Combined mean-field and semiclassical limit to Vlassov-Poisson equation from many fermionis

joint work with Li Chen and Matthew Liew

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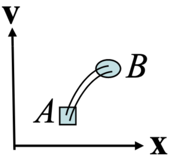
(Heuristic) Derivation of Vlasov equation

$f(\mathbf{x}, \mathbf{v}, t)dxdv$: the total # of particles in the differential volume $dxdv$



If collisions are neglected, particles in an element in A will wander in continuous curves to B.
Thus, the total number in the element is conserved.
So that we have the following continuity equation:

$$\partial_t f(\mathbf{x}, \mathbf{v}, t) + \nabla_{\mathbf{x},\mathbf{v}} \cdot [f(\mathbf{x}, \mathbf{v}, t)(\dot{\mathbf{x}}, \dot{\mathbf{v}})] = 0$$

(Heuristic) Derivation of Vlasov equation

$$\partial_t f(\mathbf{x}, \mathbf{v}, t) + \nabla_{\mathbf{x},\mathbf{v}} \cdot [f(\mathbf{x}, \mathbf{v}, t)(\dot{\mathbf{x}}, \dot{\mathbf{v}})] = 0,$$

note that

$$\begin{aligned} \nabla_{\mathbf{x},\mathbf{v}} \cdot f(\mathbf{x}, \mathbf{v}, t)(\dot{\mathbf{x}}, \dot{\mathbf{v}}) &:= \nabla_{\mathbf{x}} \cdot f(\mathbf{x}, \mathbf{v}, t)\dot{\mathbf{x}} + \nabla_{\mathbf{v}} \cdot f(\mathbf{x}, \mathbf{v}, t)\dot{\mathbf{v}} \\ &= f\nabla_{\mathbf{x}} \cdot \mathbf{v} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + f\nabla_{\mathbf{v}} \cdot \dot{\mathbf{v}} + \dot{\mathbf{v}} \cdot \nabla_{\mathbf{v}} f. \end{aligned}$$

Because

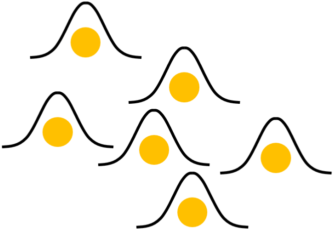
$$\nabla_{\mathbf{x}} \cdot \mathbf{v} = 0$$

$$\dot{\mathbf{v}} = \frac{q}{m}(\mathbf{E} + \frac{1}{c}\mathbf{v} \times \mathbf{B}) \implies \nabla_{\mathbf{v}} \cdot \dot{\mathbf{v}} = 0 \quad \text{if } B = 0 \text{ or } c = \infty,$$

we have that

$$\partial_t f(\mathbf{x}, \mathbf{v}, t) + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \frac{q}{m}\mathbf{E} \cdot \nabla_{\mathbf{v}} f = 0$$

N-fermionic system in 3D



$$\Psi_t(x_1, \cdots, x_N) = \frac{1}{\sqrt{N!}} \det\{\mathrm{e}_i(x_j)\}_{i,j=1}^N \in L^2_a(\mathbb{R}^{3N}).$$

N-body Hamiltonian

$$H_N = \sum_{j=1}^N \left(-\frac{1}{2}\Delta_{x_j}\right) + \lambda \sum_{i<j}^N V\left(x_i - x_j\right)$$

Fermionic mean-field regime

Consider a system of N interacting fermions with wave function:

$$H_N = -\frac{1}{2}\sum_{j=1}^{N}\Delta_{x_j} + \lambda\sum_{i\neq j}^{N} V(x_i - x_j)$$

$$E_{kin} = \langle \psi_N, \sum_{j=1}^{N}(-\Delta_{x_j})\psi_N\rangle \sim N^{5/3}$$

$$E_{int} = \langle \psi_N, \lambda\sum_{i<j}^{N} V(x_i - x_j)\psi_N\rangle \sim \lambda N^2$$

$$\implies \lambda = N^{-1/3}$$

$$H_N = -\frac{1}{2}\sum_{j=1}^{N}\Delta_{x_j} + \frac{1}{N^{1/3}}\sum_{i\neq j}^{N} V(x_i - x_j)$$

