Mean-Field Limits for Large Particle Systems
Lecture 2: From Schrödinger to Hartree

François Golse

CMLS, École polytechnique

"Frontiers of Applied and Computational Mathematics"
Shanghai Jiao-Tong University, July 9-20 2018

A CRASH COURSE ON QUANTUM N-PARTICLE DYNAMICS

T. Kato: "Perturbation theory for linear operators". Springer

N-particle wave function

The state at time t of a N-particle system in quantum mechanics is described by its wave function

$$\Psi_N \equiv \Psi_N(t, x_1, \ldots, x_N) \in \mathbf{C}$$

where x_j is the position of the jth particle
What does the wave function tell us? the probability density of having particle no.1 at the position x_1, particle no.2 at the position x_2,... and particle no. N at the position x_N is

$$|\Psi_N(t, x_1, \ldots, x_N)|^2$$

In particular

$$\int |\Psi_N(t, x_1, \ldots, x_N)|^2 dx_1 \ldots dx_N = 1$$

Quantum N-particle Hamiltonian

Classical Hamiltonian=function $\mathcal{H}_N(X_N, \Xi_N)$ with $(X_N, \Xi_N) \in \mathbf{R}^{2dN}$ ($\mathbf{R}^{2dN}$ = the N-particle phase space)
Quantum Hamiltonian=(unbounded) operator H_N on $\mathfrak{H}_N := L^2(\mathbf{R}^{dN})$ ($\mathbf{R}^{dN}$ = the N-particle configuration space)

Quantization rule for

$$\mathcal{H}_N(X_N, \Xi_N) := \sum_{j=1}^{N} \tfrac{1}{2}|\xi_j|^2 + \frac{1}{N} \sum_{1 \le j < k \le N} V(x_j - x_k)$$

(a) Function $f(X_N) \mapsto$ multiplication operator by $f(X_N)$ on $\mathfrak{H}_N$
(b) Monomial $\xi_1^{\alpha_1} \dots \xi_N^{\alpha_N} \mapsto (-i\hbar\partial_{x_1})^{\alpha_1} \dots (-i\hbar\partial_{x_N})^{\alpha_N}$

$$\mathcal{H}_N \mapsto H_N := \sum_{j=1}^{N} -\tfrac{1}{2}\hbar^2 \Delta_{x_j} + \frac{1}{N} \sum_{1 \le j < k \le N} V(x_j - x_k)$$

The (N-particle) Schrödinger equation

Planck's constant $\hbar = 1.05 \cdot 10^{-34} J \cdot s$

$$i\hbar\partial_t \Psi_N = H_N \Psi_N \,, \qquad \Psi_N\Big|_{t=0} = \Psi_N^{in}$$

Theorem (Kato, Trans. AMS '51) If $d = 3$, and if for some $R > 0$,

$$V\Big|_{B(0,R)} \in L^2(B(0,R)) \qquad \text{and } V\Big|_{\mathbf{R}^3 \setminus B(0,R)} \in L^\infty(\mathbf{R}^3 \setminus B(0,R))$$

then, for each $N \geq 1$ and each $\hbar > 0$, the quantum Hamiltonian

$$H_N := \sum_{k=1}^{N} -\tfrac{1}{2}\hbar^2 \Delta_{x_k} + \frac{1}{N} \sum_{1\leq k<l\leq N} V(x_k - x_l)$$

has a self-adjoint extension on $\mathfrak{H}_N := L^2(\mathbf{R}^{3N})$ and generates a unitary group e^{-itH_N} on $\mathfrak{H}_N$

Dirac's notation

Dirac's notation Denote $|\Phi_N\rangle :=$ the vector $\Phi_N \in \mathfrak{H}_N = L^2(\mathbf{R}^{dN})$

$$\langle\Psi_N| := \text{linear functional on } \mathfrak{H}_N \ni \phi_N \mapsto \int_{\mathbf{R}^{dN}} \overline{\Psi_N}\phi_N(X_N)dX_N$$

Hence

$$\langle\Psi_N|\Phi_N\rangle = \int_{\mathbf{R}^{dN}} \overline{\Psi_N}\Phi_N(X_N)dX_N \in \mathbf{C}$$

while

$$|\Phi_N\rangle\langle\Psi_N| = \text{ projection on } \mathbf{C}|\Phi_N\rangle \text{ along } (\mathbf{C}|\Psi_N\rangle)^\perp$$

Hilbert-Schmidt operators

Let $\mathfrak{H} := L^2(\mathbf{R}^n)$, let $\mathcal{L}(\mathfrak{H})$ = set of bounded operators on $\mathfrak{H}$ and let $\mathcal{K}(\mathfrak{H})$ be the set of compact operators on $\mathfrak{H}$ (2-sided ideal of $\mathcal{L}(\mathfrak{H})$)
Hilbert-Schmidt operators on $\mathfrak{H}$ are integral operators of the form

$$T\psi(x) := \int_{\mathbf{R}^d} \tilde{T}(x,y)\psi(y)dy \quad \text{s.t. } \tilde{T} \in L^2(\mathbf{R}^n \times \mathbf{R}^n)$$

