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To cite this version:

Rémi Carles, Clotilde Fermanian Kammerer, Caroline Lasser. On the Cauchy problem for the Hartree approximation in quantum dynamics. Nonlinearity, 2023, 36 (6), pp.3158-3181. 10.1088/1361-6544/accf5a . hal-03738486

HAL Id: hal-03738486

https://hal.science/hal-03738486v1

Submitted on 26 Jul 2022

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ON THE CAUCHY PROBLEM FOR THE HARTREE APPROXIMATION IN QUANTUM DYNAMICS

RÉMI CARLES, CLOTILDE FERMANIAN KAMMERER, AND CAROLINE LASSER

Abstract. We prove existence and uniqueness results for the time-dependent Hartree approximation arising in quantum dynamics. The Hartree equations of motion form a coupled system of nonlinear Schrödinger equations for the evolution of product state approximations. They are a prominent example for dimension reduction in the context of the the time-dependent Dirac–Frenkel variational principle. We handle the case of Coulomb potentials thanks to Strichartz estimates. Our main result addresses a general setting where the nonlinear coupling cannot be considered as a perturbation. The proof uses a recursive construction that is inspired by the standard approach for the Cauchy problem associated to symmetric quasilinear hyperbolic equations.

1. Introduction

We consider the time-dependent Schrödinger equation

$$i\partial_t\psi = H\psi, \tag{1.1}$$

where the total Hamiltonian is given by

$$H = H_x + H_y + w(x,y), \quad H_x = -\frac{1}{2}\Delta_x + V_1(x), \quad H_y = -\frac{1}{2}\Delta_y + V_2(y)$$

with $x \in \mathbb{R}^{d_1}$ and $y \in \mathbb{R}^{d_2}$, $d_1, d_2 \geq 1$. The potentials V_1, V_2 and w are always real-valued, we will make extra regularity and decay assumptions later on . It is common wisdom that for dealing with quantum systems "a solution of the wave equation in many-dimensional space is far too complicated to be practicable" (Dirac 1930) and one aims at approximative methods that effectively reduce the space dimension. Here, we focus on initial data that decouple the space variables,

$$\psi(0,x,y) = \phi_0^x(x)\phi_0^y(y).$$

Such a form of initial data indeed suggests a dimension reduction approach. Of course, if there is no coupling ($w(x,y) = 0$), the full solution is itself a product state $\psi(t,x,y) = \phi_x(t,x)\phi_y(t,y)$, with

$$\begin{cases} i\partial_t\phi^x = H_x\phi^x, & \phi^x(0,x) = \phi_0^x(x), \\ i\partial_t\phi^y = H_y\phi^y, & \phi^y(0,y) = \phi_0^y(y). \end{cases}$$

RC was supported by Rennes Métropole through its AIS program, and by Centre Henri Lebesgue, program ANR-11-LABX-0020-0. CL was supported by the Centre for Advanced Study in Oslo, Norway, research project *Attosecond Quantum Dynamics Beyond the Born-Oppenheimer Approximation*.

When the coupling is present, one seeks for approximate solutions $u(t) \approx \psi(t)$ of product form $u(t,x,y) = \phi^x(t,x)\phi^y(t,y)$ in order to reduce the initial system (1.1) in $\mathbb{R}^{d_1+d_2}$ to two systems on spaces of smaller dimensions, $\mathbb{R}^{d_1}$ and $\mathbb{R}^{d_2}$. In situations, where the overall configuration space has a natural decomposition of its dimension $d_1 + \cdots + d_N$, a corresponding product ansatz of N factors is sought. Here we only investigate the case $N = 2$, mentioning that repeated application of the binary construction yields the more general case. Applying the time-dependent Dirac–Frenkel variational principle to the manifold

$$\mathcal{M} = \left\{ u = \varphi^x \otimes \varphi^y \mid \varphi^x \in L^2(\mathbb{R}^{d_1}),\ \varphi^y \in L^2(\mathbb{R}^{d_2}) \right\}$$

yields the so-called *time-dependent Hartree approximation*,

$$\psi(t,x,y) \approx \phi^x(t,x)\phi^y(t,y) \in \mathcal{M},$$

where the pair (ϕ^x, ϕ^y) solves the nonlinearly coupled system

$$\begin{cases} i\partial_t \phi^x = H_x \phi^x + \langle w \rangle_y \phi^x, & \phi^x(0,x) = \phi_0^x(x), \\ i\partial_t \phi^y = H_y \phi^y + \langle w \rangle_x \phi^y, & \phi^y(0,y) = \phi_0^y(y). \end{cases} \tag{1.2}$$

