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

Kinetic theory based on the random initial value problem and coarse graining

Jim Ellison

Department of Math&Stat, UNM

In collaboration with

Gabriele Bassi BNL and Klaus Heinemann UNM

December 5, 2016

Applied Math Seminar Presentation

[1] Partial support from DOE:DE -FG02-99ER41104

Outline

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

1. Relation of $6N$-Dimensional KM as random IVP to associated 6-Dimensional VM IVP for N large
2. General Framework: N particle motion with random IID initial conditions, associated PDF and random Klimontovich density (KD), coarse grained KD, large N statistics, BBGKY
3. Four examples of evolution laws with random initial conditions
    - Non-interacting particle case (Non-collective)
    - Two particle interaction force
    - Simple relativistic KM system
    - $6N$-Dimensional KM
4. Main two questions
    - How well does the coarse grained mean of KD approximate the the coarse grained KD?
    - Kinetic theory: Find a good approximate evolution law for the mean of the KD

6D microscopic Klimontovich-Maxwell (KM) System

Goal today: Framework for KM $\rightarrow$ VM

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

The coupled KM system for $i = 1, \ldots, N$ is [2]

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

$$W_{0i} = (\mathbf{R}_i(0), \mathbf{P}_i(0)) \text{ as IID random vectors}$$

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

$$\partial_t \mathbf{B} = -\nabla \times \mathbf{E}, \quad \partial_t \mathbf{E} = c^2 \nabla \times \mathbf{B} - cZ_0 \mathbf{J}^K(\mathbf{R}, t; W_0),$$

$$\mathbf{J}^K(\mathbf{R}, t; W_0) = \sum_{n=1}^{N} q\mathbf{v}(\mathbf{P}_n(t; W_0))\delta(\mathbf{R} - \mathbf{R}_n(t; W_0))$$

Primary interest: Random 6D Klimontovich phase space density

$$K(\mathbf{R}, \mathbf{P}, t; W_0) = \frac{1}{N} \sum_{n=1}^{N} \delta(\mathbf{R} - \mathbf{R}_n(t; W_0))\delta(\mathbf{P} - \mathbf{P}_n(t; W_0))$$

[2] Needs slight revision as fields are infinite at particles

6D macroscopic Vlasov-Maxwell system

Goal today: Framework for KM $\rightarrow$ VM

Second: Macroscopic Vlasov-Maxwell (VM)

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

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

$$f(\mathbf{R}, \mathbf{P}, 0) = f_0(\mathbf{R}, \mathbf{P}) \text{ smooth}$$

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

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

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

Goal: Relate Klimontovich and Vlasov phase space densities, K, f

Let $\bar{K}$ be expected value of K, and $K_A(t; W_0) = \int_A dv K(v, t; W_0)$

Issue 1: How close are K_A and $\bar{K}_A$ for large N?

Issue 2: How close are $\bar{K}_A$ and f for large N?

General Framework- I

Particle motion and probability distribution

1. N electron evolution in d-dimensional phase space

$$w_i(t; W_0) \in \mathbb{R}^d; \ i = 1, N; \ t \geq 0; \ \ w_i(0; W_0) = W_{0i},$$
$$W_0 = (W_{01}, \cdots, W_{0iN})^T, \ \{W_{0i}\} \text{ IID RVs with PDF } \psi_0$$
$$W(t; W_0) = [w_1(t; W_0), \cdots, w_N(t; W_0)]^T \in \mathbb{R}^{Nd}$$

2. $\Psi(w, t)$ denotes joint PDF of the $w_i(t, W_0)$. It is assumed to have permutation symmetry (PS), i.e., $\Psi(\cdots, w_i, \cdots, w_j, \cdots, t) = \Psi(\cdots, w_j, \cdots, w_i, \cdots, t) \Rightarrow$ marginal PDFs, $\Psi_s(w_{i_1}, \cdots, w_{i_s}, t)$, of any s-particles are equal, thus Ψ_s given by integrating out any $N - s$ variables from Ψ.