Set of Hilbert-Schmidt operators on $\mathfrak{H}$ denoted $\mathcal{L}^2(\mathfrak{H}) \subset \mathcal{K}(\mathfrak{H})$; closed 2-sided ideal of $\mathcal{L}(\mathfrak{H})$
Hilbert-Schmidt inner product and norm

$$(R|S)_{\mathcal{L}^2(\mathfrak{H})} := \iint_{\mathbf{R}^d \times \mathbf{R}^d} \overline{R(x,y)} S(x,y)dxdy$$

$$\|T\|_{\mathcal{L}^2(\mathfrak{H})} := (T|T)^{1/2}_{\mathcal{L}^2(\mathfrak{H})} = \|\tilde{T}\|_{L^2(\mathbf{R}^n \times \mathbf{R}^n)}$$

Trace-class operators

Set of trace-class operators

$$\mathcal{L}^1(\mathfrak{H}) := \{RS \text{ s.t. } R \text{ and } S \in \mathcal{L}^2(\mathfrak{H})\}$$

Trace of a trace-class operator: for each $T \in \mathcal{L}^1(\mathfrak{H})$,

$$\mathrm{tr}(T) := \int_{\mathbf{R}^d} \tilde{T}(x,x)dx$$

Trace norm

$$\|T\|_{\mathcal{L}^1(\mathfrak{H})} = \mathrm{tr}(|T|) = \||T|^{1/2}\|^2_{\mathcal{L}^2(\mathfrak{H})}, \quad \text{where } |T| = \sqrt{T^*T}$$

Exercise Let $T \in \mathcal{L}(\mathfrak{H})$ with integral kernel $\tilde{T}$.
(1) If $T \in \mathcal{L}^1(\mathfrak{H})$, the map $z \mapsto \tilde{T}(x+z,x)$ belongs to $C(\mathbf{R}^d; L^1(\mathbf{R}^d))$
(2) Assume $x \mapsto \tilde{T}(x,x)$ integrable on $\mathbf{R}^d$. Does $T \in \mathcal{L}^1(\mathfrak{H})$?

$$\|AT\|^2_{\mathcal{L}^2(\mathfrak{H})} = \sum_{k\geq 1} \|ATe_k\|^2_{\mathfrak{H}} \leq \|A\|^2 \sum_{k\geq 1} \|ATe_k\|^2_{\mathfrak{H}} = \|A\|^2 \|T\|^2_{\mathcal{L}^2(\mathfrak{H})}$$

With the polar decompositions $AT = |AT|V$ and $T = |T|U$, one has

$$\begin{aligned}\|AT\|_{\mathcal{L}^1(\mathfrak{H})} = \operatorname{tr}(|AT|) = \operatorname{tr}(A|T|UV^*) &= \operatorname{tr}(A|T|^{1/2}|T|^{1/2}UV^*) \\ &\leq \|A|T|^{1/2}\|_{\mathcal{L}^2(\mathfrak{H})} \||T|^{1/2}UV^*\|_{\mathcal{L}^2(\mathfrak{H})} \\ &\leq \|A\| \||T|^{1/2}\|^2_{\mathcal{L}^2(\mathfrak{H})} \|UV^*\| \\ &= \|A\| \|T\|_{\mathcal{L}^1(\mathfrak{H})}\end{aligned}$$

Density operators

A density operator on a separable Hilbert space $\mathfrak{H}$ is $R \in \mathcal{L}(\mathfrak{H})$ s.t.

$$R = R^* \geq 0\,, \quad \text{and} \quad \mathrm{tr}(R) = 1\,.$$

Set of density operators on $\mathfrak{H}$ denoted $\mathcal{D}(\mathfrak{H})$

Examples

(1) If $\psi \in \mathfrak{H}$ satisfies $\|\psi\|_{\mathfrak{H}} = 1$, then $|\psi\rangle\langle\psi| \in \mathcal{D}(\mathfrak{H})$ (pure state)

(2) If $(\psi_k)_{k\geq 1} \in \mathfrak{H}$ satisfies $\langle\psi_k|\psi_l\rangle = \delta_{kl}$, then

$$\sum_{k\geq 1} \lambda_k |\psi_k\rangle\langle\psi_k| \in \mathcal{D}(\mathfrak{H}) \quad \text{iff} \quad \lambda_k \geq 0 \text{ and } \sum_{k\geq 1} \lambda_k = 1$$

(mixed state)

Key observation Let $\Psi_N \equiv \Psi_N(t, X_N) \in \mathfrak{H}_N = L^2(\mathbf{R}^{dN})$, then

$$i\hbar\partial_t\Psi_N = H_N\Psi_N \quad \Rightarrow \quad i\hbar\partial_t|\Psi_N\rangle\langle\Psi_N| = [\,H_N, |\Psi_N\rangle\langle\Psi_N|\,]$$

Proof compute the time-derivative of

$$e^{-itH_N/\hbar}\left(\left|\Psi_N\big|_{t=0}\right\rangle\left\langle\Psi_N\big|_{t=0}\right|\right)e^{itH_N/\hbar}$$

Exercise Is the converse true?

von Neumann equation with unknown $t \mapsto R_N(t) \in \mathcal{D}(\mathfrak{H}_N)$

$$i\hbar\partial_t R_N(t) = [H_N, R_N(t)]\,, \qquad R_N\big|_{t=0} = R_N^{in} \in \mathcal{D}(\mathfrak{H}_N)$$

Indistinguishable particles

For $\sigma \in \mathfrak{S}_N$ and $\Psi_N \in \mathfrak{H}_N = L^2(\mathbf{R}^{dN})$, define

$$U_\sigma \Psi_N(X_N) = \Psi_N(x_{\sigma^{-1}(1)}, \ldots, x_{\sigma^{-1}(N)})$$

