Ab initio approximations for N Particles Schrödinger Equation.

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N body Schrödinger equation and densities

$$i\hbar\partial_t\Psi_N(X_N,t) = -\frac{\hbar^2}{2}\Delta\Psi_N(X_N,t) + C(N)\sum_{1\le j<k\le n} V_N(|x_j - x_k|)\Psi_N(X_N,t)$$

$$X_N = (x_1, x_2, \dots, x_N) \in \mathbb{R}^{3N}\,,\ i\hbar\partial_t\Psi_N = H_N\Psi_N\,,$$

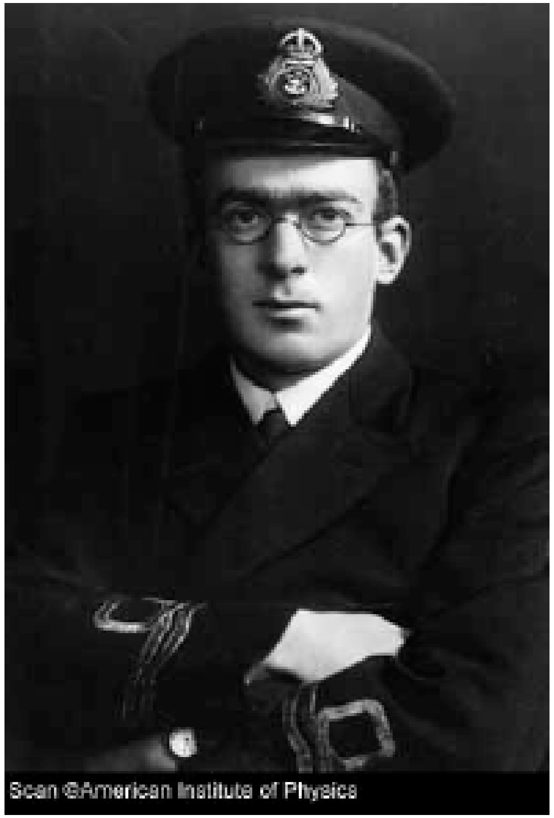
$$\int_{\mathbb{R}^{3N}} |\Psi_N(X_N,t)|^2 dX_N = 1$$

$$\int_{\mathbb{R}^{3N}} (H_N\Psi_N(X_N,t), \Psi_N(X_N,t))dX_N = \int_{\mathbb{R}^{3N}} (H_N\Psi_N(X_N,0), \Psi_N(X_N,0))dX_N$$

$$D_N = \Psi_N(X_N,t)\otimes\overline{\Psi_N(Y_N,t)}\,,\ i\hbar\partial_t D_N(X_N,t) = [H_N, D_N]\,,$$

$$\text{Trace } D_N = 1\,,\ \text{Trace } (H_N D_N(X_N,t)) = \text{Trace } (H_N D_N(X_N,0))$$

$$(\sigma f)(x_{\sigma(1)}, x_{\sigma(2)}, \dots, x_{\sigma(N)})\ \text{Indistinguishability} D_N\sigma = \sigma D_N$$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APPROXIMATIONS : Galerkin, Hartree, Hartree Fock, MCDTHF.

Multiscale Analysis, Time dependent problems

- $\hbar$ Planck constant ("small")

- N Number of particles ("large")

- Frequency of the data (Energy norm) $\Psi(X, 0) = A(X)e^{i\frac{S(X)}{\hbar}}$

- Structure of the data.

I. Catto, F. Golse, A. Gottlieb, O. Koch, C. Lubich, N. Mauser, S. Trabelsi

Galerkin

$$(\phi_i, \phi_j) = \delta ij \,, \tilde{\Psi}_N = \sum_{1 \le i \le k} a_i(t)\phi_i(X_N) \,,$$

$$i\hbar \frac{da_i(t)}{dt} + \sum_{1 \le j \le k} (H_N \phi_j, \phi_i) a_j(t) = 0 \,.$$

Hartree

$$\int |\psi(x,t)|^2 dx = 1 \, \tilde{\Psi}_N = \prod_{1 \le j \le N} \psi(x_j, t) \,,$$

$$i\hbar \partial_t \psi = -\frac{\hbar^2}{2} \Delta\psi + \int (V(x-z)|\psi(z)|^2 dz)\psi$$

