Asymptotic Solutions to Many-body Dynamics III: Quantum dynamics in random potential, Kinetic and Mean-Field Limits

Horng-Tzer Yau
New York University

Collaboration with L. Erdős

Quantum dynamics of N particles interacting with a field

Schrödinger equation $\quad i\partial_t\psi_t(x_1,\cdots,x_N) = H\psi_t(x_1,\cdots,x_N)$

Hamiltonian $\quad H = H_0 + H_{e-e} + H_{e-f} + H_f$

Electron Hamiltonian $\quad H_0 = \sum_{j=1}^{N} \Big(-\frac{1}{2}\Delta_{x_j} + \lambda\Phi(x_j) \Big)$

Two-body interaction $\quad H_{e-e} = \lambda_{e,e} \sum_{1\le i<j\le N} \Phi_{e,e}(x_i - x_j)$

Particle-field int. $\quad H_{e-f}$

Field Hamiltonian $\quad H_f$

Possible fields: phonon (lattice vibrations), random potential (impurity). Also E.M.: $-\Delta \mapsto (-i\nabla + A)^2$

GOAL: Describe the dynamics of this complex quantum system in various limiting regimes using simpler effective equations.

How do classical equations emerge and what quantum effects are retained?

We consider different models by keeping some terms and neglecting others.

COMPLEXITY:

- Complex environment (impurities)
- Many-body ($N \approx 10^{23}$ particles)
- Long time evolution (compared to the atomic time scale).

SIMPLIFICATIONS:

(i) Idealized limits:

- Micro – macro scale separation: de Broglie wavelength ($\mathring{A}$)

  vs. "naked eye" (cm): $1\mathring{A}/1cm \to 0$

- Weak coupling and/or low density of interactions.

(ii) Special initial conditions (e.g. no initial correlation)

(iii) Partial information (coarse graining, smoothing, weak limit)

(iv) Randomness.

Units: length = [Bohr radius] ($\hbar^2/me^2$), energy = [Rydberg] ($me^4/2\hbar^2$).

Furthermore: $2\pi = 1$.

List of models and equations

I. ONE-BODY MODELS ($H_{e-e} = 0$)

(1) Semiclassical limit – linear Vlasov equation

(2) Weak coupling and low density limits (random potential or phonon) – linear Boltzmann eq.

II. MANY-BODY MODELS ($H_{e-e} \neq 0$)

(1) High-density mean field limit

Bosons – nonlinear Hartree eq. (nonlinear Schrödinger)

Fermions - nonlinear Vlasov equation

(2) Weak coupling and low density limits – nonlinear Boltz. eq.

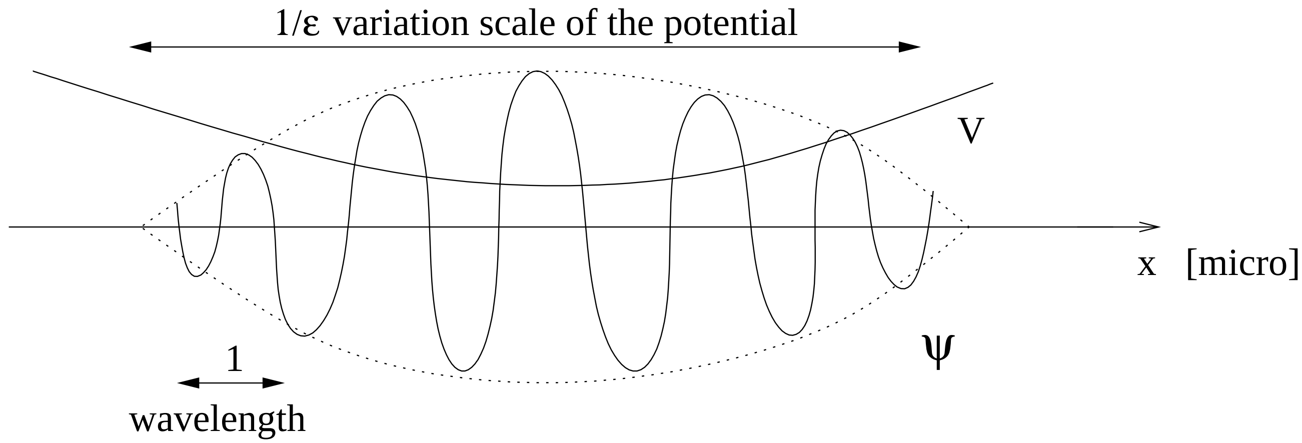
I. Noninteracting (effectively one body) models: $H_{e-e} = 0$