Observe that

$$U_{\sigma\tau} = U_\sigma U_\tau\,, \qquad U_\sigma^* = U_\sigma^{-1}$$

Density operator R_N of a system of N indistinguishable particles

$$U_\sigma R_N U_\sigma^* = R_N \quad \text{for all } \sigma \in \mathfrak{S}_N$$

Do not mix indistinguishability with

$$U_\sigma \Psi_N = \Psi_N\,, \qquad \text{Bose-Einstein statistics}$$

$$U_\sigma \Psi_N = (-1)^{|\sigma|} \Psi_N\,, \qquad \text{Fermi-Dirac statistics}$$

Lemma Let $R_N^{in} \in \mathcal{D}(\mathfrak{H}_N)$, and assume that $U_\sigma R_N^{in} U_\sigma^* = R_N^{in}$. Then, the solution $R_N(t)$ of the N-particle von Neumann equation with initial data R_N^{in} satisfies

$$U_\sigma R_N(t) U_\sigma^* = R_N(t)\,, \qquad \text{for all } t \in \mathbf{R}$$

Proof Since the N-particle Hamiltonian

$$H_N := \sum_{j=1}^{N} -\tfrac{1}{2}\hbar^2 \Delta_{x_j} + \frac{1}{N} \sum_{1 \le j < k \le N} V(x_j - x_k)$$

satisfies $[H_N, U_\sigma] = 0$, one has $U_\sigma e^{-itH_N/\hbar} U_\sigma^* = e^{-itH_N/\hbar}$ so that

$$U_\sigma (e^{-itH_N/\hbar} R_N^{in} e^{itH_N/\hbar}) U_\sigma^* = e^{-itH_N/\hbar} (U_\sigma R_N^{in} U_\sigma^*) e^{itH_N/\hbar}$$

Hartree equation (wave function formalism)

Quantum mean-field theory used mostly for bosons (for fermions, there is a correction — exchange term)

Mean-field potential in quantum mechanics

$$V_\psi(t,x) := \int_{\mathbf{R}^d} V(x-z)|\psi(t,z)|^2 dz = V \star |\psi(t,\cdot)|^2(x)$$

Mean-field quantum Hamiltonian

$$H_\psi(t) := -\tfrac{1}{2}\hbar^2\Delta_x + V_\psi(t,x)$$

Hartree equation for the 1-particle wave function $\psi \equiv \psi(t,x) \in \mathbf{C}$

$$i\hbar\partial_t\psi(t,x) = H(t)\psi(t,x)\,, \qquad \psi\big|_{t=0} = \psi^{in}$$

Hartree equation (density operator formalism)

Unknown $t \mapsto R(t) \in \mathcal{D}(\mathfrak{H})$ where $\mathfrak{H} = L^2(\mathbf{R}^d)$

Mean-field potential denoting $\tau_x f(z) := f(z-x)$, assuming (H1)

$$V_R(t,x) := \operatorname{tr}(\tau_x V R(t)) = \int_{\mathbf{R}^d} V(x-z)\tilde{R}(t,z,z)dz$$

Mean-field quantum Hamiltonian

$$H_R(t) := -\tfrac{1}{2}\hbar^2\Delta_x + V_R(t,x)$$

Hartree equation

$$i\hbar\partial_t R(t) = [H_R(t), R(t)]\,, \qquad R\Big|_{t=0} = R^{in}$$

$\boxed{\text{THE BBGKY FORMALISM}}$

C. Bardos, F. Golse, N. Mauser:
Methods Appl. Anal. **7**, 275–293 (2000)

H. Spohn: Rev. Mod. Phys. **52**, 600–640 (1980)

C. Bardos, L. Erdös, F. Golse, N. Mauser, H.T. Yau:
C.R. Math. Acad. Sci. Paris **334**, 515–520 (2002)

Marginals of N-particle quantum densities

Let $R_N \in \mathcal{D}(\mathfrak{H}_N)$ satisfy $U_\sigma R_N U_\sigma^* = R_N$ for all $\sigma \in \mathfrak{S}_N$

Theorem One has $\mathcal{L}^1(\mathfrak{H}_N) = \mathcal{K}(\mathfrak{H}_N)'$ and $\mathcal{L}(\mathfrak{H}_N) = \mathcal{L}^1(\mathfrak{H}_N)'$

Definition For each $R_N \in \mathcal{D}(\mathfrak{H}_N)$ and each $n = 1, \ldots, N-1$, there exists a unique $R_{N:n} \in \mathcal{D}(\mathfrak{H}_n)$ s.t.

$$\mathrm{tr}_{\mathfrak{H}_n}(R_{N:n}A) = \mathrm{tr}_{\mathfrak{H}_N}(R_N(A \otimes I_{\mathfrak{H}_{N-n}})) \qquad \text{for all } A \in \mathcal{L}(\mathfrak{H}_n)$$

(Indeed, the r.h.s. defines a linear functional on finite rank operators A which is continuous for the operator norm)

For integral operators, denoting $Z_N^{n+1} = (z_{n+1}, \ldots, z_N)$, one has

$$\tilde{R}_{N:n}(X_n, Y_n) = \int_{\mathbf{R}^{d(N-n)}} \tilde{R}_N(X_n, Z_N^{n+1}, Y_n, Z_N^{n+1}) dZ_N^{n+1}$$