Hartree Fock

$$\tilde{\Psi}_N(x_1,\dots,x_N) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \psi_1(x_1) & \psi_1(x_2) & \cdots & \psi_1(x_N) \\ \psi_2(x_1) & \psi_2(x_2) & \cdots & \psi_2(x_N) \\ \vdots & \vdots & & \vdots \\ \psi_N(x_1) & \psi_N(x_2) & \cdots & \psi_N(x_N) \end{vmatrix}, (\psi_i,\psi_j)=\delta_{ij}$$

$$i\hbar\frac{\partial}{\partial t}\psi_k(t,x) = -\frac{\hbar^2}{2}\Delta_x\psi_k(t,x) + \Bigg\{\psi_k(t,x)\sum_{l=1}^{N}\int V(x-z)|\psi_l(t,z)|^2dz - \sum_{l=1}^{N}\psi_l(t,x)\int V(x-z)\psi_k(t,z)\overline{\psi_l(t,z)}dz\Bigg\}$$

MCTDHF $K \geq N$

Galerkin + Hartree Fock

$$\Phi = (\phi_1(x,t), \cdots, \phi_K(x,t))^T, \int_{\mathbb{R}^3} \phi_i(x,t)\bar{\phi}_j(x,t)dx = \delta_{i,j},$$

$$\Sigma = \{\sigma : \{1 \ldots N\} \mapsto \{1 \ldots K\}, i < j \Rightarrow \sigma(i) < \sigma(j)\}$$

$$\tilde{\Phi} = \sum_{\sigma \in \Sigma} a_\sigma \phi_\sigma(X_N, t), \phi_\sigma(X_N, t) = \frac{1}{\sqrt{N!}} det(\phi_{\sigma(i)}(x_i, t)), 1 \leq i \leq N.$$

$$i\frac{da_\sigma}{dt} = \sum_{\sigma' \in \Sigma} (\sum_{1 \leq i < j \leq N} V(|x_i - x_j|)\Phi_{\sigma'}, \Phi_\sigma) a_{\sigma'} \text{ Galerkin}$$

$$\Gamma i\hbar\partial_t \Phi = -\frac{\hbar^2}{2}\Gamma\Delta\Phi + (I - P)(W_{C,\Phi}\Phi), \text{ Hartree Fock}$$

$P = \sum_{1 \leq i \leq K} \phi_i\rangle\langle\phi_i$, Γ and $W_{C,\Phi}$ next pages...

Remarks concerning all the above examples

• All the approximations are as the initial Schrödinger equation time reversible. No irreversibility appears in the process.

• The total L^2 norm is conserved : $\int_{\mathbb{R}^{3N}} |\tilde{\Psi}_N(X_N)|^2 dX_N = 1$ probability

• For Galerkin, Hartree Fock and MCTDHF conservation of orthogonality of "orbitals" $\phi_i(x,t)$

- All the "Ansatz" $\tilde{\Phi}(X_N)$ are defined from a set $\mathcal{F}$ of parameter by "simple" algebraic map $\pi : \mathcal{F} \to L^2(\mathbb{R}^{3N})$

Galerkin $\mathcal{F} = \{a = (a_1, a_2, \dots a_k) \in \mathbb{C}^k, \sum_{1\le i\le k} |a_i|^2 = 1\}$

$$\pi(a) = \sum_{1\le i\le k} a_k(t)\phi_k(x)$$

Hartree $\mathcal{F} = \{\phi(x) \in L^2(\mathbb{R}^3) \int_{\mathbb{R}^3} |\phi(x)|^2 dx = 1\}$,

$$\pi(\phi) = \prod_{1\le i\le N} \phi(x_i)$$

Hartree Fock $\mathcal{F} = \{\Phi = (\phi_1(x), \phi_2(x), \dots, \phi_N(x)), (\phi_i, \phi_j) = \delta_{ij})\}$

$$\pi(\Phi) = \frac{1}{\sqrt{N!}} det(\phi_i(x_j)) .$$

MCTDHF $K \ge N$,

$$\mathcal{F} = \{\Phi = (\phi_i(x))1 \le i \le K, (\phi_i, \phi_j) = \delta_{ij})\} \times \{a = (a_\sigma) \sum_{\sigma\in\Sigma} |a_\sigma|^2 = 1\},$$

$$\pi(\Phi, a) = \sum_{\sigma\in\Sigma} \frac{a_\sigma}{\sqrt{N!}} det(\phi_{\sigma(i)}(x_j)) .$$

