

# Asymptotics for the Hartree equation

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DISPERSIVE EQUATIONS WITH RANDOM INITIAL DATA  
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# Hamiltonian

We consider a system of  $N$  particles represented by a wave function  $\psi$  and evolving according to the energy :

$$\mathcal{E}_N = -\frac{1}{2} \sum_i \int \bar{\psi} \Delta_i \psi + \frac{1}{2} \sum_{i \neq j} w(x_i - x_j) \bar{\psi} \psi.$$

Here, we assume that the particles are fermions, which means that they satisfy Pauli's principle, in other words for all permutation  $\sigma$

$$\psi(x_{\sigma(1)}, \dots, x_{\sigma(n)}) = \varepsilon(\sigma) \psi(x_1, \dots, x_n).$$

We take  $\psi$  to be equal to

$$\psi = \frac{1}{\sqrt{N!}} \sum_{\sigma} \varepsilon(\sigma) \prod_i u_{\sigma(i)}(x_i)$$

with  $u_i$  orthogonal and normalised (Slater determinant).

# Hartree-Fock

We get the following energy :

$$\mathcal{E}_N = \mathcal{E}_{kin} + \mathcal{E}_{mf} + \mathcal{E}_{exch}$$

with

$$\mathcal{E}_{kin} = -\frac{1}{2} \sum_i u_i \Delta u_i$$

$$\mathcal{E}_{mf} = \frac{1}{2} \sum_{i \neq j} \int w * |u_i|^2 |u_j|^2$$

$$\mathcal{E}_{exch} = \frac{1}{2} \sum_{i \neq j} \int w * (\bar{u}_i u_j) \bar{u}_j u_i.$$

# Hartree-Fock

By assuming  $\mathcal{E}_{exch} \ll \mathcal{E}_N$  and  $\mathcal{E}_{mf} \sim \frac{1}{2} \sum_{i,j} \int w * |u_i|^2 |u_j|^2$ , we get the equations

$$i\partial_t u_j = -\Delta u_j + w * \left( \sum_k |u_k|^2 \right) u_j.$$

This equation was derived from many body quantum mechanics in a mean-field or semi-classical limit :

- ▶ Bardos Erdos Golse Mauser Yau '02
- ▶ Bardos Golse Gottlieb Mauser '03
- ▶ Elgart Erdos Schlein Yau '04
- ▶ Frohlich Knowles '11
- ▶ Benedikter Porta Schlein '13

## Equation on operators

Take  $\gamma = \sum_k |u_k\rangle\langle u_k|$  where  $|u_k\rangle\langle u_k|$  is the projection over  $\mathbb{C}u_k$ .  
Note that  $\text{Tr } \gamma = N$  is the number of particles. It satisfies

$$i\partial_t \gamma = [-\Delta + w * \rho_\gamma, \gamma] \quad (1)$$

where  $[\cdot, \cdot]$  is the commutator and  $\rho_\gamma$  is the diagonal of the integral kernel of  $\gamma$ , that is

$$\rho_\gamma(x) = \tilde{\gamma}(x, x)$$

with

$$(\gamma v)(x) = \int \tilde{\gamma}(x, y)v(y)dy.$$

Rk : Nonlinearity induced by  $\rho_\gamma$ .

Well-posed if  $(-\Delta)^s \gamma$  is trace class (the regularity depends on the assumptions on  $w$ ).

# Stationary solutions

$\gamma_f$  : Fourier multiplier by  $f$ .

$$\widehat{\gamma_f v}(\xi) = f(\xi)\hat{v}(\xi).$$

$$\tilde{\gamma}_f(x, y) = \int d\xi f(\xi) e^{i\xi(x-y)}$$

$$\rho_{\gamma_f} = \int f(\xi) d\xi.$$

$\gamma_f$  commutes with  $\Delta$  and  $w * \rho_{\gamma_f}$  is a constant hence  $\gamma_f$  is a stationary solution. Rk :  $\gamma_f$  is not trace class ( $\text{Tr}(\gamma) = \int dx \rho_\gamma(x)$ ).

$$Q = \gamma - \gamma_f$$

$$i\partial_t Q = [-\Delta, Q] + [w * \rho_{Q+\gamma_f}, \gamma_f + Q]. \quad (2)$$

# Global well-posedness

Lewin-Sabin :  $f = 1_{[-\mu, \mu]}$ ,  $d \geq 2$ ,  $w \in L^1 \cap L^\infty$ , defocusing, GWP in the energy space

Bose and Fermi gas at positive temperature :  $d \in \{1, 2, 3\}$ ,  $w \in L^1 \cap L^\infty$  (+ other assumptions depending on the dimension), defocusing, GWP in the entropy space.