BBGKY hierarchy 1

Goal to write an equation for $R_{N:1}$

Pick $A \in \mathcal{L}(\mathfrak{H}_1)$ s.t. $[\Delta, A] \in \mathcal{L}(\mathfrak{H}_1)$; then

$$i\hbar\partial_t \operatorname{tr}_{\mathfrak{H}_1}(AR_{N:1}(t)) = -\operatorname{tr}_{\mathfrak{H}_N}([H_N, A \otimes I_{\mathfrak{H}_{N-1}}]R_N(t))$$

Denoting by V_{kl}(= the multiplication by)$V(x_k - x_l)$, one has

$$[H_N, A \otimes I_{\mathfrak{H}_{N-1}}] = -\tfrac{1}{2}\hbar^2[\Delta_{x_1}, A] \otimes I_{\mathfrak{H}_{N-1}} + \frac{1}{N}\sum_{k=2}^{N}[V_{1k}, A \otimes I_{\mathfrak{H}_{N-k}}]$$

Since $U_\tau R_N(t) U_\tau^* = R_N(t)$, where τ is the transposition $2 \leftrightarrow k$

$$\operatorname{tr}_{\mathfrak{H}_N}([V_{1k}, A \otimes I_{\mathfrak{H}_{N-1}}]R_N(t)) = \operatorname{tr}_{\mathfrak{H}_2}([V_{12}, A \otimes I_{\mathfrak{H}_1}]R_{N:2}(t))$$

Thus

$$i\hbar\partial_t \operatorname{tr}_{\mathfrak{H}_1}(AR_{N:1}(t)) = -\operatorname{tr}_{\mathfrak{H}_1}\left(-\tfrac{1}{2}\hbar^2[\Delta_{x_1}, A]R_{N:1}(t)\right) - \tfrac{N-1}{N}\operatorname{tr}_{\mathfrak{H}_2}([V_{12}, A \otimes I_{\mathfrak{H}_1}]R_{N:2}(t))$$

for all $A \in \mathcal{L}(\mathfrak{H}_1)$ s.t. $[\Delta, A] \in \mathcal{L}(\mathfrak{H}_1)$

This is the weak formulation of the 1st BBGKY equation:

$$i\hbar\partial_t R_{N:1} = [-\tfrac{1}{2}\hbar^2\Delta_{x_1}, R_{N:1}] + \tfrac{N-1}{N}[V_{12}, R_{N:2}]_{:1}$$

This is **not** a closed equation on $R_{N:1}$, since it involves $R_{N:2}$

Seek an equation for $R_{N:2}(t)$. Pick $B \in \mathcal{L}(\mathfrak{H}_2)$ s.t. $[\Delta_{x_j}, B] \in \mathcal{L}(\mathfrak{H}_2)$ for $j = 1, 2$; then

$$i\hbar\partial_t \operatorname{tr}_{\mathfrak{H}_2}(BR_{N:2}(t)) = -\operatorname{tr}_{\mathfrak{H}_N}([H_N, B \otimes I_{\mathfrak{H}_{N-2}}]R_N(t))$$

Then

$$[H_N, B \otimes I_{\mathfrak{H}_{N-2}}] = \sum_{j=1}^{2}[-\tfrac{1}{2}\hbar^2\Delta_{x_j}, B] \otimes I_{\mathfrak{H}_{N-2}} + \frac{1}{N}[V_{12}, B] \otimes I_{\mathfrak{H}_{N-2}}$$
$$+ \frac{1}{N}\sum_{j=1}^{2}\sum_{k=3}^{N}[V_{jk}, B \otimes I_{\mathfrak{H}_{N-2}}]$$

BBGKY hierarchy 2

By indistinguishability, for $j = 1, 2$ and $k \geq 3$

$$\begin{aligned}\mathrm{tr}_{\mathfrak{H}_N}([V_{jk}, A \otimes I_{\mathfrak{H}_{N-2}}]R_N) &= \mathrm{tr}_{\mathfrak{H}_N}(([V_{j3}, A \otimes I] \otimes I_{\mathfrak{H}_{N-3}})R_N) \\ &= \mathrm{tr}_{\mathfrak{H}_N}(([V_{j3}, A \otimes I]R_{N:3})\end{aligned}$$

so that, arguing as above

$$\begin{aligned}i\hbar\partial_t R_{N:2} = &\sum_{j=1}^{2}[-\tfrac{1}{2}\hbar^2\Delta_{x_j}, R_{N:2}] \\ &+ \underbrace{\tfrac{N-2}{N}\sum_{j=1}^{2}[V_{j3}, R_{N:3}]_{:2}}_{\text{interaction term}} + \underbrace{\tfrac{1}{N}[V_{12}, R_{N:2}]}_{\text{recollision term}}\end{aligned}$$

BBGKY hierarchy n

More generally, for each $n = 1, \ldots, N-1$

$$i\hbar\partial_t R_{N:n} = \sum_{j=1}^{n}[-\tfrac{1}{2}\hbar^2\Delta_{x_j}, R_{N:n}]$$
$$+ \underbrace{\tfrac{N-n}{N}\sum_{j=1}^{n}[V_{j,n+1}, R_{N:n+1}]_{:n}}_{\text{interaction term}} + \underbrace{\tfrac{1}{N}\sum_{j,k=1}^{n}[V_{jk}, R_{N:n}]}_{\text{recollision term}}$$

For $n = N$, one has $R_{N:N} = R_N$, and the Nth equation in the BBGKY hierarchy is the N-particle von Neumann equation