DENSITIES

Schrödinger $D_N = \Psi_N(X_N, t) \otimes \overline{\Psi_N(Y_N, t)}$, $i\hbar\partial_t D_N(X_N, t) = [H_N, D_N]$;

$D_{N:n} = \int_{\mathbb{R}^{3(N-n)}} D(X_n, Z_n^N, Y_n, Z_n^N) dZ_n^N$

Galerkin $D_N = \sum_{ij} a_i(t)\overline{a}_j(t)\phi_i(x) \otimes \overline{\phi_j(y)}$

Hartree $D_{N:1} = \phi(x,t) \otimes \overline{\phi(y,t)}$

Hartree Fock $D_{N:1} = \frac{1}{N} \sum_{1 \le i \le K} \phi_i(x,t) \otimes \overline{\phi_i(y,t)}$

MCTDHF $D_{N:1} = \sum_{1 \le ij \le K} \gamma_{ij}\phi_i(x,t) \otimes \overline{\phi_j(y,t)}$

$1 \le i \le k$, $s(i,\sigma) = 0$ if $i \notin \sigma(\{1 \dots N\})$ otherwise $s(i,\sigma) = \sigma^{-1}(j)$;

$$\gamma_{ij} = \sum_{\sigma(\{1 \dots N\})-\{i\}=\sigma'(\{1 \dots N\})-\{j\}} (-1)^{s(i,\sigma)} a_\sigma (-1)^{s(i,\sigma')} \overline{a'_\sigma}$$

Fibration and Variation

• The mapping π from $\mathcal{F}$ with value in the "Ansatz" is not always a bijection.

• It is a bijection for Galerkin and Hartree. For Hartree Fock any special unitary transformation $S(t)$ of $\mathbb{C}^N$ gives the same determinant.

• For MCTDHF the rank of the matrix $\Gamma = \{\gamma_{ij}\}$ is the rank of the operator $D_{N:1}$. It is assumed to be constant and equal to K. Then any special unitary transformation of U of $\mathbb{C}^K$ induces by the formula : $\pi(\Phi, a) = \pi(U\Phi, a')$ a special unitary transformation on $\mathbb{C}^{\#\Sigma}$ and one has $\Gamma' = U\Gamma U^T$.

• In all the above cases $\mathcal{F}$ is a fiber bundle with π being the projection on the basis and any local section s being differentiable. Variation on the ansatz imply local variation on $T(\mathcal{F})$ and all the above approximation are designed to satisfy :

$$(\partial_t \tilde{\Phi}_N + iH_N \tilde{\Phi}_N, \delta \tilde{\Phi}_N) = 0 \,.$$

This gives in particular the equation :

$$\Gamma i\hbar\partial_t\Phi = -\frac{\hbar^2}{2}\Gamma\Delta\Phi + (I-P)(W_{C,\Phi}\Phi)\,,\quad \text{Hartree Fock}$$

with

$$\Gamma = (\gamma_{ij}) = \sum_{\sigma(\{1...N\})-\{i\}=\sigma'(\{1...N\})-\{j\}} (-1)^{s(i,\sigma)}a_\sigma(-1)^{s(i,\sigma')}\overline{a'_\sigma}\,;$$

$$(W_{C,\Phi})_{ij} = \frac{N(N-1)}{2}\sum_{kl}\sum_{\sigma(\{1...N\})-\{ij\}=\sigma'(\{1...N\})-\{kl\}} (-1)^{s(i,k,\sigma)}a_\sigma(-1)^{s(i,l,\sigma')}\overline{a'_\sigma} \int_{\mathbb{R}^3}\overline{\phi_l(y)}\phi_k(y)V(x-y)dy\,.$$