The time-dependent potentials result from the averaging process

$$\langle w \rangle_y(t,x) := \int_{\mathbb{R}^{d_2}} w(x,y)|\phi^y(t,y)|^2 dy,$$
$$\langle w \rangle_x(t,y) := \int_{\mathbb{R}^{d_1}} w(x,y)|\phi^x(t,x)|^2 dx,$$

under the assumption, made throughout this paper, that

$$\|\phi_0^x\|_{L^2(\mathbb{R}^{d_1})} = \|\phi_0^y\|_{L^2(\mathbb{R}^{d_2})} = 1. \tag{1.3}$$

For any "reasonable" solution (at least with the regularity considered in this paper), the L^2-norms of $\phi^x(t,\cdot)$ and $\phi^y(t,\cdot)$, respectively, are independent of time, hence

$$\|\phi^x(t)\|_{L^2(\mathbb{R}^{d_1})} = \|\phi^y(t)\|_{L^2(\mathbb{R}^{d_2})} = 1,$$

for all t in the time interval where the solution to (1.2) is well-defined; see §6.3 for a proof.

Even though the time-dependent Hartree approximation is one of the most fundamental approximations in quantum dynamics, mathematical existence and uniqueness proofs are rather scarce. Existence and uniqueness have been studied in the case where the interaction potential is of convolution type, i.e. for $w(x,y) = W(x-y)$ and with one of the subsystems moving by classical mechanics (see [7, 2, 6] for example). A related investigation has targeted the time-dependent self-consistent field system [12] with coupling potentials of Schwartz class. However, our aim here is to discuss the existence and uniqueness of solutions for system (1.2) when the potentials $\langle w \rangle_x$ or $\langle w \rangle_y$ need not be bounded, and cannot be considered as a perturbation of V_2 or V_1, respectively. This framework requires a different approach. In particular, our result provides the Cauchy theory for the systems discussed in the articles [3, 4] where the accuracy of the Hartree approximation is studied in the broader context of composite quantum dynamics and scale separation.

The steps for our existence and uniqueness proof are strongly inspired by the method which is classical in the study of quasilinear hyperbolic systems, see e.g. [1]. With $n \in \mathbb{N}$, we associate the iterative scheme of recursive equations

$$\begin{cases} i\partial_t \phi^x_{n+1} = H_x \phi^x_{n+1} + \langle w_n \rangle_y \phi^x_{n+1}, & \phi^x_{n+1}(0,x) = \phi^x_0(x), \\ i\partial_t \phi^y_{n+1} = H_y \phi^y_{n+1} + \langle w_n \rangle_x \phi^y_{n+1}, & \phi^y_{n+1}(0,y) = \phi^y_0(y), \end{cases} \tag{1.4}$$

with

$$\langle w_n \rangle_y(t,x) = \int_{\mathbb{R}^n} w(x,y) |\phi^y_n(t,y)|^2 dy, \quad \langle w_n \rangle_x(t,y) = \int_{\mathbb{R}^d} w(x,y) |\phi^x_n(t,x)|^2 dx. \tag{1.5}$$

The main steps of the proof of our existence and uniqueness result are then:

(1) The iterative scheme is well-defined and enjoys bounds in "large" norm, which control second order derivatives and polynomial growth of order two for some finite time horizon.
(2) The solution of the scheme converges in "small" norm, which is the L^2 norm.
(3) It is possible to pass to the limit $n \to +\infty$ in the equation, which leads to the construction of a solution that one then proves to be unique and global in time (provided the initial data is regular enough).