Hence

$$\text{von Neuman} \ \subset \ \text{BBGKY} \ \Leftarrow \ \text{von Neumann}$$

Hartree hierarchy

Passing to the limit formally in the nth BBGKY equation as $N \to \infty$, assuming that $R_{N:n}(t) \to R_n(t) \in \mathcal{D}(\mathfrak{H}_n)$

$$i\hbar\partial_t R_n = \sum_{j=1}^{n}[-\tfrac{1}{2}\hbar^2\Delta_{x_j}, R_n] + \sum_{j=1}^{n}[V_{j,n+1}, R_{n+1}]_{:n}\,, \qquad n \geq 1$$

since the recollision term is formally of order $O(n^2/N)$

Hartree hierarchy formally similar to the BBGKY hierarchy; however, the following differences are fundamental

•it is an infinite hierarchy

•there are no recollision terms

A key observation

Let $R \equiv R(t) \in \mathcal{D}(\mathfrak{H}_1)$ be he solution of the Hartree equation

$$i\hbar\partial_t R(t) = [H_R(t), R(t)]\,, \qquad R\Big|_{t=0} = R^{in}$$

Then

$$i\hbar\partial_t R(t)^{\otimes n} = \sum_{j=1}^{n}[-\tfrac{1}{2}\hbar^2\Delta_{x_j}, R(t)^{\otimes n}] + \sum_{j=1}^{n}[V_{j,n+1}, R(t)^{\otimes(n+1)}]_{:n}$$

I.e. the sequence of tensor powers of the solution of the Hartree equation is an exact solution of the infinite Hartree hierarchy
Not true in general for the BBGKY hierarchy! (another difference between both hierarchies...)

The strategy

(1) Justify rigorously the "formal" limit from the BBGKY to the Hartree hierarchy (relatively easy)

Idea with $R_{N:n} := 0$ for $n > N$, the sequence of sequences $(R_{N:n})_{n\geq 1}$ indexed by N is bounded in

$$\prod_{n\geq 1} L^\infty(\mathbf{R}_+;\mathcal{L}^1(\mathfrak{H}_n))$$

By Banach-Alaoglu+diagonal extraction, one can find an increasing sequence of integers $\phi(N)$ such that

$$R_{\phi(N):n} \to R_n \text{ in } L^\infty(\mathbf{R}_+;\mathcal{L}^1(\mathfrak{H}_n)) \text{ weakly} - * \text{ as } N \to \infty$$

(2) Prove that the solution of the Hartree hierarchy is uniquely determined by its initial data (quite difficult in general)

The mean-field limit theorem

Assume that $V \in L^\infty(\mathbf{R}^d)$. Let $R^{in} \in \mathcal{D}(\mathfrak{H}_1)$ satisfy $[\Delta, R^{in}] \in \mathcal{L}(\mathfrak{H}_1)$. Let $R \equiv R(t)$ be the solution of the Hartree equation

$$i\hbar\partial_t R(t) = [H_R(t), R(t)]\,, \qquad R\Big|_{t=0} = R^{in}$$

and let $R_N(t)$ be the solution of the N-body von Neumann equation

$$i\hbar\partial_t R_N(t) = [H_N, R_N(t)]\,, \qquad R_N\Big|_{t=0} = (R^{in})^{\otimes N}$$

Then, for each $n \geq 1$, one has

$$R_{N:n} \to R^{\otimes n} \text{ in } L^\infty(\mathbf{R}_+; \mathcal{L}^1(\mathfrak{H}_n)) \text{ weak-*}$$

as $N \to \infty$.

Differential equation $\dot{u}(t) = F(t, u(t))$

Scale of Banach spaces $(B_r)_{r\geq 0}$, norms $\|\cdot\|_r$ s.t.

$$r' \leq r \Rightarrow B_r \subset B_{r'} \text{ with } \|\cdot\|_{r'} \leq \|\cdot\|_r$$

Assumptions on F

(a) there exists $r_0 > 0$ s.t.

$$0 < r' < r < r_0 \Rightarrow F \in C(\mathbf{R} \times B_r, B_{r'})$$

$$\text{and } B_r \ni z \mapsto F(t,z) \in B_{r'} \text{ is linear for all } t \in \mathbf{R}$$

(b) there exists $C > 0$ s.t.

$$0 < r' < r < r_0 \Rightarrow \|F(t,z)\|_{r'} \leq C\frac{\|z\|_r}{r - r'}$$

Thm. (Ovcyannikov DAN'71, Nirenberg J Diff Geo '72)
For all $r \in (0, r_0)$ and all $\alpha > 0$, the only solution of

$$\dot{u}(t) = F(t, u(t)), \quad u(0) = 0$$

in $C^1((-\alpha, \alpha), B_r)$ is $u = 0$.

What does this have to do with CK? Consider PDE

$$\partial_t u(t, z) = P(t, z, \partial_z) u(t, z), \quad u\big|_{t=0} = 0$$

where P is a 1st order linear differential operator with coefficients bounded and analytic on strip $|\Im(z)| < r_0$

Assumption (b) is Cauchy estimate for $\partial_z u$ on the strip $|\Im(z)| < r'$ by u on the bigger strip $|\Im(z)| < r$

Application to infinite hierarchy

Sequence of Banach spaces $(E_n)_{n\geq 1}$, norm $|\cdot|_n$, with strongly continuous groups of isometries $U_n(t)$ in E_n