Consequences

- With $\partial_t \tilde{\Phi}_N = \delta \tilde{\Phi}_N$

$$(\partial_t \tilde{\Phi}_N + iH_N \tilde{\Phi}_N, \delta \tilde{\Phi}_N) = 0$$

gives *the conservation of energy*

$$\frac{d}{dt} \Re (H_N \tilde{\Phi}_N, \tilde{\Phi}_N) = 0$$

$$\frac{1}{2} \int |\nabla \phi|^2 + \int V(|x-y|) |\phi(x)|^2 |\phi(y)|^2 dxdy = Cte\,, \text{ Hartree.}$$

$$\frac{N}{2} \sum_i \int |\nabla \phi_i|^2 + \frac{N(N-1)}{2} (\sum_i \int V(|x-y|) |\phi_i(x)|^2 |\phi_i(y)|^2 dxdy$$

$$- \sum_{i<j} \sum_i \int V(|x-y|) |\phi_i(x)|^2 |\phi_i(y)|^2 dxdy) = Cte \text{ Hartree Fock.}$$

$$\frac{1}{2} \int (\Gamma \nabla \Phi, \nabla \Phi) + \sum_{kl} \sum_{\sigma(\{1...N\})-\{ij\}=\sigma'(\{1...N\})-\{kl\}} (-1)^{s(i,k,\sigma)} a_\sigma (-1)^{s(i,l,\sigma')} \overline{a'_\sigma}$$

$$\int_{\mathbb{R}^3} \overline{\phi_l(y)} \phi_k(y) \phi_j(x) \overline{\phi_i(x)} V(|x-y|) dxdy = Cte \text{ MCTDHF.}$$

• The conservation of energy leads to regularity estimates (in the MCDTHF only with the hypothesis rang$(\Gamma) = K$) giving existence and uniqueness of solutions of the corresponding equations with *singular* (Coulomb for instance) potential.

• The variationnal principle gives a posteriori and a priori erreur estimates : **Lubich.**

• In the case of Galerkin one has (with same initial data) denoting by $\pi(\mathcal{F})$ le subspace spanned by $(\phi_1, \phi_2, \ldots, \phi_n)$:

$$\|\Psi(t) - \tilde{\Psi}(t)\| \leq \int_0^t dist(iH\tilde{\Psi}_N, \pi(\mathcal{F}))ds \quad \text{A posteriori}$$

$$\|\Psi(t) - \tilde{\Psi}(t)\| \leq \int_0^t dist(\Psi, \pi(\mathcal{F}))ds \quad \text{A priori}$$

• In the case of MCTDHF one has (with same initial data and with the constant rank hypothesis) introducing the tangent space $T_{\pi(C,\Phi)}(\pi(\mathcal{F}))$ the a posteriori estimate.

$$\|\Psi(t) - \tilde{\Psi}(t)\| \leq \int_0^t dist(iH\tilde{\Psi}_N, \pi(\mathcal{F}))ds \quad \text{A posteriori.}$$

For the a priori estimate defines a notion of bound of curvature for a submanifold $\mathcal{M}$ of an Hilbert space $\mathcal{H}$ κ is a local bound of the curvature of $\mathcal{M}$ if "locally" one has the estimates :

$$\|P_{(T_u(\mathcal{M}))}\phi - P_{(T_v(\mathcal{M}))}\| \leq \kappa\|u - v\|\|\phi\|\,, \; \|(I - P_{(T_u(\mathcal{M}))})(u - v)\| \leq \|u - v\|^2$$

Assume

$$0 < s < \bar{t} \Rightarrow d(s) = dist(\Psi(s), \pi(\mathcal{F}) \leq \frac{1}{2\kappa} \text{ curvature } of \pi(\mathcal{F}(s))$$

Then a priori estimate :

$$\|\Psi(t) - \tilde{\Psi}(t)\| \leq d(t) + Ce^{K(\kappa t)} \int_0^t d(s)ds$$

• Estimates are models solutions dependent!!

”Mean Field limits, Hartree ansatz and Semiclassical limit”

N large, $\hbar$ small, frequency ? ?

lin. N-body Schrödinger equation	$\xrightarrow{\hbar\to 0}$	lin.N-body Hamiltonian
$\downarrow$ $\xrightarrow{1/N\to 0}$ $\downarrow$		$\downarrow$ $\xrightarrow{1/N\to 0}$ $\downarrow$
1-body “nonlin. Schrödinger”	$\xrightarrow{\hbar\to 0}$	1-body “Vlasov”

Reversibility is present everywhere in the above diagramm Wigner transform. This makes the derivation much easier. Much more difficult will be the derivation of macroscopic equations from Vlasov

Spohn, Brown and Hepp, Golse, Gottlieb, Mauser, Erdos, Schlein, Yau

Hartree Derivation

Partial traces, reduced densities.