General Framework- II

The random Klimontovich density (KD)

1. Random Klimontovich density (KD)

$$K(v,t;W_0) = \frac{1}{N}\sum_1^N \delta(v - w_i(t;W_0)),$$

$$K_A(t,W_0) = \int_A dvK(v,t;W_0) = \frac{1}{N}\cdot \#\text{ particles in } A$$

2. Moments of KRD in terms of PDF Ψ

$$\bar{K}(v,t) := \overline{K(v,t;W_0)} = \Psi_1(v,t)$$

$$\bar{K}_A(t) := \overline{K_A(t;W_0)} = \int_A dv\Psi_1(v,t)$$

Thus the expected value of K is the probability density of $w_i(t;W_0)$ and the expected value of K_A is the probability that $w_i(t;W_0) \in A$

General Framework- IIA

Remarks on Klimontovich density

1. $\delta(v - w_i(t; W_0))$ has three possible interpretations: (1) standard physics, (2) delta sequences, (3) generalized functions. But in (2) what would be the sequence for the electron as a point source? Here we use (1). K. Heinemann is working on (3).
2. Using interpretation (1) : $\overline{\delta(v - w_i(t; W_0))} = \int dw_0 \Psi_0(w_0)\delta(v - w_i(t; w_0)) = \int dw \Psi(w, t)\delta(v - w_i) = \int dw_i \Psi_1(w_i, t)\delta(v - w_i) = \Psi_1(v, t)$.
   This justifies the formula $\bar{K}(v, t) = \Psi_1(v, t)$ on the previous slide.
3. For a special A, $K_A(t, W_0)$ is the so-called empirical distribution function. The related Glivenko-Cantelli theorem applies in the IID case.

General Framework- III

Basic Issues for KRD: coarse grained K and evolution law for K

Issue 1 How close are spiky K and smooth $\bar{K}$? [3] We compare K_A and $\bar{K}_A$ and call K_A a coarse grained version of K. [4]

Issue 2 Given an evolution law for K, what is the evolution law for $\bar{K}$? Once an evolution law for the w_i is defined, an evolution law for K follows. We explore three examples with increasing complexity below. The last example raises the main issues of importance for the 6D KM system mentioned above which is our main interest.

[3] K is an empirical density and $\bar{K} = \Psi_1$ is a probability density, so we are comparing densities.

[4] There is a similarity to Glivenko-Cantelli in IID case

General Framework IV

Coarse Graining leads to a sum of Bernoulli RVs

We show K_A is a sum of (L^2) Bernoulli RVs.

1. $K(v,t;W_0) = \frac{1}{N}\sum_1^N \delta(v - w_i(t;W_0))$ and integrating over A gives $K_A(t;W_0) = \frac{1}{N}\sum_1^N X_i(t)$ where $X_i(t) = 1_A(w_i(t;W_0))$ Ready for probabilistic analysis of large sum of RVs
2. The $X_i(t)$ are Bernoulli RVs with $\Pr\{X_i(t)=1\} = \int_A dv\Psi_1(v,t) =: p(t)$ thus $\overline{X_i(t)} = p(t)^5$, $\mathrm{Var}X_i(t) = p(t)(1-p(t))$
3. X_iX_j is also a Bernoulli RV. Here $\Pr\{X_iX_j = 1\} = \Pr\{X_i \in A \,\&\, X_j \in A\} = \int_{A\times A} dvdv'\Psi_2(v,v',t) \Rightarrow$ $\overline{X_iX_j} = \int_{A\times A} dvdv'\Psi_2(v,v',t) \Rightarrow$ $\mathrm{Cov}(X_iX_j) = \int_{A\times A} dvdv'(\Psi_2(v,v',t) - \Psi_1(v,t)\Psi_1(v',t))$ Recall Ψ_2 is the joint PDF of $w_i(t;W_0)$ and $w_j(t;W_0)$ for any $i \neq j$.

[5] Expected value is a probability in analogy with $\bar{K}_A(t) = \int_A dv\Psi_1(v,t)$

General Framework V

Moments of K_A and Weak Law

The variance of K_A is the square of the L^2 difference of K_A and $\bar{K}_A$

1. $K_A(t; W_0) = \frac{1}{N}\sum_1^N X_i(t) \Rightarrow \bar{K}_A(t) = \overline{X_i} = p(t) \Rightarrow$
   $\text{Var}\, K_A(t; W_0) = \frac{1}{N}p(t)(1-p(t)) + \frac{N(N-1)}{N^2}\text{Cov}\,(X_1, X_2)$ [6]
2. Issue 1: Thus $K_A \approx \bar{K}_A$ in the L^2 sense for N large if $\text{Cov}(X_1, X_2)$ is small, i.e., if $\Psi_2(v, v', t) \approx \Psi_1(v, t)\Psi_1(v', t))$. So Issue 1 reduces to a study of Ψ_2 for large N and its behavior in t. Surely Ψ depends on N in a complicated way and likely some mixing/chaotic behavior of the w_i will be needed .
3. Issue 2: Given that $K_A \approx \bar{K}_A$, it then becomes important to study $\bar{K}$. This is discussed in the following examples.