Family of bounded linear operators $L_{n,n+1} : E_{n+1} \to E_n$ for $n \geq 1$

Infinite hierarchy: for each $n \geq 1$

$$\dot{u}_n(t) = U_n(t) L_{n,n+1} U_{n+1}(-t) u_{n+1}(t)\,, \qquad u_n(0) = 0$$

Theorem (Bardos-FG-Erdös-Mauser-Yau CRAS02) Assume that

$$\|L_{n,n+1}\|_{\mathcal{L}(E_{n+1},E_n)} \leq Cn\,, \qquad n \geq 1$$

Let $u_n \in C^1([0,t^*], E_n)$ for $n \geq 1$ satisfy the infinite hierarchy and

$$\sup_{0\leq t\leq t^*} \|u_n(t)\|_n \leq R^n \text{ for all } n \geq 1$$

Then $u_n = 0$ on $[0,t^*]$ for all $n \geq 1$

Application to infinite hierarchies

Scale of Banach spaces

$$B_r := \left\{ v = (v_n)_{n\geq 1} \in \prod_{n\geq 1} E_n \text{ s.t. } \|v\|_r := \sum_{n\geq 1} r^n |v_n|_n < \infty \right\}$$

Function F:

$$F(t,v) := (U_n(t) L_{n,n+1} U_{n+1}(-t) v_{n+1})_{n\geq 1}$$

so that

$$\|F(t,v)\|_{r'} \leq C \sum_{n\geq 1} n r'^n |v_n|_n \leq C \sum_{n\geq 1} \frac{r^{n+1} - r'^{n+1}}{r - r'} |v_n|_n$$
$$\leq \frac{C}{r - r'} \sum_{n\geq 1} r^{n+1} |v|_{n+1} \leq \frac{C|v|_r}{r - r'}$$

$\boxed{\text{PICKL'S METHOD}}$

P. Pickl: Lett. Math. Phys. **97**, 151–164 (2011)

Assume that V is even, that $V \in L^{2r}(\mathbf{R}^3)$ for some $r \geq 1$, and that $V\mathbf{1}_{|z|>R} \in L^\infty(\mathbf{R}^3)$ for some $R > 0$.
Set $\hbar = 1$.

Assume that the Cauchy problem for Hartree's equation has a unique solution $\psi \in C(\mathbf{R}; L^{2r'}(\mathbf{R}^3))$, with $r' = \frac{r}{r-1}$, with initial data $\psi^{in} \in L^2(\mathbf{R}^3)$ satisfying $\|\psi^{in}\|_{L^2} = 1$.
Let $\Psi_N = e^{-itH_N}(\psi^{in})^{\otimes N}$, and let $R_N = |\Psi_N\rangle\langle\Psi_N|$.

Then

$$\| R_{N:1}(t) - |\psi(t,\cdot)\rangle\langle\psi(t,\cdot)| \|$$
$$\leq 3 \min\left(1, \frac{1}{\sqrt{N}}\left(\exp\left|\int_0^t 10\|V\|_{L^{2r}}\|\psi(s,\cdot)\|_{L^{2r'}} ds\right| - 1\right)^{1/2}\right)$$

Pickl's functional 1

Let $\hbar = 1$ and $R_N(t) := |\Psi_N(t,\cdot)\rangle\langle\Psi_N(t,\cdot)|$, where Ψ_N is the solution of the N-particle Schrödinger equation

$$i\partial_t\Psi_N = H_N\Psi_N\,, \qquad \Psi_N\big|_{t=0} = \Psi_N^{in}$$

Assume that, for all $\sigma \in \mathfrak{S}_N$

$$U_\sigma\Psi_N^{in} = \Psi_N^{in} \quad \text{so that } U_\sigma\Psi(t,\cdot) = \Psi(t,\cdot) \quad \text{for all } t \in \mathbf{R}$$

Let $\psi \equiv \psi(t,x) \in \mathbf{C}$ be the wave function solution of

$$i\partial_t\psi = H_\psi(t)\psi\,, \qquad \psi\big|_{t=0} = \psi^{in}$$

Set $\rho(t) := |\psi(t,\cdot)\rangle\langle\psi(t,\cdot)|$ and define

$$\mathcal{E}_N(t) := \mathrm{tr}_{\mathfrak{H}_1}(R_{N:1}(t)(I - \rho(t)))$$

$\mathcal{E}_N$ controls the operator norm

Lemma $\|R_{N:1}-\rho\| \le 2\mathcal{E}_N^{1/2}+\mathcal{E}_N$

Proof Observe that

$$R_{N:1}=(p+\rho)R_{N:1}(p+\rho)\,,\quad \rho R_{N:1}\rho=\langle\psi|R_{N:1}|\psi\rangle\rho=\mathrm{tr}(R_{N:1}\rho)\rho$$

so that

$$R_{N:1}-\rho=R_{N:1}-\mathrm{tr}(R_{N:1}\rho)\rho-\mathcal{E}_N\rho=pR_{N:1}+\rho R_{N:1}p-\mathcal{E}_N\rho$$

Since

$$\mathcal{E}_N=\mathrm{tr}_{\mathfrak{H}_1}(R_{N:1}p)=\mathrm{tr}_{\mathfrak{H}_N}(R_N(p\otimes I_{\mathfrak{H}_{N-1}}))=\|(p\otimes I_{\mathfrak{H}_{N-1}})\Psi_N\|^2_{\mathfrak{H}_N}$$

one has

$$\|pR_{N:1}\|=\|\,|(p\otimes I_{\mathfrak{H}_{N-1}})\Psi_N\rangle\langle\Psi_N|\,\|\le\mathcal{E}_N^{1/2}$$
$$\|\rho R_{N:1}p\|\le\|R_{N:1}p\|=\|(R_{N:1}p)^*\|=\|pR_{N:1}\|$$