$$D_{N:n}(X_N, Y_N) = \int D_N(x_1, x_2, \dots x_n, Z_n^N, y_1, y_2, \dots, y_n, Z_n^N) dZ_n^N$$

$$\forall K \in \mathcal{L}(L^2(\mathbb{R}^{3n}) \text{ Trace } ((K \otimes I_{n+1} \otimes \dots I_N) D_N) = \text{ Trace } (K D_{N:n})$$

$$D_N \text{ sym. pos. } \Rightarrow D_{N:n} \text{ sym. pos. }, \text{ Trace } (D_N) = 1 \Rightarrow \text{ Trace } (D_{N:n}) = 1$$

$$i\hbar \partial_t D_{N:n}(X_n, Y_n, t) = -\frac{\hbar^2}{2}[\Delta_{X_n} - \Delta_{Y_n}] D_{N:n}(X_n, Y_n, t)$$

$$+\frac{1}{N} \sum_{1 \le j < k \le n} [V(|x_j - x_k|) - V(|y_j - y_k|)] D_{N:n}(X_n, Y_n, t)$$

$$+\frac{N-n}{N} \sum_{1 \le j \le n} \int [V(|x_j - z|) - V(|y_j - z|)] D_{N:n+1}(X_n, z, Y_n, z, t) dz$$

$$i\hbar \partial_t D_n(X_n, Y_n, t) = -\frac{\hbar^2}{2}[\Delta_{X_n} - \Delta_{Y_n}] D_n(X_n, Y_n, t)$$

$$\sum_{1 \le j \le n} \int [V(|x_j - z|) - V(|y_j - z|)] D_{(n+1)}(X_n, z, Y_n, z, t) dz\,.$$

$$\partial_t D_n = i\mathcal{A}_n D_n + \mathcal{C}_{n+1,n} D_n\,, \|\mathcal{C}_{n+1,n}\| \simeq O(n)!!???$$

Strategies for Proofs

1 Show that an Ansatz generates a solution of the infinite Hierachy

2 Convergence of the finite Hierachy to the infinite Hierachy

3 Uniqueness and \ or stability of the Hierarchy.

In general 3 implies 2

1. Start from Schrödinger Poisson

$$i\hbar\partial_t\psi = -\frac{\hbar^2}{2}\Delta\psi + \int (V(x-z)|\psi(z)|^2 dz)\psi$$

Then

$$d(x,y,t) = \psi(x,t)\otimes\overline{\psi(y,t)}\,;\, D_n = \prod_{1\le i\le n} d(x_i,y_i,t)$$

is a solution of the infinite hierarchy.

3. Compare with the Riccati equation⇒ Riccati Hierarchy ;

$$y' = y^2\, y_n = y^n\,, (y_n)' = ny^{n-1} \Rightarrow (y_n)' = ny^{n+1}\,, Y' = C(Y).$$

With $V \in L^\infty$

$$\| \int [V(|x_j - z|) - V(|y_j - z|)] D_{(n+1)}(X_n, z, Y_n, z, t) dz \|_{\mathcal{L}^1} \leq$$
$$2 \| V(|x_j - x_{n+1}|) D_{(n+1)}(X_n, x_{n+1}, Y_n, y_{n+1}, t)|) \|_{\mathcal{L}^1} \leq \| V D_{n+1} \|_{\mathcal{L}^1}$$
$$\leq \|V\|_{L^\infty} \|D_{n+1}\|_{\mathcal{L}^1}$$

With V Coulomb like $V(|x|) = C|x|^{-1}$ compressed trace :

$$\|K\|_{\mathcal{L}^{1,1}(L^2(\mathbb{R}^{3n})} = \| \prod_{1 \leq i \leq n} (I - \Delta_{x_i})^{\frac{1}{2}} K \prod_{1 \leq i \leq n} (I - \Delta_{x_i})^{\frac{1}{2}} \|_{\text{trace}}$$

$$\| |\nabla_x| \int \frac{1}{|x - z|} d_2(x, z, y, z) dz |\nabla_y| \|_{\text{trace}}$$

Several terms and for typical Hardy inequality :

$$\| \int \frac{1}{|x-z|^2} \nabla_y d_2(x,z,y,z)\, dz \|_{\text{trace}}$$

$$\int \frac{|\phi(x)|^2}{|x|^2} dx \le 4 \int |\nabla \phi(x)|^2 dx \,.$$

$V_N \to b\delta$ Non linear Schrodinger equation.