Chen, Hong, Pavlovic :  $d = 2, 3$ ,  $f = 1_{[-\mu, \mu]}$ ,  $w = \delta$ , GWP in the energy space



# Stability

Lewin-Sabin :  $d = 2$ ,  $w \in W^{1,1}$  + assumptions on  $f$  and  $w$  that are not smallness assumptions, scattering in Schatten  $\frac{4}{3}$  for small data.

Chen, Hong, Pavlovic :  $d \geq 3$ , same assumptions on  $f$ ,  $w = w_+ * w_-$ ,  $w_{\pm} \in L^{2d/(d+2)}$ ,  $|\nabla|^{\pm\frac{1}{2}} w_{\pm} \in W^{\pm\alpha_0,1}$ , ( $\alpha_0$  depends on the regularity of the initial datum) + assumptions on  $f$  and  $w$  that are not smallness assumptions, scattering in Schatten  $2d$  for small data.

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# Model

Operators	Random Fields
$\gamma = \mathbb{E}( X\rangle\langle X )$	$X$
$\rho_\gamma$	$\mathbb{E}( X ^2)$
$i\partial_t \gamma = [-\Delta + w * \rho_\gamma, \gamma]$	$i\partial_t X = -\Delta X + w * \mathbb{E}( X ^2)X$
$\gamma_{ f ^2}$	$Y_f = \int f(k) e^{ikx - it(m+k^2)} dW(k)$

with  $\mathbb{E}(dW(k)\overline{dW(l)}) = \delta(k-l)dkdl$  and  $\mathbb{E}(|Y|^2) = \int |f|^2$  and  $m = w * \int |f|^2$ .

Rk : Law of  $Y_f$  is invariant by translations in both time and space.

$$Z = X - Y_f$$

$$i\partial_t Z = (m - \Delta)Z + w * (2\text{Re}\mathbb{E}(\bar{Y}_f Z) + |Z|^2)(Y_f + Z)$$

GWP in the energy space  $L^2_{\text{prob}}, H^1(\mathbb{R}^3)$ .

## Retrieving the system

If one takes the probability space  $\Omega = \{1, \dots, N\}$  with uniform probability, the random field  $X$  becomes

$$\sqrt{N}(u_1, \dots, u_N)$$

and

$$\mathbb{E}(|X|^2) = \sum_{k=1}^N |u_k|^2$$

and we retrieve the initial system.

# GWP at the operator level

Existence :

$$\begin{array}{ccc} \gamma_0 & \longrightarrow & X_0 \\ \downarrow & & \downarrow \\ \gamma & \longleftarrow & X \end{array}$$

$X_0$  : Gaussian field with cov op  $\gamma_0$

Uniqueness :  $\gamma_0$  induces  $X_0$ .

$\gamma_1, \gamma_2$  two solutions with id  $\gamma_0 \Rightarrow X_1, X_2$  two solutions with id  $X_0$  and such that  $\gamma_i = \mathbb{E}(|X_i\rangle\langle X_i|)$ .

Continuity : Choice of appropriate metric space for  $\gamma$ .

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# Equilibrium

The equation is for this section :  $i\partial_t X = -\Delta X + \mathbb{E}(|X|^2)X$ .

Write  $Y_f = e^{-it} \int f(\xi) dW(\xi)$  with  $\int |f(\xi)|^2 d\xi = 1$ .

It solves  $i\partial_t Y_f = -\Delta Y_f + \mathbb{E}(|Y_f|^2)Y_f$ .

$X = Z + Y_f(t)$

$$i\partial_t Z = (1 - \Delta)Z + (\mathbb{E}(|Z|^2) + 2\operatorname{Re}\mathbb{E}(\bar{Y}_f Z))(Y_f + Z).$$

$Z_1 = \mathbb{E}(\bar{Y}_f Z)$ ,  $Z_2 = Z - Z_1 Y_f$

$$\begin{cases} i\partial_t Z_1 = (1 - \Delta)Z_1 + 2\operatorname{Re}Z_1 + (\mathbb{E}(|Z_2|^2) + |Z_1|^2)(1 + Z_1) + 2\operatorname{Re}(Z_1)Z_1 \\ i\partial_t Z_2 = (1 - \Delta)Z_2 + (\mathbb{E}(|Z_2|^2) + |Z_1|^2 + 2\operatorname{Re}Z_1)Z_2 \end{cases}$$

# Stability of $e^{-it}$ for the Schrödinger equation

Gustafson-Nakanishi-Tsai :

$$i\partial_t u = (1 - \Delta)u + 2\operatorname{Re}u + |u|^2(1 + u) + 2\operatorname{Re}uu$$

scattering for small data of regularity  $d/2 - 1$  for  $d \geq 4$ . + dim 3

Guo-Hani-Nakanishi : same equation,  $d = 3$ , scattering for small data of regularity of one more angular derivative than the energy space.