Evolution of $\mathcal{E}_N(t)$

Lemma Denote $p(t) = I - \rho(t)$; then

$$\dot{\mathcal{E}}_N(t) = \mathcal{F}_N(t) = 2\Im \operatorname{tr}(R_{N:2}(t)(\rho(t)\otimes I)W(t)(p(t)\otimes I))$$

with

$$W(t) := \tfrac{N-1}{N}V_{12} - (V \star |\psi(t,\cdot)|^2) \otimes I$$

The core result in Pickl's argument is the following proposition

Proposition Let $r \geq 1$, and set $r' = \frac{r}{r-1}$; then

$$|\mathcal{F}_N(t)| \leq 10\|V\|_{L^{2r}}\|\psi(t,\cdot)\|_{L^{2r'}}\left(\mathcal{E}_N(t) + \tfrac{1}{N}\right)$$

Expand $\mathcal{F}_N(t)$ as

$$\begin{aligned}\mathcal{F}_N(t) =& 2\Im \operatorname{tr}(R_{N:2}(t)(\rho(t)\otimes I)W(t)(p(t)\otimes I))\\ =& 2\Im \operatorname{tr}(R_{N:2}(t)((\rho(t)\otimes \rho(t))W(t)(p(t)\otimes \rho(t)))\\ &+ 2\Im \operatorname{tr}(R_{N:2}(t)((\rho(t)\otimes \rho(t))W(t)(p(t)\otimes p(t)))\\ &+ 2\Im \operatorname{tr}(R_{N:2}(t)((\rho(t)\otimes p(t))W(t)(p(t)\otimes p(t)))\\ =& 2\Im(\,(1)+(2)+(3)\,)\end{aligned}$$

since, by indistinguishability

$$\operatorname{tr}(R_{N:2}((\rho\otimes p)W(p\otimes\rho)) = \operatorname{tr}((p\otimes\rho)W(\rho\otimes p)R_{N:2}) \in \mathbf{R}$$

Goal to control $\mathcal{F}_N$ by a linearly growing function of $\mathcal{E}_N$ and apply Gronwall's inequality

Writing $\rho \otimes p = (\rho \otimes I)(I \otimes p)$ and $p \otimes p = (p \otimes I)(I \otimes p)$, one has

$$\begin{aligned}(3) &\le \|(\rho \otimes I)W(p \otimes I)\| \operatorname{tr}_{\mathfrak{H}_2}((I \otimes p)R_{N:2}(I \otimes p)) \\ &\le \|(\rho \otimes I)W\| \operatorname{tr}_{\mathfrak{H}_1}(R_{N:1}p) = \|(\rho \otimes I)W\|\mathcal{E}_N\end{aligned}$$

Observe that

$$\langle \psi | \tau_{x_2} V^2 | \psi \rangle = (V^2)_\psi(x_2) \text{ so that } (\rho \otimes I)V_{12}^2(\rho \otimes I) = \rho \otimes (V^2)_\psi$$

and therefore

$$\begin{aligned}\|(\rho \otimes I)W\|^2 &= \|(\rho \otimes I)W^2(\rho \otimes I)\| \\ \le (2\|V^2\|_{L^r} + 2\|(V \star |\psi(t,\cdot)|^2)^2\|_{L^r})\| \, |\psi(t,\cdot)|^2\|_{L^{r'}} \\ &\le 4\|V\|_{L^{2r}}^2 \|\psi(t,\cdot)\|_{L^{2r'}}^2\end{aligned}$$

Bounding (1)

Since $\|R_{N:2}\| \leq \mathrm{tr}(R_{N:2}) = 1$ and $\|p\| \leq 1$

$$(1) \leq \|(\rho \otimes \rho)W(t)(p \otimes \rho)\| \leq \|(\rho \otimes I)(I \otimes \rho)W(I \otimes \rho)\|$$

Observe that

$$(I \otimes \rho)W(I \otimes \rho) = -\frac{1}{N}(V \star |\psi(t,\cdot)|^2) \otimes \rho$$

Hence

$$\begin{aligned}\|(\rho \otimes I)(I \otimes \rho)W(I \otimes \rho)\|^2 &\leq \|(\rho \otimes I)((I \otimes \rho)W(I \otimes \rho))^2(\rho \otimes I)\| \\ &= \frac{1}{N^2}\|\langle\psi|V_\psi^2|\psi\rangle\rho \otimes \rho\| \leq \frac{1}{N^2}\int |V_\psi(t,x)|^2|\psi(t,x)|^2 dx \\ &\leq \frac{1}{N^2}\|V_\psi(t,\cdot)\|_{L^{2r}}^2\|\psi(t,\cdot)\|_{L^{2r'}}^2 \leq \frac{1}{N^2}\|V\|_{L^{2r}}^2\|\psi(t,\cdot)\|_{L^{2r'}}^2\end{aligned}$$

Key lemma

Notation

(1) For $T \in \mathcal{L}(\mathfrak{H}_1)$, set $T_{j,N} = I_{\mathfrak{H}_{j-1}} \otimes T \otimes I_{\mathfrak{H}_{N-j}} \in \mathcal{L}(\mathfrak{H}_N)$