$$i\hbar\partial_t \Psi_N(X_N,t) = -\frac{\hbar^2}{2}\Delta\Psi_N(X_N,t) + \frac{1}{N}\sum_{1\le j<k\le n} V_N(|x_j - x_k|)\Psi_N(X_N,t)$$

$$\Psi_N(X_N,0) = \prod_{1\le i\le N}\psi_i(x)\,, \quad D_N = \Psi_N(x,t)\otimes\overline{\Psi(y,t)}$$

$$i\hbar\partial_t D_{N:n}(X_n,Y_n,t) = -\frac{\hbar^2}{2}[\Delta_{X_n} - \Delta_{Y_n}]D_{N:n}(X_n,Y_n,t)$$

$$+\frac{1}{N}\sum_{1\le j<k\le n}[V_N(|x_j-x_k|) - V_N(|y_j-y_k|)]D_{N:n}(X_n,Y_n,t)$$

$$+\frac{N-n}{N}\sum_{1\le j\le n}\int[V_N(|x_j-z|) - V_N(|y_j-z|)]D_{N:n+1}(X_n,z,Y_n,z,t)dz$$

$$i\hbar\partial_t D_n(X_n,Y_n,t) = -\frac{\hbar^2}{2}[\Delta_{X_n},D_n] + \sum_{1\le j\le n}(D_n(X_n,x_j,Y_n,x_j,t) - D_n(X_n,y_j,Y_n,y_j,t))$$

$$i\hbar\partial_t\psi(x,t) = -\frac{\hbar^2}{2}\Delta_x\psi(x,t) + b|\psi(x,t)|^2\cdot\psi(x,t)\,,\ D_n(X_n,Y_n) = \prod_{1\le i\le n}\psi(x_i,t)\overline{\psi(y_i,t))}$$

The method of Erdos, Schlein and Yau

1 Use Duhamel expansion :

$$D_n(t) = \int_0^t ds_1 \int_0^{s_1} ds_2 \dots \int_0^{s_{m-1}} ds_m$$
$$U^n(t-s_1)C_{n+1,n}U^{k+1}(s_1-s_2)C_{n+2,n+1}\cdots$$
$$U^{n+m-1}(s_{m-1}-s_m)C_{n+m-1,m}D_{n+m}(s_m)$$

2 Express the above operator in term of elements of a Feynmann Graph

$$\sum_{\Gamma\in\mathcal{F}_{n,m}} (\mathcal{L}_\Gamma)_{n,n+m}\,,\ \#\mathcal{F}_{n,m} = 2^{4n+m}$$

By a Strichartz type regularising effect prove for that for $m > 10 + n/2$

$$\| \prod_{1\le i\le n} (I+(-\Delta_{x_i})^2)^{-1}(\mathcal{L}_\Gamma)_{n,m}D_{n+m}\|_{\mathrm{Tr}} \le C^m t^{\frac{m}{4}}\mathrm{Tr}\left(\prod_{1\le i\le n+m}(I+(-\Delta_{x_i}))D_{n+m}\right)$$

Fermions versus Bosons The Hartree Fock Ansatz

The TDHF equations is a system of N coupled Schrödinger equations for orthonormal orbitals $\psi_1(t,x), \psi_2(t,x), \ldots, \psi_N(t,x)$:

$$i\hbar\frac{\partial}{\partial t}\psi_k(t,x) = -\frac{\hbar^2}{2}\Delta_x\psi_k(t,x) + \frac{1}{N}\Big\{\psi_k(t,x)\sum_{l=1}^{N}\int V(x-z)|\psi_l(t,z)|^2 dz$$
$$- \sum_{l=1}^{N}\psi_l(t,x)\int V(x-z)\psi_k(t,z)\overline{\psi_l(t,z)}dz\Big\}$$

The N orbitals remain orthonormal at all times. This provides an approximation for the solution $\Psi(X_N,t)$ in agreement with the Pauli exclusion principle by

$$\Psi_N(x_1,\ldots,x_N) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \psi_1(x_1) & \psi_1(x_2) & \cdots & \psi_1(x_N) \\ \psi_2(x_1) & \psi_2(x_2) & \cdots & \psi_2(x_N) \\ \vdots & \vdots & & \vdots \\ \psi_N(x_1) & \psi_N(x_2) & \cdots & \psi_N(x_N) \end{vmatrix}.$$

$$D_N^{\text{Slater}} = \Psi_{\text{Slater}}(X_N,t)\otimes\overline{\Psi_{\text{Slater}}(Y_N,t)}$$