Time-dependent Schrödinger equation

$$E_{kin} \sim N^{5/3} \sim N v^2 \implies v \sim N^{1/3}$$

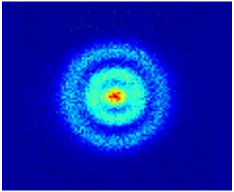
Relevant time scale $\sim N^{-1/3}$

$$N^{\frac{1}{3}} \mathrm{i}\partial_t \psi_{N,t} = \left[-\frac{1}{2} \sum_{j=1}^{N} \Delta_{x_j} + \frac{1}{2N^{1/3}} \sum_{i \neq j}^{N} V_N(x_i - x_j) \right] \psi_{N,t},$$

Setting $\hbar = N^{-1/3}$ and multiplying $\hbar^2$ on both sides, we get

$$\mathrm{i}\hbar\partial_t \psi_{N,t} = \left[-\frac{\hbar^2}{2} \sum_{j=1}^{N} \Delta_{x_j} + \frac{1}{2N} \sum_{i \neq j}^{N} V_N(x_i - x_j) \right] \psi_{N,t}.$$

Particle systems



- Classical System: Follows Vlasov equation

$$\partial_t f + 2p \cdot \nabla_q f - \nabla(V * \rho_t) \cdot \nabla_p f = 0$$

- Quantum System: Follows N-particle Schrödinger equation

$$\mathrm{i}\hbar\partial_t \Psi_{N,t} = \sum_{j=1}^{N} \left(-\frac{\hbar^2}{2m}\Delta \right) \Psi_{N,t} + \frac{1}{N} \sum_{i<j}^{N} V(x_i - x_j)\Psi_{N,t}$$

Problem

$$
\begin{tikzcd}
\boxed{N\text{-fermionic Schrödinger (S)}} \arrow[r, "N\to\infty"] \arrow[d, "\hbar\to 0"] \arrow[dr, "\hbar=N^{-1/3}\to 0"] & \boxed{\text{Hartree-Fock (HF)}} \arrow[d, "\hbar\to 0"] \\
\boxed{\text{Liouville (L)}} \arrow[r, "N\to\infty"] & \boxed{\text{Vlasov (V)}}
\end{tikzcd}
$$

Figure: N-fermionic Schrödinger systems to other equations

Literature review I

Mean field limit (S) $\rightarrow$ (HF)

- 2003: Elgart, Erdős, Schlein, Yau
- 2013: Benedikter, Porta, Schlein
- 2015: Benedikter, Jakšić, Porta, Saffirio, Schlein
- 2017: Porta, Rademacher, Saffirio, Schlein
- 2018: Saffirio

Semiclassical Limit (HF) $\rightarrow$ (V)

- 1993: Lions, Paul
- 2014: Figalli, Ligabò, Paul.
- 2017-19: Golse, Paul, Pulvirenti, Laflèche
- 2009: Athanassoulis, Paul, Pezzotti, Pulvirenti
- 2016: Benedikter, Porta, Saffirio, Schlein
- 2019: Saffirio

Literature review II

Semiclassical Limit (S) $\rightarrow$ (L)

- 1993: Lions, Paul

Mean field limit (L) $\rightarrow$ (HF)

- 1979: Dobrushin

Combined limit (S) $\rightarrow$ (HF)

- 1981: Narnhofer, Swell
- 1981: Spohn
- 2017: Golse, Paul
- 2021: Chen, L. Liew
- 2021: Chong, Laflèche, Saffirio
- 2021: Chen, L. Liew

How can we compare two systems?

Remark that

- Classical System: Follows Vlasov equation, domain is in phase space

$$\partial_t f + 2p \cdot \nabla_q f - \nabla(V * \rho_t) \cdot \nabla_p f = 0$$

- Quantum System: Follows N-particle Schrödinger equation

$$\mathrm{i}\hbar\partial_t \Psi_{N,t} = \sum_{j=1}^{N} \left(-\frac{\hbar^2}{2m}\Delta \right) \Psi_{N,t} + \lambda \sum_{i<j}^{N} V(x_i - x_j)\Psi_{N,t}.$$

Note that

$$f : \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R} \to \mathbb{R}_{\geq 0}$$
$$\Psi : \mathbb{R}^{3N} \times \mathbb{R} \to \mathbb{C}$$

Wigner-Weyl transform

Weyl transform of a function f

$$\Phi[f] = \frac{1}{(2\pi)^{2d}} \iiiint f(q,p) \left(e^{i(a(Q-q)+b(P-p))} \right) \mathrm{d}q\, \mathrm{d}p\, \mathrm{d}a\, \mathrm{d}b.$$

