Long-Time Behaviour of the Density Functional Theory

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joint work with Fabio Pusateri (in progress)

Banff, July, 2019

Self-consistent Approximation

Dynamics of a system of n identical bosons or fermions is given by the many-body Schrödinger equation (SE)

$$i\partial_t \psi = H_n \psi.$$

Restricting the SE to the Hartree or Hartree-Fock states

$$\otimes_1^n \psi \qquad \text{and} \qquad \wedge_1^n \psi_i,$$

we obtain the celebrated Hartree or Hartree-Fock equation,

$$i\partial_t \gamma = [h_\gamma, \gamma], \tag{1}$$

where $\gamma = nP_\psi$ for bosons and $\gamma = \sum_1^n P_{\psi_i}$ for fermions and h_γ is a (self-consistent) one-particle Schrödinger operator depending on γ.

Trade-off: large dimensions for the nonlinearity.

Hartree, Hartree-Fock and DFT Equations

We summarize the resulting self-consistent equation,

$$i\partial_t\gamma = [h_\gamma, \gamma],$$

where h_γ is self-consistent one-particle Schródinger operator,

$$h_\gamma := -\Delta + \underbrace{v * \rho_\gamma}_{\text{direct self-interact}} + \underbrace{ex(\gamma)}_{\text{exch self-interact}} \quad (2)$$

Here v is a pair potential,

$$\rho_\gamma(x,t) := \gamma(x;x,t) \text{ is the charge density,}$$

$$ex(\gamma) := \begin{cases} 0 & \text{for the Hartree model} \\ -v^\sharp\gamma & \text{for the Hartree-Fock case} \\ xc(\rho_\gamma) & \text{for the density functional theory (DFT).} \end{cases}$$

Example of $xc(\rho)$ is the Dirac term $-c\rho^{1/3}$.

Time-dependent density functional equations

The time-dependent density functional theory (DFT) is based on the time-dependent Kohn-Sham equation for an operator γ:

$$\partial_t \gamma = i[h_\gamma, \gamma] \qquad \text{(KSE)}$$

where $h_\gamma := -\Delta + g(\rho_\gamma)$, with $g : L^1_{\mathrm{loc}}(\mathbb{R}^d) \to \mathbb{R}$ and

$$\rho_\gamma(x,t) := \gamma(x,x,t), \text{ the one-particle density.}$$

Here $\gamma \geq 0$, called the density operator. For fermions, $\gamma \leq 1$ (the Pauli exclusion principle).

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We assume $g(\rho)$ is a tansl/rot covariant functional:

$$U_\lambda g(\rho) U_\lambda^{-1} = g(U_\lambda \rho) \tag{3}$$

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(here $g(\rho)$ is considered as a multiplication operator). A typical g:

$$g(\rho) = v * \rho + xc(\rho), \qquad (5)$$

with v a pair potential and $xc(\rho)$ an exch-correl energy term, e.g. $v(x) = \lambda/|x|$ (the Coulomb or Newton potential in $3D$) and $v(x) = \lambda\delta(x)$ (the local potential) and $xc(\rho) = -c\rho^{1/3}$ (Dirac).

Key problems

- Existence theory
- Asymptotic behaviour as $t \to \infty$ (scattering theory, return to equilibrium)
- Static, self-similar and travelling wave solutions and their stability (related to the previous item)

The existence theory: Chadam-Glassey (75), Bove-Da Prato-Fano (76), Zagatti (92) (H and HF eqs, $\mathrm{Tr}\,\gamma_0 < \infty$)

Lewin-Sabin (15) (regular potentials), Th. Chen-Hong-Pavlović (17) (delta potential) (H eq, $\mathrm{Tr}\,\gamma_0 = \infty$)

Scattering: Ginibre-Velo (80), Hayashi-Tsutsumi (87), Hayashi-Naumkin (97), Kato-Pusateri (12) (H eq, scalar case)

Asympt. stab. of transl. invar. solns: Lewin-Sabin (15), Th. Chen-Hong-Pavlović (17)

Results

Assume $\gamma_0 \geq 0$ are trace class with the weight $< x >^d$.