1. SEMICLASSICAL MODELS: Macro potential profile vs. micro wavelength

In micro coordinates: $$i\partial_t \psi(x) = \Big[-\tfrac{1}{2}\Delta_x + V(\varepsilon x)\Big]\psi(x)$$

In macro coordinates: $$i\varepsilon\partial_T \Psi(X) = \Big[-\tfrac{\varepsilon^2}{2}\Delta_X + V(X)\Big]\Psi(X)$$

under Euler scaling $(x\varepsilon, t\varepsilon) = (X, T)$, $\varepsilon \to 0$.



Wavefunction and potential scales in semiclassics

Limiting macroscopic equation: (linear) **Vlasov equation**

$$(\partial_T + V \cdot \nabla_X) W_T(X,V) = \nabla V(X) \cdot \nabla_V W_T(X,V)$$

for the weak limit of the rescaled Wigner transform

$$W_\psi(x,v) = \int \overline{\psi}\Big(x + \frac{z}{2}\Big) \psi\Big(x - \frac{z}{2}\Big) e^{ivz} dz$$

$$W_T^{(\varepsilon)}(X,V) := \varepsilon^{-d} W_{\psi_{T/\varepsilon}}\Big(\frac{X}{\varepsilon}, V\Big)$$

$$W_T(X,V) := \lim_{\varepsilon \to 0} W_T^{(\varepsilon)}(X,V)$$

Wigner transform (usually not positive) – phase space density:

$$\int W_\psi(x,v) dv = |\psi(x)|^2, \qquad \int W_\psi(x,v) dx = |\widehat{\psi}(v)|^2$$

KEY: WKB analysis, $\Psi_T(X) \sim A_T(X)e^{iS_T(X)/\varepsilon}$ form preserved.

Result is fully classical: no remnant of quantum mechanics.

2. RANDOM POTENTIAL MODELS. $H = -\frac{1}{2}\Delta_x + V_\omega(x)$

V_ω is unscaled but random.

In $d = 1$, then localization occurs for all λ.

Frohlich-Spencer, Aizenman: In all dimensions, localization occurs for λ large. V_ω dominates.

Question: How does conduction occur?

1. phenomenological model: Boltzmann equation. $\Longrightarrow$ Long time dynamics of the electrons are diffusive.

2. Perturbation theory: Boltzmann equation is basically correct up to re-normalization of diffusion coefficient for $d \geq 3$; localization for all λ for $d \leq 2$.

Recall $(x\varepsilon, t\varepsilon) = (X, T)$, where x, t are microscopic (Schrödinger) coordinates, so this is very long time ($t \sim \varepsilon^{-1}$) for Schr. eq.

GOAL: describe the dynamics for arbitrary macro time $T > 0$.

We reduce V_ω and look for the first nontrivial regime beyond free dynamics. Two possibilities:

(i) Low density limit (LDL) (Quantum Lorenz gas)

(ii) Weak coupling limit (WCL) (van Hove limit)

(i) Low density limit (LDL)

$$-\frac{1}{2}\Delta_x + \sum_{\alpha=1}^{M} V_0(x - x_\alpha) \qquad \text{in a box } [-L, L]^d$$