1.1. **Outline.** In the next Section 2, we recall elementary properties of the time-dependent variational principle and formally derive the Hartree equations (1.2). Then we discuss coupling potentials $w(x,y)$ of Coulombic and of polynomial type in Section 3, where we also present our main result Theorem 3.11, which establishes existence and uniqueness of the solutions to the Hartree system for coupling with polynomial growth. The different steps of the proof of Theorem 3.11 are the subject of Section 4 (analysis of the iterative scheme), Section 5 (convergence in small norms) and Section 6 (passing to the limit). A sufficient condition for the growth of the coupling potential is verified in Section 7. The Appendices A and B summarize some technical arguments.

1.2. **Notations.** We write L^∞_T for $L^\infty([0,T])$. The notations L^2_x, L^2_y, $L^2_{x,y}$ stand for $L^2(\mathbb{R}^{d_1}_x)$, $L^2(\mathbb{R}^{d_2}_y)$, $L^2(\mathbb{R}^{d_1+d_2}_{x,y})$, respectively. We denote by $\langle \cdot,\cdot \rangle_{L^2_x}$, $\langle \cdot,\cdot \rangle_{L^2_y}$, $\langle \cdot,\cdot \rangle_{L^2_{x,y}}$ the corresponding inner products. For $f,g \geq 0$, we write $f \lesssim g$ whenever there exists a "universal" constant (in the sense that it does not depend on time, space, or n, typically) such that $f \leq Cg$.

2. Variational principle

The time-dependent Hartree approximation results from the Dirac–Frenkel variational principle applied to the manifold

$$\mathcal{M} = \left\{ u = \varphi^x \otimes \varphi^y \mid \varphi^x \in L^2_x,\ \varphi^y \in L^2_y \right\}, \tag{2.1}$$

see also [15, §II.3.1] for the analogous discussion with Hartree products of N orbitals in $L^2(\mathbb{R}^3)$. The reader can also refer to [14]. The principle determines an approximate solution

$u(t) \in \mathcal{M}$ for the time-dependent Schrödinger equation

$$i\partial_t \psi = H\psi$$

with initial data $\psi(0) \in \mathcal{M}$ by requiring that for all times t

$$\begin{cases} \partial_t u(t) \in \mathcal{T}_{u(t)}\mathcal{M}, \\ \langle v, i\partial_t u(t) - Hu(t)\rangle = 0 \quad \text{for all} \quad v \in \mathcal{T}_{u(t)}\mathcal{M}, \end{cases} \tag{2.2}$$

where $\mathcal{T}_{u(t)}\mathcal{M}$ denotes the tangent space of $\mathcal{M}$ at $u(t)$. For deriving the Hartree equations, we first have to understand the manifold $\mathcal{M}$ and its tangent space. Note that the representation of a Hartree function is non-unique, since $\varphi^x \otimes \varphi^y = (a\varphi^x) \otimes (a^{-1}\varphi^y)$ for any $a \in \mathbb{C} \setminus \{0\}$. However, we can have unique representations in the tangent space once appropriate gauge conditions are set.

Lemma 2.1 (Tangent space)**.** *For any $u = \varphi^x \otimes \varphi^y \in \mathcal{M}$, $u \neq 0$,*

$$\mathcal{T}_u\mathcal{M} = \left\{ v^x \otimes \varphi^y + \varphi^x \otimes v^y \mid v^x \in L^2_x,\ v^y \in L^2_y \right\}.$$

Any $v \in \mathcal{T}_u\mathcal{M}$ has a unique representation of the form $v = v^x \otimes \varphi^y + \varphi^x \otimes v^y$, if we impose the gauge condition $\langle \varphi^x, v^x\rangle = 0$. The tangent spaces are complex linear subspaces of $L^2_{x,y}$ such that $u \in \mathcal{T}_u\mathcal{M}$ for all $u \in \mathcal{M}$.