# What we expect

$d=4$ ; GP with quadratic and cubic terms + Schrödinger with quadratic and cubic terms, should have scattering in the same way.

$d=3$  ; Problem comes from quadratic terms in the Schrödinger equation. Proof of relies on normal form. It is not obvious that it would work with the coupling.

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# Equilibrium

$$Y = \frac{m}{2}(g_+ e_+ + g_- e_-)$$

with  $e_{\pm} = e^{\pm i\xi_0 x - it(m + \xi_0^2)}$  and  $g_+, g_-$  two gaussians  $\mathcal{N}(0, 1)$  independent.

$$\mathbb{E}(|Y|^2) = m \text{ and } i\partial_t Y = (m - \Delta)Y.$$

Write  $Z = g_+ e_+ z_+ + g_- e_- z_-$ .

$$i\partial_t z_{\pm} = -\Delta z_{\pm} - 2i(\pm\xi_0) \cdot \nabla z_{\pm} + (|z_+|^2 + |z_-|^2 + 2\operatorname{Re}(z_+ + z_-))\left(\frac{m}{2} + z_{\pm}\right).$$

## Linearised

$$i\partial_t z_{\pm} = -\Delta z_{\pm} - 2i(\pm\xi_0) \cdot \nabla z_{\pm} + m\text{Re}(z_+ + z_-).$$

$$A = \begin{pmatrix} -2\xi_0 \cdot \nabla & -\Delta & 0 & 0 \\ \Delta - m & -2\xi_0 \cdot \nabla & -m & 0 \\ 0 & 0 & 2\xi_0 \cdot \nabla & -\Delta \\ -m & 0 & \Delta - m & 2\xi_0 \cdot \nabla \end{pmatrix}$$

## Particular cases

$$m = 0 \text{ Dz}$$

$$A = \text{Diag} (-2\xi_0 \cdot \nabla + i\Delta; -2\xi_0 \cdot \nabla - i\Delta; 2\xi_0 \cdot \nabla + i\Delta; 2\xi_0 \cdot \nabla - i\Delta).$$

$$\xi_0 = 0 \text{ Dz}$$

$$A = \text{Diag} (i\sqrt{-\Delta(2m-\Delta)}; -i\sqrt{-\Delta(2m-\Delta)}; i\Delta; -i\Delta).$$

Otherwise, one always get spectral instability, as in : Let  $\xi_0 \neq 0$  and  $m \neq 0$ . There exist  $\varepsilon_1, \varepsilon_2 > 0$  such that for all  $\kappa \in \mathbb{S}^{d-1}$  and  $r \in \mathbb{R}_+$ ;  $|\kappa \cdot \xi_0| \leq \varepsilon_1$  and  $r \leq \varepsilon_2$  implies that  $\hat{A}(\xi)$  has real eigen values.

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# Problem

We are back with  $w \neq \delta$  and  $f$  smooth.

The perturbation  $Z$  satisfies the equation :

$$i\partial_t Z = (m - \Delta)Z + w * (2\text{Re}\mathbb{E}(\bar{Y}_f Z) + \mathbb{E}(|Z|^2))(Y_f + Z)$$

with

$$Y_f = \int f(k) e^{ikx - it(m+k^2)} dW(k).$$

# Result

Non-smallness assumption on  $f$  and  $w$ .

$$\|\hat{w}_-\|_{L^\infty} \lesssim \left( \int_{\mathbb{R}^d} \frac{|h(x)|}{|x|^{d-2}} dx \right)^{-1}$$

where  $h$  is the inverse Fourier transform of  $|f|^2$ .

$$\hat{w}(0)_+ < \varepsilon_f$$

where  $\varepsilon_f$  depends on the behaviour of  $f$  in 0.



## Result

**THEOREM** [Collot, dS] Assume  $|\xi|^{-1/2-\varepsilon} \hat{w} \in L^\infty$ , and  $w \in W^{d/2-1,1}$  and  $f$  of Schwartz class (simplification). Let  $X$  be the solution to

$$i\partial_t X = -\Delta X + w * \mathbb{E}(|X|^2)X$$

with initial datum  $X_0 = Y_f(0) + Z_0$  with  $Z_0 \in L^2_{\text{prob}}, H^{d/2-1}$ ,  $Z_0$  independent from  $Y_f(0)$  (simplification, there is a space) and small enough. Then, there exists  $Z_{\pm\infty} \in L^2_{\text{prob}}, H^{d/2-1}$  such that

$$\|X(t) - Y_f(t) - S(t)Z_{\pm\infty}\|_{H^{d/2-1}}$$

goes to 0 when  $t \rightarrow \pm\infty$ .