Wigner map of an operator Φ

$$f(q,p) = 2 \int_{-\infty}^{\infty} \mathrm{d}y \; e^{-2ipy/\hbar} \; \langle q+y|\Phi[f]|q-y\rangle$$

Let $R \in \mathcal{L}(\mathfrak{h})$ be the integral operator having kernel r

$$R\phi(x) = \int_{\mathbb{R}^d} r(x,y)\phi(y)dy$$

Wigner transform of R

$$W_\hbar[R](q,p) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} r\Big(q + \frac{\hbar}{2}y, q - \frac{\hbar}{2}y\Big) e^{ip\cdot y} dy$$

Husimi measure

- k-**particle Husimi measure**: For $1 \le k \le N$,

$$\mathfrak{m}_{N,t}^{(k)} := \frac{N(N-1)\cdots(N-k+1)}{N^k} W_{N,t}^{(k)} * \mathcal{G}^{\hbar},$$

where

$$\mathcal{G}^{\hbar}(q_1, p_1, \dots, q_k, p_k) := \frac{1}{(\pi\hbar)^{3k}} \exp\Big(- \frac{\sum_{j=1}^{k} {q_j}^2 + {p_j}^2}{\hbar} \Big).$$

- **generalized** k-**particle Husimi measure**: For $p, q \in \mathbb{R}^3$ and $\psi_{N,t} \in L_a^2(\mathbb{R}^{3N})$

$$m_{N,t}^{(k)}(q_1, p_1, \dots, q_k, p_k) = \big\langle \psi_{N,t}, a^*(f_{q_1,p_1}^{\hbar}) \cdots a^*(f_{q_k,p_k}^{\hbar}) a(f_{q_k,p_k}^{\hbar}) \cdots a(f_{q_1,p_1}^{\hbar}) \psi_{N,t} \big\rangle$$

where $a^*(f_{q,p}^{\hbar})$ and $a(f_{q,p}^{\hbar})$ are standard creation- and annihilation-operator respectively with respect to the coherent state $f_{q,p}^{\hbar}$ given by

$$f_{q,p}^{\hbar}(y) := \hbar^{-\frac{3}{4}} f\left(\frac{y-q}{\sqrt{\hbar}}\right) e^{\frac{i}{\hbar} p \cdot y},$$

for any real-valued function f satisfying $\|f\|_2 = 1$.

Properties of k-Husimi measure

For all $t \geq 0$ and $1 \leq k \leq N.$, the following properties hold true for $m^{(k)}_{N,t}$,

1. $m^{(k)}_{N,t}$ is symmetric,
2. $\frac{1}{(2\pi)^{3k}} \int \cdots \int (dqdp)^{\otimes k} m^{(k)}_{N,t} = \frac{N(N-1)\cdots(N-k+1)}{N^k}$,
3. $\frac{1}{(2\pi\hbar)^3} \iint dq_k dp_k \; m^{(k)}_{N,t} = (N-k+1) m^{(k-1)}_{N,t}$,
4. $0 \leq m^{(k)}_{N,t} \leq 1$ a.e.,
5. If chose $f(x) = \pi^{-3/4} e^{-|x|^2/2}$, then

$$m^{(k)}_{N,t} = \frac{N(N-1)\cdots(N-k+1)}{N^k} W^{(k)}_{N,t} * \mathcal{G}^{\hbar},$$

   where
   $\mathcal{G}^{\hbar}(q_1, p_1, \ldots, q_k, p_k) := (\pi\hbar)^{-3k} \exp\big(-\hbar^{-1}(\sum_{j=1}^{k} |q_j|^2 + |p_j|^2)\big)$.

Main goal

Vlasov Equation: For given initial data m_0, let m_t be the solution to the following Vlasov equation

$$\begin{cases} \partial_t m_t(q,p) + p \cdot \nabla_q m_t(q,p) = \nabla_q \big(V * \varrho_t\big)(q) \cdot \nabla_p m_t(q,p), \\ m_t(q,p)\big|_{t=0} = m_0(q,p), \end{cases}$$

where $\varrho_t(q) := \int m_t(q,p)dp$.

Goal: To prove that $m_{N,t}^{(1)}$ converges to m_t in the sense of distribution as $N \to \infty$.

Theorem (L. Chen, J. L. , M. Liew (AHP 2021))

Let $m^{(1)}_{N,t} := m_{N,t}$ *be the 1-particle Husimi measure and suppose the following assumptions hold:*

(1) V_N *is the truncated Coulomb potential with* $\beta_N := N^{-\epsilon}$, $0 < \epsilon < \frac{1}{24}$.