The lemma is proved in Appendix A. The following formal arguments show that, in case that the variational solution $u(t)$ is well-defined and sufficiently regular, the L^2 norm and the energy expectation value are conserved automatically. Indeed, we differentiate with respect to time t and use the variational condition (2.2) for $v = u(t)$,

$$\frac{d}{dt}\|u(t)\|^2_{L^2_{x,y}} = 2\,\mathrm{Re}\langle u(t), \partial_t u(t)\rangle_{L^2_{x,y}} = 2\,\mathrm{Re}\langle u(t), \tfrac{1}{i}Hu(t)\rangle_{L^2_{x,y}} = 0,$$

due to self-adjointness of the Hamiltonian. Similarly, using self-adjointness and the variational condition (2.2) for $v = \partial_t u(t)$,

$$\frac{d}{dt}\langle u(t), Hu(t)\rangle_{L^2_{x,y}} = 2\,\mathrm{Re}\langle \partial_t u(t), Hu(t)\rangle_{L^2_{x,y}} = 2\,\mathrm{Re}\langle \partial_t u(t), i\partial_t u(t)\rangle_{L^2_{x,y}} = 0.$$

Let us now formally derive the Hartree system (1.2). We write

$$u(t) = \varphi^x(t) \otimes \varphi^y(t),$$

with $\|\varphi^x(t)\|_{L^2_x} = \|\varphi^y(t)\|_{L^2_y} = 1$. We have

$$\begin{aligned} i\partial_t u &= (i\partial_t \varphi^x(t)) \otimes \varphi^y(t) + \varphi^x(t) \otimes (i\partial_t \varphi^y(t)), \\ Hu &= H_x\varphi^x(t)) \otimes \varphi^y(t) + \varphi^x(t) \otimes (H_y\varphi^y(t)) + w(x,y)\varphi^x(t) \otimes \varphi^y(t). \end{aligned}$$

Choosing elements $v = v^x \otimes \varphi^y + \varphi^x \otimes v^y \in \mathcal{T}_{u(t)}\mathcal{M}$ and evaluating (2.2), we obtain the following necessary and sufficient conditions:

(i) If v^y=0, we obtain that for all $v^x \in L^2_x$ such that $\langle v^x, \varphi^x(t)\rangle_{L^2_x} = 0$,

$$\langle v^x, (i\partial_t - H_x)\varphi^x(t)\rangle_{L^2_x} = \int_{\mathbb{R}^{d_1+d_2}} w(x,y)v^x(x)\varphi^x(t,x)|\varphi^y(t,y)|^2 dxdy.$$

(ii) If v^x=0, we obtain that for all $v^y \in L^2_y$ such that $\langle v^y, \varphi^y(t)\rangle_{L^2_y} = 0$,

$$\langle v^y, (i\partial_t - H_y)\varphi^y(t)\rangle_{L^2_y} = \int_{\mathbb{R}^{d_1+d_2}} w(x,y)v^y(y)\varphi^y(t,y)|\varphi^x(t,x)|^2 dxdy.$$

The choice of $\varphi^x(t)$ and $\varphi^y(t)$ satisfying the Hartree system (1.2) guarantees (i) and (ii).

3. Main result

We present existence and uniqueness results for the solution of the time-dependent Hartree system (1.2). In §3.1, we discuss how Strichartz estimates may be applied to Coulombic coupling. In §3.2, we give detailed assumptions on polynomial growth conditions. Then, in §3.3 we state our main result Theorem 3.11.

3.1. **Coupling potentials of Coulombic form.** The case of Coulomb singularities (in combination with classical nuclear dynamics) has already been addressed in [7, 2] by Schauder and Picard fixed point arguments, respectively. We briefly revisit the main result from [7], and show how it may be adapted thanks to Strichartz estimates. We suppose $d_1 = d_2 = 3$, and have in mind the case

$$w(x,y) = \frac{\varepsilon}{|x-y|}, \quad \varepsilon \in \mathbb{R}. \tag{3.1}$$

We consider more generally the case $w(x,y) = W(x-y)$, for a possibly singular W. We assume that the potentials V_1 and V_2 are perturbations of smooth and at most quadratic potentials:

$$V_j = \mathbf{V}_j + v_j,$$

where

$$\mathbf{V}_j \in \mathcal{Q} = \left\{V \in C^\infty(\mathbb{R}^3;\mathbb{R}),\ \partial^\alpha V \in L^\infty(\mathbb{R}^3),\ \forall |\alpha| \geq 2\right\},$$

and

$$v_j \in L^p(\mathbb{R}^3) + L^\infty(\mathbb{R}^3), \quad \text{for some } p > 3/2.$$