## Duhamel formulation

With  $V = 2\text{Re}\mathbb{E}(\bar{Y}_f Z) + \mathbb{E}(|Z|^2)$  and  $S(t) = e^{-it(m-\Delta)}$  :

$$Z(t) = S(t)Z_0 - i \int_0^t S(t-\tau) w * V(\tau) Y_f(\tau) d\tau - i \int_0^t S(t-\tau) V(\tau) Z(\tau) d\tau.$$

$$\begin{aligned} V(t) = & \mathbb{E}(|Z(t)|^2) + 2\text{Re}\mathbb{E}(\overline{Y_f(t)} S(t) Z_0) \\ & - 2\text{Re}\mathbb{E}\left(\overline{i Y_f(t)} \int_0^t S(t-\tau) w * V(\tau) Y_f(\tau) d\tau\right) \\ & - 2\text{Re}\mathbb{E}\left(\overline{i Y_f(t)} \int_0^t S(t-\tau) w * V(\tau) Z(\tau) d\tau\right). \quad (3) \end{aligned}$$

# Discussion on spaces

Space for  $V$

$$\Theta_V = L^2, L^2 \cap L^{1+d/2}, L^{1+d/2}$$

cannot have  $V \in L^p, L^p$  with  $p < 2$ , or derivatives in  $V$ , implies loss of derivatives in  $w : s = \frac{d}{2} - 1$ .

Space for  $Z$

$$\Theta = L^4, L^4 \cap L^{d+2}, L^{d+2} \cap L^{2(2+d)/d}, W^{s, 2(2+d)/d} \cap C(\mathbb{R}, H^s)$$

$$\|S(t)g\|_{\Theta} \lesssim \|g\|_{H^s}.$$

## Linear term

The assumptions of “non smallness” on  $f$  are the same assumptions on  $f$  as in Lewin-Sabin, or Chen-Hong-Pavlovic.

Linear term :

$$-2\operatorname{Re}\mathbb{E}\left(i\overline{Y_f(t)} \int_0^t S(t-\tau)V(\tau)Y_f(\tau)d\tau\right) = -L(V)$$

Problem : Proving that  $1 + L$  is continuously invertible without a smallness assumption on  $Y_f$ .

$$\widehat{L(V)} = -2 \int_0^t d\tau \sin((t-\tau)\xi^2) h(2(t-\tau)\xi) \widehat{W}(\xi) \widehat{V}(\tau, \xi).$$

## Linear term

$$L(V) = K *_{t,x} V.$$

We have

$$\|L(V)\|_{\Theta_V} \lesssim \|\mathcal{F}_{t,x}(L(V))\|_{L^2, L^2 \cap L^{(d+2)/d}, (d+2)/d}.$$

Hence it suffices to bound  $\mathcal{F}_{t,x}(K)$  in  $L^2, L^2 \cap L^p, L^p$  with  $p = 2\frac{d+2}{d-2}$ .

If it is small enough we get that  $1 + L$  is invertible.

The sine helps for small  $\xi$  otherwise one may use the decay of  $h$  at infinity.

## Additional difficulties

Bounding

$$I = -i \int_0^t S(t-\tau) V(\tau) Y_f(\tau) d\tau$$

in the space for  $Z$ . Requires  $\hat{w}(k) = O(|k|^{1/2+})$ .

Indeed,

$$\mathbb{E}(|I|^2) = \int d\eta |f(\eta)|^2 \left| \int_0^t S_\eta(t-\tau) (w * V(\tau)) d\tau \right|^2$$

where

$$S_\eta(t) = S_\eta(t) = e^{-it(-\Delta - 2i\eta \cdot \nabla)}.$$

It reduces using Strichartz inequalities to bound

$$\int_0^\infty dt_1 \int_{-t_1}^\infty dt \int d\xi e^{it\xi^2} h(-2t\xi)(1 + \xi^2)^s |\hat{w}(\xi)|^2 \hat{V}(t_1, \xi) \overline{\hat{V}(t_1 + t, \xi)}.$$

We would use the  $L^2, L^2$  norm of  $V$ . The issue is the lack of sine. That is where we use the hypothesis on the behaviour at 0 of  $\hat{w}$ .

## Additional difficulties, II

Bounding

$$-2\operatorname{Re}\mathbb{E}\left(i\overline{Y_f(t)}\int_0^t S(t-\tau)V(\tau)Z(\tau)d\tau\right).$$

by iteration.

Calling  $W_V(g) = \int_0^t S(t-\tau)V(\tau)g(\tau)d\tau$ , this means bounding

$$-2\operatorname{Re}\mathbb{E}\left(i\overline{Y_f(t)}W_V^n(Y)d\tau\right).$$

We can compute this term explicitly and use the same technique as in the linear term and  $I$ .



Thank you for your attention !