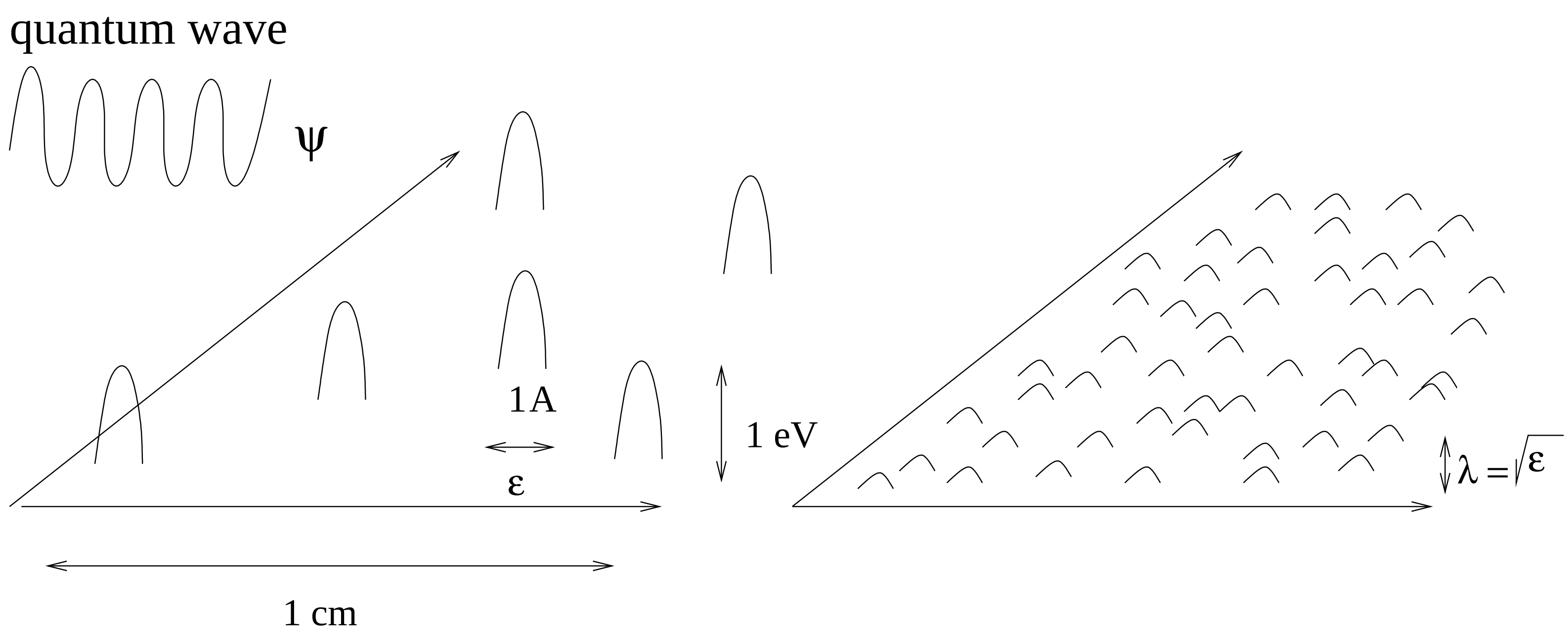
$\{x_\alpha\}_{\alpha=1,\dots M}$ random point process (e.g. uniform or Poisson) with density $\varrho := \frac{M}{L^d} \to 0$ (as $\varrho \sim \varepsilon$, $L \gg \varepsilon^{-1}$)

(ii) Weak coupling limit (WCL)

$$-\frac{1}{2}\Delta_x + \lambda V_\omega(x) \qquad \lambda \to 0, \quad (\lambda \sim \sqrt{\varepsilon})$$

V_ω time independent random field, e.g. Gauss, with correlation on micro scale:

$$R^2(x - y) = \mathbf{E} V_\omega(x) V_\omega(y)$$



Low density scenery

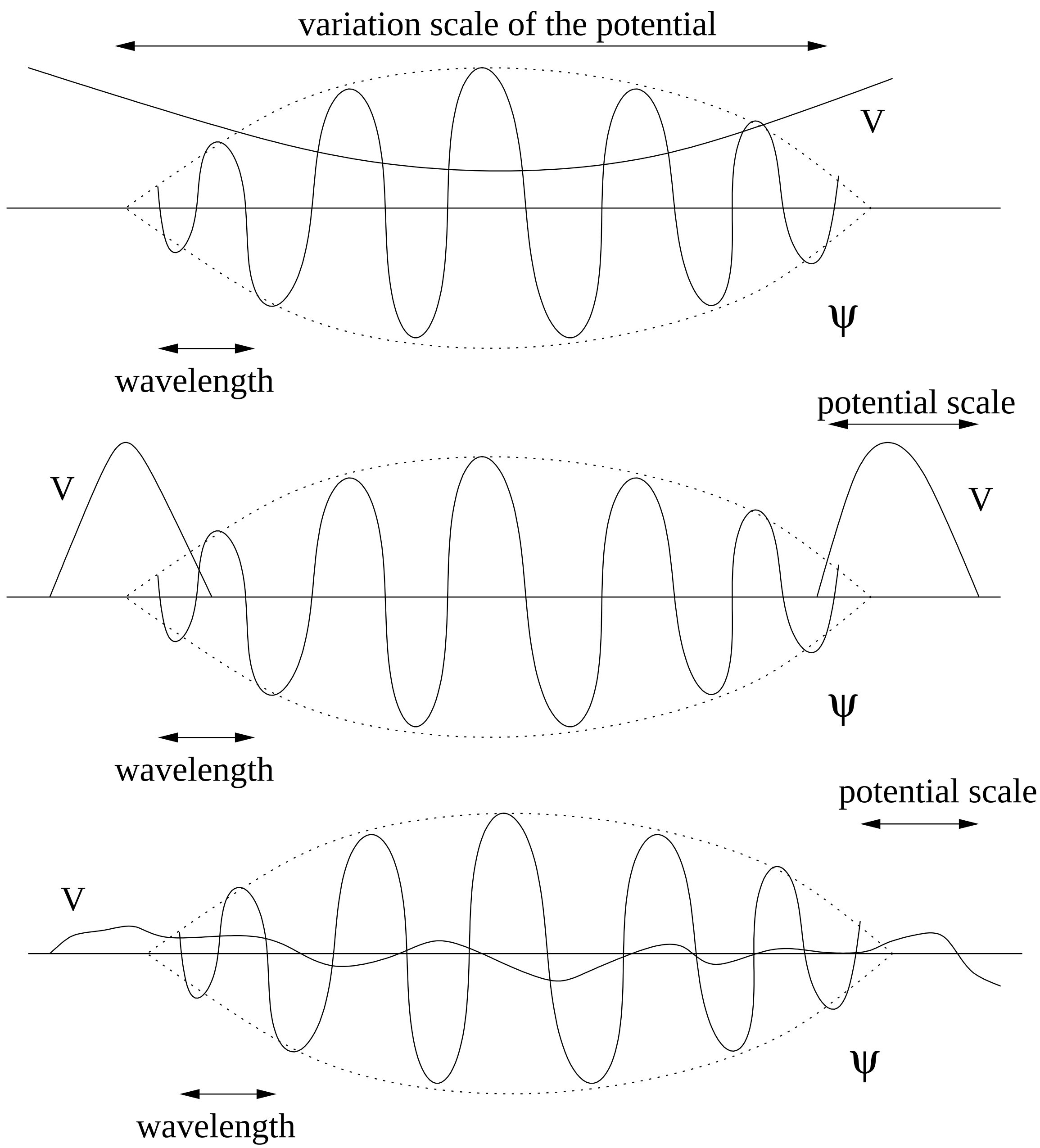
Number of obstacles: ε^{-2}

Density: O (ε)

Weak coupling scenery

Number of obstacles: ε^{-3}

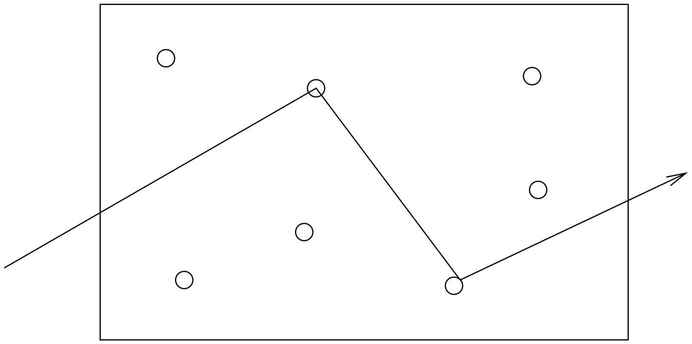
Density: O(1)



Semiclassical

Low density

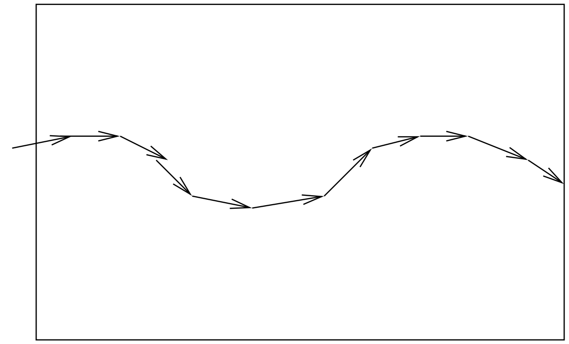
Weak coupling



Typical LDL picture leads to Boltzmann

Few big collisions. Collision number is

finite (seen also from Dyson expansion)



Typical WCL picture leads to

Brownian motion in velocity (classical).