Typically, we may consider Coulomb potentials, as

$$\frac{1}{|x|} = \frac{1}{|x|}\mathbf{1}_{|x|<1} + \frac{1}{|x|}\mathbf{1}_{|x|\geq 1}.$$

The first term on the right hand side belongs to $L^p(\mathbb{R}^3)$ for any $1 \leq p < 3$, and the second term is obviously bounded. We then make the same assumption on W. Denote

$$\mathbf{H}_x = -\frac{1}{2}\Delta_x + \mathbf{V}_1, \quad \mathbf{H}_y = -\frac{1}{2}\Delta_y + \mathbf{V}_2.$$

Then $e^{-it\mathbf{H}_x}$ and $e^{-it\mathbf{H}_y}$ enjoy Strichartz estimates, and (1.2) can be solved at the L^2 level, by a straightforward adaptation of [10, Corollary 4.6.5]:

Theorem 3.1. *Assume $d_1 = d_2 = 3$, $\mathbf{V}_1, \mathbf{V}_2 \in \mathcal{Q}$, $v_1, v_2, W \in L^p(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ for some $p > 3/2$, and $\phi_0^x, \phi_0^y \in L^2(\mathbb{R}^3)$. Then (1.2) has a unique solution $(\phi^x, \phi^y) \in C(\mathbb{R}; L^2(\mathbb{R}^3))^2 \cap L^q_{\mathrm{loc}}(\mathbb{R}; L^r(\mathbb{R}^3))^2$, where $1 = 2/r + 1/p$ and q is such that*

$$\frac{2}{q} = 3\left(\frac{1}{2} - \frac{1}{r}\right).$$

The L^2-norms of ϕ^x and ϕ^y are independent of $t \in \mathbb{R}$, hence in view of (1.3),

$$\|\phi^x(t)\|_{L^2(\mathbb{R}^3)} = \|\phi^y(t)\|_{L^2(\mathbb{R}^3)} = 1, \quad \forall t \in \mathbb{R}.$$

The proof is presented shortly in Appendix B.

Remark 3.2. The sign of ε in (3.1) plays no role here. Indeed, the proof relies on local in time Strichartz estimates associated to $\mathbf{H}_x$ and $\mathbf{H}_y$, respectively, and the potentials v_1, v_2 and W are treated as perturbations, whose sign is irrelevant in order to guarantee the above global existence result. On the other hand, Theorem 3.1 brings no information regarding the quality of the dynamics or the existence of a ground state.

Remark 3.3. Under extra assumptions on the potentials v_1 and v_2 (no extra assumption is needed for W, as it is associated to a convolution), it is possible to consider higher regularity properties. In particular, working at the level of H^1-regularity makes it possible to show the conservation of the energy

$$\begin{aligned} E(t) = {} & \langle H_x \phi^x(t), \phi^x(t)\rangle_{L^2_x} + \langle H_y \phi^y(t), \phi^y(t)\rangle_{L^2_y} \\ & + \iint_{\mathbb{R}^3\times\mathbb{R}^3} W(x-y)|\phi^x(t,x)|^2|\phi^y(t,y)|^2 dxdy, \end{aligned}$$

provided that ∇v_1 and ∇v_2 also belong to $L^p(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ for some $p > 3/2$. We refer to Remark B.5 for more details.

Remark 3.4. The role of the set $\mathcal{Q}$ is to guarantee that (local in time) Strichartz estimates are available for $\mathbf{H}_x$ and $\mathbf{H}_y$. The same would still be true for a larger class of potentials, including for instance Kato potentials ([20]) or potentials decaying like an inverse square ([5]). The choice of this set $\mathcal{Q}$ is made in order to simplify the presentation, and because it is delicate to keep track of all the classes of potentials for which Strichartz estimates have been proved.

3.2. **Coupling potentials with polynomial growth.** The core of this paper addresses the case where the coupling potential w may grow polynomially. To be more concrete, we recall the example addressed in [4].