(2) For $a \in \{0,1\}^{\{1,\ldots,N\}}$ and $\pi = \pi^* = \pi^2 \in \mathcal{L}(\mathfrak{H}_1)$, set

$$P_N[a,\pi] := \prod_{j=1}^{N} \pi_{N,j}^{1-a(j)} (I - \pi_{N,j})^{a(j)}$$

Lemma The spectral decomposition of

$$M_N := \frac{1}{N} \sum_{j=1}^{N} p_{j,N} \quad \text{is} \quad M_N = \sum_{k=1}^{N} \frac{k}{N} \Pi_{k,N}[\rho]$$

where the spectral projections are

$$\Pi_{k,N}[\rho] = \sum_{a(1)+\ldots+a(N)=k} P_N[a,\rho] = \Pi_{k,N}[\rho]^*$$

$$\Pi_{k,N}[\rho]\Pi_{l,N}[\rho] = \delta_{kl}\Pi_{k,N}[\rho]\,.$$

Bounding (2)

Corollary Let $M_N^{-1/2}$ be the pseudo-inverse of $M_N^{1/2}$ extended by 0 on $\ker(M_N)$; then

$$M_N^{1/2} M_N^{-1/2} = I - \Pi_{0,N}[\rho] = I - \rho^{\otimes N} \Rightarrow M_N^{1/2} M_N^{-1/2} p_{j,N} = p_{j,N}$$

Therefore

$$\begin{aligned}
(2) &= \mathrm{tr}_{\mathfrak{H}_2}(R_{N:2}((\rho \otimes \rho) W (p \otimes p)) \\
&= \mathrm{tr}_{\mathfrak{H}_N}(R_N \rho_{1,N} \rho_{2,N} W p_{1,N} p_{2,N}) \\
&= \mathrm{tr}_{\mathfrak{H}_N}(R_N \rho_{1,N} \rho_{2,N} W M_N^{1/2} M_N^{-1/2} p_{1,N} p_{2,N}) \\
&\leq \underbrace{\|M_N^{-1/2} p_{1,N} p_{2,N} \Psi_N\|_{\mathfrak{H}_N}}_{(2a)} \underbrace{\|M_N^{1/2} W \rho_{1,N} \rho_{2,N} \psi_N\|_{\mathfrak{H}_N}}_{(2b)}
\end{aligned}$$

Bounding (2a)

By the bosonic symmetry (symmetry of the wave function Ψ_N)

$$\begin{aligned}N(N-1)(2a)^2 =& N(N-1)\langle\Psi_N|M_N^{-1}p_{1,N}p_{2,N}|\Psi_N\rangle\\ =& 2\sum_{1\le j<k\le N}\langle\Psi_N|M_N^{-1}p_{j,N}p_{k,N}|\Psi_N\rangle\\ \le& \langle\Psi_N|M_N^{-1}(NM_N)^2|\Psi_N\rangle = N^2\langle\Psi_N|M_N|\Psi_N\rangle\end{aligned}$$

Hence

$$N(N-1)(2a)^2 = \operatorname{tr}_{\mathfrak{H}_N}(R_N p_{1,N}) = N^2\operatorname{tr}_{\mathfrak{H}_1}(R_{N:1}p) = N^2\mathcal{E}_N$$

Bounding (2b)

Using again the bosonic symmetry

$$\begin{aligned}\|M_N^{1/2} W \rho_{1,N}\rho_{2,N}\psi_N\|^2_{\mathfrak{H}_N} &= \langle \Psi_N | \rho_{1,N}\rho_{2,N} W M_N W \rho_{1,N}\rho_{2,N} | \Psi_N\rangle \\ &= \tfrac{N-2}{N} \langle \Psi_N | \rho_{1,N}\rho_{2,N} W p_{3,N} W \rho_{1,N}\rho_{2,N} | \Psi_N\rangle \\ &\quad + \tfrac{2}{N} \langle \Psi_N | \rho_{1,N}\rho_{2,N} W p_{1,N} W \rho_{1,N}\rho_{2,N} | \Psi_N\rangle \\ &= (2b1) + (2b2)\end{aligned}$$

Since $p_{3,N} = p_{3,N}^* = p_{3,N}^2$ commutes with $\rho_{1,N}$, $\rho_{2,N}$ and W

$$\begin{aligned}(2b1) &\le \tfrac{N-2}{N} \|p_{3,N}\Psi_N\|^2_{\mathfrak{H}_N} \|\rho_{1,N}\rho_{2,N} W^2 \rho_{1,N}\rho_{2,N}\| \\ &\le \|\rho_{1,N} W^2 \rho_{1,N}\| \mathcal{E}_N \le 4\|V\|^2_{L^{2r}} \|\psi(t,\cdot)\|^2_{L^{2r'}} \mathcal{E}_N\end{aligned}$$

Since $\rho_{2,N}$ commutes with $\rho_{1,N}$ and $p_{1,N}$ is a projection

$$\begin{aligned}(2b2) &\le \tfrac{2}{N} \|\rho_{1,N}\rho_{2,N} W p_{1,N} W \rho_{1,N}\rho_{2,N}\| \le \tfrac{2}{N} \|\rho_{1,N}\rho_{2,N} W p_{1,N}\|^2 \\ &\le \tfrac{2}{N} \|\rho_{1,N} W\|^2 \le \tfrac{2}{N} \|\rho_{1,N} W^2 \rho_{1,N}\| \le \tfrac{8}{N} \|V\|^2_{L^{2r}} \|\psi(t,\cdot)\|^2_{L^{2r'}}\end{aligned}$$