Theorem (Local decay)

Let $g(\rho)$ satisfy, for $d < 4$, the conditions

$$g(\rho) = v * \rho + \lambda \rho^{\beta}, \tag{6}$$

with $v \in L^r_w, 1 < r < \infty$, $\beta > 1/2$ and $\|v\|_{L^r_w} + |\lambda| \ll 1$.
Then KSE is GWP and has the scattering property:
$\forall$ initial condition $\gamma_0 \in I^1$, $\exists$ an operator $\gamma_\infty \in I^1$ s.t., as $t \to \infty$, the solution, $\gamma(t)$, satisfies

$$\left\|\gamma(t) - e^{it\Delta}\gamma_\infty e^{-i\Delta t}\right\|_{I^1} \to 0. \tag{7}$$

Conjecture: The result holds for $\beta > 1/d$ (short-range or subcritical nonlinearity).

Properties of the Kohn-Sham equation (KSE)

- Galilean invariance
- Conservation of energy and number of particles
- Preservation of positivity
- Hamiltonian structure

Scattering criticality

Recall the time-dependent Kohn-Sham equation (KSE):

$$\partial_t \gamma = i[h_\gamma, \gamma], \; h_\gamma := -\Delta + g(\rho_\gamma).$$

Let $U_\lambda : \psi(x) \to \lambda^d \psi(\lambda x)$. Consider $g(\rho)$ satisfying

$$U_\lambda g(\rho) U_\lambda^{-1} = \lambda^{-\alpha} g(U_\lambda \rho), \qquad \text{(Scal)}$$

($g(\rho)$ is a multiplication operator and ρ, a function). We say $g(\rho)$ is scattering subcritical/critical/supercritical iff

$$\alpha > 1/ \; \alpha = 1/ \; \alpha < 1.$$

E. g. $g(\rho) = |x|^{-\alpha} * \rho$ and $g(\rho) = \rho^\beta, \beta = \frac{\alpha}{d}$, satisfy (Scal).

($\rho^{\frac{\alpha}{d}}$ is a 'semi-classical limit' of $|x|^{-\alpha} * \rho$.)

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More generally, $g(\rho)$ is short-range (scatt. subcritical) iff $\forall f$ nice,

$$\int_1^\infty \|g(f_t)\|_\infty dt < \infty, \; f_t(x) := t^{-d} f(\frac{x}{t})$$

and long-range (scattering critical or supercritical) otherwise.

Passing to a Hilbert space (mini-GNS)

To work on a Hilbert space pass from γ to $\sqrt{\gamma}$, or more generally to κ, s.t. $\kappa^*\kappa = \gamma$. Then the KSE becomes

$$\partial_t \kappa = i[h_\kappa, \kappa] \qquad (\sqrt{KSE})$$

where $h_\kappa := -\Delta + g(\kappa)$, with $g(\kappa)$ having the gauge symmetry

$$e^{i\chi} g(\kappa) e^{-i\chi} = g(e^{i\chi}\kappa e^{-i\chi}), \ \forall \chi \qquad (8)$$

Proposition

- *$\sqrt{KSE} \iff KSE$, with $\kappa^*\kappa = \gamma$;*
- *Well Pos(κ) $\Rightarrow$ Well Pos(γ);*
- *Scat Th(κ) $\Rightarrow$ Scat Th(γ).*

Local decay

If γ is trace-class, then $\kappa = \sqrt{\gamma}$ is a Hilbert-Schmidt operator.
Let $\kappa(y,x) = \tilde{\kappa}(r,c)$, where $r := y - x, c := \frac{1}{2}(y+x)$.
Define the norm

$$\|\kappa\|_{L^q_r L^p_c} \equiv \|\tilde{\kappa}\|_{L^q_r L^p_c} := \|\|\tilde{\kappa}\|_{L^p_c}\|_{L^q_r}. \tag{9}$$

Theorem [Local decay] *Let $g(\rho)$ satisfy the conditions*

$$\|dg(\rho)\xi\|_p \ll \|\xi\|_q, \tag{10}$$

where $1 + 1/p - 1/q > 1/d$, etc , and g be small. Then

$$\|\kappa\|_{L^2_r L^s_c} \lesssim t^{-b}\|x^b\kappa_0\|_{HS} \qquad (b = d(\frac{1}{2} - \frac{1}{s})).$$

Corollary: The *GWP* and *scattering* $\Longrightarrow$ the same for KSE.