[6] $\text{Var}\,(X_1 + \cdots + X_N) = N\,\text{Var}\, X_1 + N(N-1)\text{Cov}(X_1, X_2)$ which are given in terms of Ψ_1 and Ψ_2

Example 1 (Non-interacting particles) - 1

Particle evolution law for the w_i

The non-interacting particle motions w_i are defined by

$$\dot{w}_i = G(w_i, t), \quad w_i(0; W_0) = W_{0i} \text{ IID random ICs}$$

The ODEs and ICs are uncoupled hence the $w_i(t; W_0)$ are IID random vectors.

• Without self fields the 6D Klimontovich-Maxwell system reduces to these uncoupled EOM for the N-electrons.

Example 1 (Non-interacting particles) - 2

Probabilistic Limit Theorems and Issue 1

The $X_i(t) = 1_A(w_i(t; W_0))$ are IID Bernoulli RVs with $p(t) = \int_A dv \Psi_1(v,t)$, thus:

- LLNs: $K_A(t; W_0) \to p(t)$ in probability, in L^2 and a.s., as $N \to \infty$.
- CLT: $K_A(t, W_0) \approx p(t) + (\frac{p(t)-p(t)^2}{N})^{1/2}\chi$ in the sense of convergence in distribution. χ is a normal $(0,1)$ random variable.
- LD: Large Deviation bounds for $\delta \in [0,1]$[7] :
  $\Pr\{K_A(t; W_0) \geq (1+\delta)p(t)\} \leq \exp(-N\delta^2 p(t)/3)$ and
  $\Pr\{K_A(t; W_0) \leq (1-\delta)p(t)\} \leq \exp(-N\delta^2 p(t)/2)$
  The bounds are small if $N\delta^2$ is large.
- GC: Glivenko-Cantelli applies here

Thus we have a complete answer to Issue 1

[7] From http://cs.brown.edu/courses/cs155/slides/Chapter-4.pdf

Example 1 (Non-interacting particles) - 3

Klimontovich density evolution law and Issue 2

The Klimontovich random density satisfies

$$\partial_t K + \nabla_v \cdot G(v,t)K = 0,$$
$$K(v,0) = \frac{1}{N}\sum_{i=1}^{N} \delta(v - W_{0i}),$$

and taking expected value we obtain

$$\partial_t \bar{K} + \nabla_v \cdot G(v,t)\bar{K} = 0,$$
$$\bar{K}(v,0) = \frac{1}{N}\overline{\sum_{i=1}^{N} \delta(v - W_{0i})} = \psi_0(v)$$

Thus the equations for K and $\bar{K} \equiv \Psi_1$ are the same, the evolutions differ only because of the initial data. The equation for $\bar{K}$ is called the Kinetic Equation.

Thus we have a complete answer to Issue 2.

We have not seen these results for single particle dynamics in accelerators.

Example 2 (Two particle interaction force) - 1

Particle evolution law and KD

The particle motions and associated KD are given by
$\dot{\theta}_i = \omega(\epsilon_i), \ \dot{\epsilon}_i = \sum_1^N F(\theta_i - \theta_j)$
$K(\theta, \epsilon, t; W_0) = \frac{1}{N} \sum_1^N \delta(\theta - \theta_i(t; W_0))\delta(\epsilon - \epsilon_i(t; W_0))$

As in the general case
$\text{Var}\, K_A(t; W_0) = \frac{1}{N} p(t)(1 - p(t)) + \frac{N(N-1)}{N^2} \text{Cov}\,(X_1, X_2)$
$\text{Cov}(X_i X_j) = \int_{A \times A} d\theta d\epsilon d\theta' d\epsilon' \mathcal{C}(\theta, \epsilon, \theta', \epsilon', t)$ where
$\mathcal{C}(\theta, \epsilon, \theta', \epsilon', t) = \Psi_2(v, v', t) - \Psi_1(v, t)\Psi_1(v', t)), v = (\theta, \epsilon)$

Issue 1: If $w_i(t; W_0)$ and $w_j(t; W_0)$ are independent then $\mathcal{C} = 0$ and $\bar{K}$ is a good approximation to K. Next step : study the N and t behavior of the covariance.

