N}\sum_{n=1}^{N} \overline{a_n b_n} - \overline{a_n}\,\overline{b_n}$

Thus we need to analyze

$$\overline{\mathbf{F}_n(\mathbf{R},\mathbf{P},t)} = q[\overline{\mathbf{E}_{Tn}(\mathbf{R},t)} + \mathbf{v}(\mathbf{P}) \times \overline{\mathbf{B}_{Tn}(\mathbf{R},t)}].$$

Note: Bar and overline denote expected value with respect to the ICs. The traditional use of E is cumbersome and conflicts with electric field.

Expected value of the microscopic Maxwell equations yields

$$\partial_t \bar{\mathbf{B}}_i = -\nabla \times \bar{\mathbf{E}}_i, \;\; \partial_t \bar{\mathbf{E}}_i = c^2 \nabla \times \bar{\mathbf{B}}_i - cZ_0 \overline{\mathbf{J}_i^K(\mathbf{R},t)},$$

Now

$$\mathbf{J}^K(\mathbf{R},t) = \sum_{n=1}^{N} q\mathbf{v}(\mathbf{P}_n(t)\delta(\mathbf{R}-\mathbf{R}_n(t)) = Nq\int_{\mathbb{R}^3} d\mathbf{P}\mathbf{v}(\mathbf{P}) f^K(\mathbf{R},\mathbf{P},t)$$

and it follows that

$$\overline{\mathbf{J}_i^K(\mathbf{R},t)} = \overline{\mathbf{J}^K(\mathbf{R},t)} - q\overline{\mathbf{v}(\mathbf{P}_i(t))\delta(\mathbf{R}-\mathbf{R}_i(t))} \approx \overline{\mathbf{J}^K(\mathbf{R},t)}$$

for large N, and we obtain $\bar{\mathbf{B}}_i \approx \mathbf{B}, \bar{\mathbf{E}}_i \approx \mathbf{E}$ where

$$\partial_t \mathbf{B} = -\nabla \times \mathbf{E}, \;\; \partial_t \mathbf{E} = c^2 \nabla \times \mathbf{B} - cZ_0 \overline{\mathbf{J}^K(\mathbf{R},t)}$$

$$\overline{\mathbf{J}^K(\mathbf{R},t)} = qN\int_{\mathbb{R}^3} d\mathbf{P}\mathbf{v}(\mathbf{P})\bar{f}^K(\mathbf{R},\mathbf{P},t)$$

Thus

$$\overline{\mathbf{F}_n(\mathbf{R},\mathbf{P},t)} = q[\overline{\mathbf{E}_{Tn}(\mathbf{R},t)} + \mathbf{v}(\mathbf{P}) \times \overline{\mathbf{B}_{Tn}(\mathbf{R},t)}]$$

$$\approx q[\overline{\mathbf{E}_T(\mathbf{R},t)} + \mathbf{v}(\mathbf{P}) \times \overline{\mathbf{B}_T(\mathbf{R},t)}] =: \mathbf{F}(\mathbf{R},\mathbf{P},t)$$

Recalling

$$\partial_t \bar{f}(\mathbf{R},\mathbf{P},t) = -D_{\mathbf{R}}\bar{f}(\mathbf{R},\mathbf{P},t)\mathbf{v}(\mathbf{P})$$

$$-\frac{1}{N}\sum_{n=1}^{N} \overline{\delta(\mathbf{R}-\mathbf{R}_n(t))D\delta(\mathbf{P}-\mathbf{P}_n(t))} \quad \overline{\mathbf{F}_n(\mathbf{R},\mathbf{P},t)}$$

$$+\text{Correction Term} \equiv \text{CT}.$$

we obtain the approximation

$$\partial_t \bar{f}(\mathbf{R},\mathbf{P},t) = -D_{\mathbf{R}}\bar{f}(\mathbf{R},\mathbf{P},t)\mathbf{v}(\mathbf{P}) - D_{\mathbf{P}}\bar{f}(\mathbf{R},\mathbf{P},t)\mathbf{F}(\mathbf{R},\mathbf{P},t)) + \text{CT}$$

which can be rewritten

$$[\partial_t + \nabla_{\mathbf{R}} \cdot \mathbf{v}(\mathbf{P}) + \nabla_{\mathbf{P}} \cdot \mathbf{F}(\mathbf{R},\mathbf{P},t)]\bar{f}(\mathbf{R},\mathbf{P},t) = \text{CT}$$

For CT$=0$ We Have The Vlasov Equation

Summary and Mathematical issues

Approximation via probabilistic limit theorems? When is CT small?

1. We have formulated the N-particle electron dynamics with self-fields in term of the N-particle KM random IBVP. The randomness enters via density estimation from scattered data representing the initial electron positions.
2. We have taken expected value of the microscopic KM IBVP and shown that it leads, in reasonable approximation, to the macroscopic VM +CT. Is CT related to FEL dynamics?
3. Open mathematical issues
   - How well does VM with CT approximate the coarse-grained KM? Relevance of vast literature on probabilistic limit theorems? A generalized SLLN? Recall the simple non-collective case where this is likely straight forward.
   - Good estimates of CT are likely difficult. E.g., the CT must be related to the CT in the BBGKY hierarchy. Note there is no CT in the non-collective case going from Klimontovich to Liouville.