The theorem follows from the next two basic statements.

A priori bounds

Define the *Galilean 'boost generator'*

$$J_t\kappa := [j_t, \kappa], \quad \text{with} \;\; j_t := x - 2pt, \;\; p := -i\nabla.$$

and the *non-abelian Sobolev spaces* based on the space of Hilbert - Schmidt operators with the smoothness grading provided by J:

$$W_t^s := \left\{\kappa \in I^2 \; : \; \sum_{|\alpha|\leq s} \|J_t^\alpha \kappa\|_{I^2} < \infty\right\}. \tag{11}$$

Proposition (A priori bounds)

Any solution to $\sqrt{KSE}$ satisfies the estimate (for $b \geq d/2$)

$$\|\kappa(t)\|_{W_t^b} \leq 2\|\kappa_0\|_{W_0^b}. \tag{12}$$

The main idea: use almost conservation law:

$$D_\gamma J_t\kappa = J_t D_\gamma\kappa + [dg(\rho_\gamma)\rho_{J_t\gamma}, \kappa]$$

where $$D_\gamma\kappa := i\partial_t\kappa - [h_\gamma, \kappa].$$

The *gauge invariance*, more precisely the invariance under *Galilean*

Non-abelian Gagliardo-Nirenberg-Kleinerman-type ineqs

Proposition (Non-abelian GNK-type inequality)

Let $\alpha b = d(\frac{1}{2} - \frac{1}{s})$ *and* $0 \leq \alpha \leq 1$ *(d odd). Then*

$$\|\kappa\|_{L^2_r L^s_c} \lesssim t^{-\alpha b} \|\kappa\|^{\alpha}_{W^b_t} \|\kappa\|^{1-\alpha}_{W^0_t}.$$

where, recall,

$$W^s_t := \Big\{\kappa \in I^2 \, : \, \sum_{|\alpha| \leq s} \|J^\alpha_t \kappa\|_{I^2} < \infty\Big\},$$

$$J_t\kappa := [j_t, \kappa], \quad \textit{with} \;\; j_t := x - 2pt, \;\; p := -i\nabla.$$

The main idea: (a) extend the GNI to non-abelian spaces

(b) pass from the non-abelian GNI to the non-abelian GNKI by using

$$-iD = \frac{1}{2t} e^{-ix^2/4t} J_t e^{ix^2/4t}, \text{ where } D\kappa := [\partial, \kappa].$$

Completing the proof

The non-abelian Gagliardo-Nirenberg-Kleinerman-type inequality

$$\|\kappa\|_{L_r^2 L_c^s} \lesssim t^{-b} \|\kappa\|_{W_t^b}$$

with the a priori bound

$$\|\kappa(t)\|_{W_t^b} \lesssim \|\kappa_0\|_{W_0^b}$$

give the local decay estimate

$$\|\kappa(t)\|_{L_r^2 L_c^s} \lesssim t^{-b} \|\kappa_0\|_{W_0^b}$$

$\Longrightarrow$ GWP and scattering for $\sqrt{KSE}$

$\Longrightarrow$ GWP and scattering for KSE.

Summary

We discussed

- main features of the time-dependent equations of the density functional theory;
- introduced some new useful tools: (a) the Hilbert-space representation, (b) the almost conserved Galilean generator, (c) modified Sobolev spaces and (d) mixed norms;
- gave a thumbnail sketch of the local decay result, which implies GWP and scattering theory.

Future extensions:

- Scattering critical and supercritical nonlinearities
- Asymptotic stability of static solutions (return to equilibrium)

Thank-you for your attention