(2) *For fixed* $T > 0$, *let* $\Psi_{N,t} \in \mathcal{F}^N_a$, $t \in [0, T]$, *be the solution to the Schrödinger equation with the Slater determinant as the initial data .*

(3) $f \geq 0$ *is a compact supported and it is in* $H^1(\mathbb{R}^3)$ *with* $\|f\|_2 = 1$.

(4) *Let* m_N *be the initial 1-particle Husimi measure with* L^1*-weak limit* m_0 *and satisfies the uniform bound:*

$$\iint dqdp\ (|p|^2 + |q|)m_N(q,p) < \infty.$$

Then, $m_{N,t}$ *has a weak-*$\star$ *convergent subsequence in* $L^\infty((0,T]; L^1(\mathbb{R}^3 \times \mathbb{R}^3))$ *with limit* m_t, *where* m_t *is the solution of the Vlasov-Poisson equation with repulsive Coulomb potential in the sense of distribution.*

Truncated repulsive Coulomb potential

We consider the mollification of repulsive Coulomb potential, i.e.

$$V_N(x) = (V * \mathcal{G}_{\beta_N})(x)$$

where $V(x) = |x|^{-1}$ and $\mathcal{G}_{\beta_N}(x) := \frac{1}{(2\pi\beta_N^2)^{3/2}} e^{-(x/\beta_N)^2}$.

Remark

$$\|\nabla V_N\|_{L^\infty} \leq C\beta_N^{-2},$$

we will set $\beta_N \sim N^{-\epsilon}$ with $0 < \epsilon < 1/24$.

Proof strategy

Recall,

$$m^{(1)}_{N,t}(q,p) = \left\langle \psi_{N,t}, a^*(f^{\hbar}_{q,p}) a(f^{\hbar}_{q,p}) \psi_{N,t} \right\rangle$$

where $\Psi_{N,t}$ is the solution to the Schrödinger equation.
Taking the $i\hbar\partial_t m_{N,t}$ and divide both side with $i\hbar$, we will obtain the following term:

$$\begin{aligned}
&\partial_t m_{N,t}(q,p) + p\cdot\nabla_q m_{N,t}(q,p) - \nabla_q \cdot \left(\hbar \operatorname{Im} \left\langle \nabla_q a(f^{\hbar}_{q,p})\psi_{N,t}, a(f^{\hbar}_{q,p})\psi_{N,t} \right\rangle\right) \\
&= \frac{1}{(2\pi)^3} \nabla_p \cdot \int dw_1 du_1 dw_2 du_2 dq_2 dp_2 \left(f^{\hbar}_{q,p}(w) \overline{f^{\hbar}_{q,p}(u)} \right)^{\otimes 2} \\
&\qquad \times \int_0^1 ds\; \nabla V_N\big(su_1 + (1-s)w_1 - w_2\big) \langle \Psi_{N,t}, a_{w_1} a_{w_2} a^*_{u_2} a^*_{u_1} \Psi_{N,t} \rangle
\end{aligned}$$

where we denote

$$\left(f^{\hbar}_{q,p}(w) \overline{f^{\hbar}_{q,p}(u)} \right)^{\otimes 2} := f^{\hbar}_{q,p}(w_1)\overline{f^{\hbar}_{q,p}(u_1)} f^{\hbar}_{q_2,p_2}(w_2)\overline{f^{\hbar}_{q_2,p_2}(u_2)}.$$

Proof strategy: Vlasov equation with remainders I

$$\partial_t m_{N,t} + p \cdot \nabla_q m_{N,t} = \frac{1}{(2\pi)^3} \nabla_q (V_N * \varrho_{N,t}) \nabla_p \cdot m_{N,t} + \nabla_q \cdot \widetilde{\mathcal{R}} + \nabla_p \cdot \mathcal{R},$$

where $\varrho_{N,t}(q) := \int \mathrm{d}p \, m_{N,t}(q,p)$, $\widetilde{\mathcal{R}}$ and $\mathcal{R} = \mathcal{R}_{\mathrm{s}} + \mathcal{R}_{\mathrm{m}}$ are given by