Many small collisions

Mean free path	ϱ^{-1}	$O(1)$
Time	$t \sim \varepsilon^{-1}$	$t \sim \varepsilon^{-1}$
No. of coll.	$vt/\varrho^{-1} \sim \varrho\varepsilon^{-1}$	$vt/O(1) \sim \varepsilon^{-1}$

Total effect	$\varrho\varepsilon^{-1}$	$\varepsilon^{-1}\lambda^2$ (variance!)
	$\Longrightarrow \quad \varrho = \varepsilon$	$\Longrightarrow \quad \lambda = \sqrt{\varepsilon}$

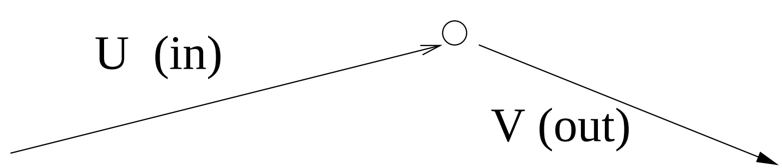
BOLTZMANN EQUATION: phenomenological. Describes a free evolution + a (random) Markovian collision mechanism.

Linear Boltzmann eq. (on macro scale)

$$(\partial_T + V \cdot \nabla_X) f_T(X,V) = \int \Big[\sigma(V,U) f_T(X,U) - \sigma(U,V) f_T(X,V)\Big] dU$$

- $f_T(X,V)$ – one particle phase space density

- $\sigma(U,V)$ collision kernel (U incoming, V outgoing velocity). Supported on $\delta(U^2 - V^2)$ if collision is elastic.



Theorem [Erdos-Y]. $d \geq 2$. If the weak limit

$$f_T(X,V) = \lim_{\varepsilon \to 0} \mathbf{E} W_T^{(\varepsilon)}(X,V)$$

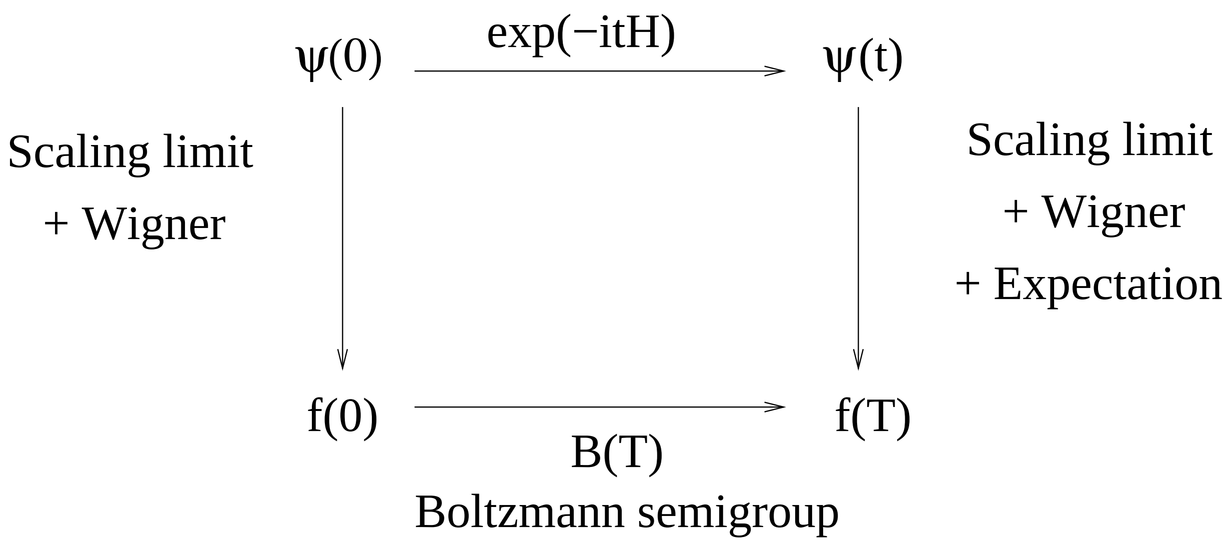
exists for $T = 0$, then it exists for any $T > 0$ and it solves the linear Boltzmann equation with collision kernel

(i) (LDL) $\sigma(U,V) = |T(U,V)|^2 \delta(U^2 - V^2)$, where $T(U,V)$ is the quantum scattering cross section for $-\frac{1}{2}\Delta + V_0$

(ii) (WCL) $\sigma(U,V) = |\widehat{R^2}(U-V)|^2 \delta(U^2-V^2)$ (Born approximation of the scattering cross section)

• Spohn: for short time and WCL Gaussian case.