With the orthogonality one has :

$$D^{\text{Slater}}_{N:1}(x,y,t)=\frac{1}{N}\sum_{1\leq k\leq N}\psi_k(x,t)\overline{\psi_k(y,t)}=F_N(t)\,.$$

$$\begin{aligned} D^{\text{Slater}}_{N:n}(x,y,t) &= \frac{N^n(N-n)!}{N!}F_N(t)^{\otimes n}\sum_{\pi\in\Pi_n}\text{sgn}(\pi)U_\pi \\ &= \frac{N^n(N-n)!}{N!}\text{det}(F_N(x_i,y_j,t))_{1\leq i,j\leq n} \end{aligned}$$

$$\lim_{N\to\infty}\frac{N^n(N-n)!}{N!}=1$$

A closed equation for $F_N(t)$

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}F_N(t,x,y) &= -\frac{\hbar^2}{2}(\Delta_x-\Delta_y)F_N(t,x,y)+ \\ \int(V(x-z) &- V(y-z))(F_N(t,x,y)F_N(t,z,z)-F_N(t,x,z)F_N(t,z,y))dz\,. \end{aligned}$$

$$\|F(t)\|_{\text{trace}} = 1, \ \|F(t)\|_{\text{op}} = \frac{1}{N} \,.$$

Theorem with $V \in L^\infty$

$$\|D_{N:n}(x,y,t)\|_{\text{trace}} = \|D^{\text{Slater}}_{N:n}(x,y,t)\|_{\text{trace}} = 1$$

$$\lim_{N\to\infty} \|D_{N:n}(x,y,t) - D^{\text{Slater}}_{N:n}(x,y,t)\|_{\text{trace}} = 0$$

Good news

- Compare with WKB approximation for waves!!!

- As for the Hartree approximation, non linear Schrödinger, Boltzmann etc... $N \to \infty$. the constitutive laws are preserved.

- The proof can be adapted to Coulomb potential with density in the compressed trace class.

Bad news

- For bounded potential no use for the exchange term when $N \to \infty$.

$$\| \int V(x-z) F_N(x,z,t) F_N(z,y,t) dz \|_{\mathrm{Tr}} \leq \|V\|_\infty \|F_N\|_{\mathrm{Tr}} \|F_N\|_{\mathrm{op}} \leq \frac{\|V\|_\infty}{N}$$

- For Coulomb potential, with the compressed trace norm :

$$\mathrm{Tr}(I - \Delta) F_N(x,y,0) \leq C$$

With the Lieb Thirring inequality

$$\int \Big(\sum_{1 \leq i \leq N} |\psi_i(x)|^2 \Big)^{\frac{5}{3}} dx \leq C \int \sum_{1 \leq j \leq N} |\nabla \psi_j(x,0)|^2 dx$$

all the non linear terms in the Hartree Fock approximation vanishes with $N \to \infty$.

$$F(x,y) = \frac{1}{N} \sum_{1 \leq i \leq N} \psi_i(x) \otimes \overline{\psi_i(y)}$$

$$\|\int(\frac{1}{(|x-z|}-\frac{1}{|y-z|})F(z,z)F(x,y)dz\|_{\mathsf{Tr}} \le 2\iint\frac{F(z,z)}{|x-z|}F(x,x)dxdz =$$
$$\iint_{|x-z|\le R}\frac{F(z,z)}{|x-z|}F(x,x)dxdz + \int_{|x-z|>R}\int\frac{F(z,z)}{|x-z|}F(x,x)dxdz$$
$$\le \frac{1}{R} + \sup_x \int_{|x-z|>R}\frac{F(z,z)}{|x-z|}dz \le \frac{1}{R} + CR^{1/5}\left(\int(F(z,z))^{\frac{5}{3}}dz\right)^{\frac{3}{5}}$$
$$\le \frac{1}{R} + CR^{1/5}N^{-2/5}\mathsf{Tr}(-\Delta F)$$

which implies

$$\|\int(\frac{1}{(|x-z|}-\frac{1}{|y-z|})F(z,z)dzF(x,y)\|_{\mathsf{Tr}} \le CN^{-\frac{1}{3}}\mathsf{Tr}(-\Delta F)^{\frac{1}{2}}.$$