$$\begin{aligned}
\widetilde{\mathcal{R}} &:= \hbar \,\mathrm{Im} \left\langle \nabla_q a(f^{\hbar}_{q,p}) \Psi_{N,t}, a(f^{\hbar}_{q,p}) \Psi_{N,t} \right\rangle , \\
\mathcal{R}_{\mathrm{s}} &:= \frac{1}{(2\pi)^3} \int \mathrm{d}w_1 \mathrm{d}u_1 \mathrm{d}w_2 \mathrm{d}u_2 \mathrm{d}q_2 \mathrm{d}p_2 \left(f^{\hbar}_{q,p}(w) \overline{f^{\hbar}_{q,p}(u)} \right)^{\otimes 2} \\
&\qquad \times \left[\int_0^1 \mathrm{d}s \; \nabla V_N \big(s u_1 + (1-s) w_1 - w_2 \big) - \nabla V_N (q - q_2) \right] \gamma^{(2)}_{N,t}(u_1, u_2; w_1, w_2), \\
\mathcal{R}_{\mathrm{m}} &:= \frac{1}{(2\pi)^3} \int \mathrm{d}w_1 \mathrm{d}u_1 \mathrm{d}w_2 \mathrm{d}u_2 \mathrm{d}q_2 \mathrm{d}p_2 \left(f^{\hbar}_{q,p}(w) \overline{f^{\hbar}_{q,p}(u)} \right)^{\otimes 2} \\
&\qquad \times \nabla V_N (q - q_2) \Big[\gamma^{(2)}_{N,t}(u_1, u_2; w_1, w_2) - \gamma^{(1)}_{N,t}(u_1; w_1) \gamma^{(1)}_{N,t}(u_2; w_2) \Big].
\end{aligned}$$

Proof Strategy

Lemma

For $g \in C_0^\infty(\mathbb{R}^3)$ *and*

$$\Omega_\hbar := \{x \in \mathbb{R}^3;\ \max_{1\leq j\leq 3} |x_j| \leq \hbar^\alpha\},$$

it holds that for every $\alpha \in (0,1)$, $s \in \mathbb{N}$, *and* $x \in \mathbb{R}^3 \backslash \Omega_\hbar$,

$$\left| \int_{\mathbb{R}^3} dp\ e^{\frac{i}{\hbar} p\cdot x} g(p) \right| \leq c_1 \hbar^{(1-\alpha)s},$$

where the constant c_1 *depends on the compact support as well as the* $W^{s,\infty}$*-norm of the test function* g.

Proof strategy

For $\varphi, \phi \in C_0^\infty(\mathbb{R}^3)$, there exists a positive constant K such that

$$\left| \iint dqdp\ \varphi(q)\phi(p)\nabla_q \cdot \widetilde{\mathcal{R}}(q,p) \right| \leq K\hbar^{\frac{1}{2}-},$$
$$\left| \iint dqdp\ \varphi(q)\phi(p)\nabla_p \cdot \mathcal{R}(q,p) \right| \leq K\big(\hbar^{\frac{1}{4}-} + \hbar^{\frac{3}{4}-}\big).$$

This show that the residual terms converge to zero in the sense of distribution.

Remark

The constant K is depends on $\|\varphi\|_{W^{1,\infty}}$, $\|\nabla\phi\|_{W^{s,\infty}}$ with s depends on α_1 and α_2, $\operatorname{supp}\phi$, $\|f\|_{L^\infty\cap L^2}$, $\operatorname{supp} f$, and $\|\nabla V_N\|_\infty$.

Proof strategy

Lemma

Assuming that $V_N(x) \geq 0$ and the initial total energy is bounded in the sense that $\frac{1}{N}\langle \Psi_N, \mathcal{H}_N \Psi_N \rangle \leq C$, then the kinetic energy is bounded as follows

$$\langle \Psi_{N,t}, \mathcal{K} \Psi_{N,t} \rangle \leq CN.$$

Lemma

For $t \geq 0$, we have the following finite moments:

$$\iint dqdp \; (|q| + |p|^2) m_{N,t}(q,p) \leq C(1+t),$$

Theorem (mixed-norm estimate)

For given suitable condition, we have the following estimate

$$\left(\iint \mathrm{d}w_1 \mathrm{d}u_1 \; \left[\mathrm{Tr}^{(1)} \left| \gamma^{(2)}_{N,t} - \omega^{(1)}_{N,t} \otimes \omega^{(1)}_{N,t} \right| (u_1; w_1) \right]^2 \right)^{\frac{1}{2}} \leq C_t N,$$

where the constant C_t depends on potential V and time t.

Thank you

Grazie

감사합니다