Example 2 (Two particle interaction force) - 2

Klimontovich evolution law and the associated mean

The Klimontovich density and its expected value satisfy

$$K_t + \omega(\epsilon)K_\theta + N\mathcal{L}(K)K_\epsilon = 0$$

$$\bar{K}_t + \omega(\epsilon)\bar{K}_\theta + N\mathcal{L}(\bar{K})\bar{K}_\epsilon = -N\overline{\mathcal{L}(K)K_\epsilon - \mathcal{L}(\bar{K})\bar{K}_\epsilon} \quad \text{where}$$

$$\mathcal{L}(K)(\theta) = \int d\theta' d\epsilon' K(\theta', \epsilon'; W_0)F(\theta - \theta')$$

The equation for $\bar{K}$ in terms of Ψ_1 and Ψ_2 is

$$\Psi_{1t} + \omega(\epsilon)\Psi_{1\theta} + N\mathcal{L}(\Psi_1)\Psi_{1\epsilon} = -N\int d\theta' d\epsilon' \mathcal{C}(\theta, \epsilon, \theta', \epsilon', t) + O(1)$$

$$\mathcal{C}(\theta, \epsilon, \theta', \epsilon', t) = \Psi_2(\theta, \epsilon, \theta', \epsilon', t) - \Psi_1(\theta, \epsilon, t)\Psi_1(\theta', \epsilon', t)$$

Issue 2: Recall $\Psi_2(v, v', t)$ is the joint probability density of w_i and w_j, so independence $\Rightarrow \bar{K} = \Psi_1$ satisfies the so-called Vlasov equation. Note independence also $\Rightarrow \bar{K} \approx K$. However, this is not the case and so a study of $\Psi_2(v, v', t)$ is the next step:

Example 3 (Simple relativistic KM system) - 1

Particle Field evolution law and integral over history

We consider particle motion coupled to a Maxwell field E [8]:

$$q_i' = p_i,\ p_i' = -aE(q_i, z; W_0);\ \ q_i(0; W_0) = Q_{i0},\ p_i(0; W_0) = P_{i0},$$

$$E_z + E_q = -b\sum_{1}^{N} \delta(q - q_i(z; W_0));\quad E(q, 0; W_0) = 0$$

Using the method of characteristics the E field can be written $E(q, t; W_0) = -b\sum_{i=1}^{N}\int_0^z ds\delta(q + (s - z) - q_i(s; W_0))$.

The self-contained particle motion can be written $q_i'(z) = p_i(z),\ p_i'(z) = ab\sum_{i=1}^{N}\int_0^z ds\delta(q + (s - z) - q_i(s; W_0))$

This is a functional ODE system [9] containing an integral over history. This makes the study of Ψ_2 problematic.

[8] Based on EOM in Kim, Lindberg paper in FEL2011 proceedings, Shanghai

[9] See e.g., J. Hale's Theory of Functional Differential Equations

Example 3 (Simple relativistic KM system) - 2

Mean field evolution

The equivalent Klimontovich-Maxwell system becomes

$$K_z + pK_q - aNEK_p = 0; \quad K(q,p,0;W_0) = \frac{1}{N}\sum_1^N \delta(q - Q_{i0})\delta(p - P_{i0})$$

$$E_z + E_q = -bN\int dpK(q,p,z;W_0); \quad E(q,0;W_0) = 0$$

The mean field equations are

$$\bar{K}_z + p\bar{K}_q - aN\bar{E}\bar{K}_p = a\partial_p Cov(E,K)$$
$$\bar{E}_z + \bar{E}_q = -bN\int dp\bar{K}(q,p,z)$$

- Integral over history also a problem here.
- If $Cov(E,F)$ is small then we have the macroscopic Vlasov-Maxwell system.

Example 3 (Simple relativistic KM system) - 3

Issues 1 and 2

Issue 1 The situation is as in general case i.e., $\mathrm{Var}\, K_A(t; W_0) = \frac{1}{N} p(t)(1 - p(t)) + \frac{N(N-1)}{N^2} \mathrm{Cov}\,(X_1, X_2)$ and so $\bar{K}$ is a good approximation to K for large N if $\mathrm{Cov}\,(X_1, X_2)$ is small. A major complication over the previous example is that we do not have a clear picture of Ψ_2.

Issue 2 The work here is to estimate $Cov(E, K)$. This also appears to be major complication over the previous example in that we do not have a clear picture of Ψ_2. The BBGKY hierarchy works in Example 1 and 2, but is problematic here, as evidenced by the integral over history issue.

General Summary: This example contains the major issues for the full 6D Microscopic Klimontovich-Maxwell (KM) to Macroscopic Vlasov-Maxwell (VM) problem. So our next step is continued study of Example 3.