• Time reversibility is lost due to the weak limit (not due to the randomness)



The long time ($t = T\varepsilon^{-1}$) Schrödinger evolution is modelled by a finite time (T) Boltzmann evolution on the macroscopic scale.

Detailed short scale information is lost (irreversible).

Effective equation is classical, but quantum features are retained in the collision kernel.

Similar result holds for phonons (Erdos).

	LDL	WCL
Classical dyn	Boltzmann [Spohn/Gallavotti]	(Integrated) Brownian [KP, DSL]
Quantum dyn:	Boltzmann	Boltzmann

Classical WCL: $v_{out} = v_{in} + O(\lambda)$

$\Longrightarrow$ Many small kicks $\Longrightarrow$ Brownian motion

Quantum WCL: Single collision process

$$\psi_{out} = \psi_{free} + \psi_{coll} \qquad \psi_{free} \text{``} \perp \text{''} \psi_{coll}$$

Prob. of collision is $\|\psi_{coll}\|^2 = O(\lambda^2)$. Rarely collides, but if it does, then outgoing wave is very different. Effectively a few big kicks.

II. MANY-BODY MODELS: $H_{e-e} \neq 0$.

$$H = -\frac{1}{2} \sum_{j=1}^{N} \Delta_{x_j} + \lambda_{e,e} \sum_{1 \le i < j \le N} \Phi(x_i - x_j)$$

1. Mean field limit: N particles, $N \to \infty$. $\lambda_{e,e}$ small.

Scaling is given by setting the kinetic and potential energies comparable.

Bosons: $\lambda_{e,e} = \frac{1}{N}$. Kinetic energy $\approx$ potential energy $= O(N)$

If $\Psi = \prod_j \psi(x_j)$ (possible only for **bosons**) then each particle is subject to the same deterministic potential (LLN for x_j)

$$\frac{1}{N} \sum_{j=1}^{N} \Phi(x - x_j) |\psi(x_j)|^2 \approx \Phi_{eff}(x) := (\Phi \star |\psi|^2)(x)$$

THEOREM [Bosons] Assume $\Psi_0 = \prod_j \psi_0(x_j)$ initial N-body product state. Then $\Psi_t \approx \prod_j \psi_t(x_j)$ as $N \to \infty$, where

$$i\partial_t \psi_t = -\frac{1}{2}\Delta\psi_t + \left(\Phi \star |\psi_t|^2\right)\psi_t \qquad \textbf{(NL Hartree equation)}$$

KEY PROBLEM: Ψ_t is NOT exact product.

[Hepp, Spohn, Ginibre-Velo, Bardos-Golse-Mauser]

[Erdos-Y] $\Phi(x) = \pm|x|^{-1}$ Coulomb case. (BBGKY hierarchy)

Digression: Study asymptotic dynamics of the Hartree equation [Soffer-Weinstein, Frohlich-Tsai-Y], especially the soliton dynamics.

(ii) **Fermions:** $\lambda = \frac{1}{N^{1/3}}$ since kinetic energy $\approx N^{5/3}$. [Narnhofer-Sewell, Spohn] **nonlinear Vlasov equation**

Equation is classical, but the fermionic nature dictates the scaling and pushes it to the semiclassical regime.

2. Kinetic limit: $(x\varepsilon, t\varepsilon) = (X, T)$, $\lambda_{e,e} = \sqrt{\varepsilon}$, $\varepsilon \to 0$

Expect: **Nonlinear Boltzmann eq.**

$$(\partial_T + V \cdot \nabla_X)F = \int \sigma \Big[(1 \pm F)(1 \pm F')\tilde{F}\tilde{F}' - FF'(1 \pm \tilde{F})(1 \pm \tilde{F}') \Big]$$

$\pm$ for Bosons or Fermions. Open question. (classical model: [Lanford]).

3. Euler Limit. Euler equations.

Longer time scales $t \gg \lambda^{-2}$. Expect diffusion.

We proved: Schrödinger $\Longrightarrow$ Boltzmann if $t = T\lambda^{-2}$

λ fixed, $t \to \infty$.

$$S(t) = \int x^2 |\psi_t(x)|^2 dx \qquad \text{mean square displacement}$$

$$S(t) < C(\lambda) \quad \text{for all } t, \qquad d = 2$$

$$S(t) \sim t \qquad d \geq 3$$

Starting point: $t \sim \lambda^{-3}$.