Example 3.5. Assume $d_1 = d_2 = 1$ and that the potentials are given by

$$V_1(x) = \frac{1}{2}x^2\left(\frac{x}{2\ell} - 1\right)^2, \quad \ell > 0, \quad V_2(y) = \frac{\omega^2}{2}y^2, \quad w(x,y) = \chi(x)y^2, \ \ \chi \in C_0^\infty(\mathbb{R}).$$

Here, $V_1(x)$ corresponds to a double well and $V_2(y)$ to a harmonic bath. The coupling $w(x,y)$ could be locally cubic when choosing $\chi(x) = x$ for x in a neighborhood of zero.

We emphasize that in Example 3.5, the average $\langle w\rangle_x$ grows quadratically in y: in terms of growth, $\langle w\rangle_x$ is comparable to V_2 and cannot be considered as a perturbation as far as the Cauchy problem is concerned. This setting turns out to be very different from the one in [7, 2] (see also Theorem 3.1), and requires a different approach to be developed below.

3.2.1. *Restriction to non-negative potentials.* In the general case, we assume $d_1, d_2 \geq 1$. First, the potentials V_1 and V_2 are smooth, real-valued, $V_1 \in C^\infty(\mathbb{R}^{d_1};\mathbb{R})$, $V_2 \in C^\infty(\mathbb{R}^{d_2};\mathbb{R})$, and bounded from below:

$$\forall x \in \mathbb{R}^{d_1}, \forall y \in \mathbb{R}^{d_2}, \;\; V_1(x) \geq -C_1 \;\text{ and }\; V_2(y) \geq -C_2,$$

for some constants $C_1, C_2 > 0$. The operators H_x and H_y then are self-adjoint operators. Up to changing $\phi^x(t,x)$ to $\phi^x(t,x)e^{itC_1}$ (which amounts to replacing V_1 by V_1+C_1 in (1.2)), and $\phi^y(t,y)$ to $\phi^y(t,y)e^{itC_2}$, we may actually assume

$$\textbf{(H1)} \qquad V_1(x) \geq 1,\; \forall x \in \mathbb{R}^{d_1}, \quad \text{and} \quad V_2(y) \geq 1,\; \forall y \in \mathbb{R}^{d_2},$$

as we are only interested in existence results for the Cauchy problem (1.2). Thus H_x and H_y are sums of a nonnegative operator (Laplacian in x and y, respectively) and of a nonnegative potential. We use them to measure the regularity of the solutions of the system (1.2).

3.2.2. *Functional setting.* For $k \in \mathbb{N}$, we define the Hilbert spaces

$$\mathcal{H}^k_x = \left\{\phi \in L^2(\mathbb{R}^{d_1}),\;\; H_x^{k/2}\phi \in L^2(\mathbb{R}^{d_1})\right\} \;\text{ and }\; \mathcal{H}^k_y = \left\{\phi \in L^2(\mathbb{R}^{d_2}),\;\; H_y^{k/2}\phi \in L^2(\mathbb{R}^{d_2})\right\},$$

which are the natural analogues of Sobolev spaces H^k in the presence of (nonnegative) potentials (in view of **(H1)**), equipped with the norms given by

$$\|\phi\|^2_{\mathcal{H}^k_x} = \|\phi\|^2_{L^2_x} + \|H_x^{k/2}\phi\|^2_{L^2_x}, \quad \|\phi\|^2_{\mathcal{H}^k_y} = \|\phi\|^2_{L^2_y} + \|H_y^{k/2}\phi\|^2_{L^2_y}.$$

For $\alpha, \beta \in \mathbb{N}$, $\Phi = (\phi^x, \phi^y) \in \mathcal{H}^\alpha_x \times \mathcal{H}^\beta_y$, we set

$$\|\Phi\|^2_{\alpha,\beta} = \|\phi^x\|^2_{\mathcal{H}^\alpha_x} + \|\phi^y\|^2_{\mathcal{H}^\beta_y} = \|\phi^x\|^2_{L^2_x} + \|H_x^{\alpha/2}\phi^x\|^2_{L^2_x} + \|\phi^y\|^2_{L^2_y} + \|H_y^{\beta/2}\phi^y\|^2_{L^2_y}.$$

All along the paper, we use that in view of **(H1)**, $0 \leq H_x^\alpha \leq H_x^{\alpha+1}$ and $0 \leq H_y^\beta \leq H_y^{\beta+1}$.

As (1.2) is reversible, from now on we consider positive time only. We shall work with the time-dependent functional spaces

$$X_T^{\alpha,\beta} = \left\{\Phi(t) = (\phi^x(t), \phi^y(t)),\; \phi^x \in L^\infty\left([0,T], \mathcal{H}^\alpha_x\right),\; \phi^y \in L^\infty\left([0,T], \mathcal{H}^\beta_y\right)\right\}.$$

If $\Phi = (\phi^x, \phi^y) \in X_T^{\alpha,\beta}$, we set

$$\|\Phi\|_{X_T^{\alpha,\beta}} = \sup_{t\in[0,T]} \|\Phi(t)\|_{\alpha,\beta}.$$

We choose to consider integer exponents α and β for the sake of simplicity. We emphasize however that our approach requires $\alpha, \beta \geq 2$; see Section 4 for a more precise discussion on this aspect. We note that Theorem 3.11 allows $\alpha = \beta = 2$.

3.2.3. *Main assumptions.* We assume that the coupling potential $w \in C^\infty(\mathbb{R}^{d_1+d_2};\mathbb{R})$ satisfies

(H2) There exist $c_0, C > 0$ with $c_0 < 1$ such that for all $(x,y) \in \mathbb{R}^{d_1} \times \mathbb{R}^{d_2}$,

$$|w(x,y)| \leq c_0(V_1(x) + V_2(y) + C).$$

We emphasize that no condition is required concerning the above constant C: for instance if V_1 and V_2 are bounded, then we may always pick $c_0 < 1$ so that **(H2)** is satisfied. For unbounded potentials, the requirement $c_0 < 1$ can be understood as some smallness property, in the sense that $w(x,y)$ is a perturbation of $V_1(x)+V_2(y)$. This actually corresponds to the physical framework where the system (1.2) is introduced in order to approximate the exact solution ψ of (1.1) through the formula $\psi \approx \phi^x \otimes \phi^y$; see [3] for a derivation of error estimates. We also note that the assumption $c_0 < 1$ implies that w is $(H_x + H_y)$-bounded with relative bound $c_0 < 1$, hence by Kato–Rellich Theorem (see e.g. [18, Theorem X.12]), H is self-adjoint.

Remark 3.6. If w is at most quadratic, in the sense that $w \in C^\infty(\mathbb{R}^{d_1+d_2};\mathbb{R})$

$$\partial^\gamma_{x,y} w \in L^\infty(\mathbb{R}^{d_1+d_2}), \quad \forall \gamma \in \mathbb{N}^{d_1+d_2},\ |\gamma| \geq 2,$$

then the assumption **(H2)** is not needed to guarantee that H is self-adjoint (see the Faris–Lavine Theorem, [18, Theorem X.38]). Such a framework corresponds to the assumptions made for the error analysis in [3, 4]. For such potentials w, the assumption $c_0 < 1$ in **(H2)** is needed only in order to ensure that the Hartree solutions are global in time.

We also assume some conditions on the regularity of commutators of the coupling potential with the operators H_x and H_y. For integers $\alpha, \beta \geq 1$, we consider the condition:

(H3)$_{\alpha,\beta}$. There exist $c_1, c_2 > 0$ such that for all $k \in \{1, \cdots, \alpha\}$, $\ell \in \{1, \cdots, \beta\}$, for all $f_j = f_j(x)$, $g_j = g_j(y)$ in the Schwartz class ($j \in \{1,2\}$),

$$\begin{aligned}
&\left|\langle H_x^{k-1}[w(\cdot,y), H_x]f_1, f_2\rangle_{L^2_x}\right| + \left|\langle [w(\cdot,y), H_x]H_x^{k-1}f_1, f_2\rangle_{L^2_x}\right| \\
&\qquad\qquad \leq c_1\left(1 + V_2(y)\right)\|f_1\|_{\mathcal{H}^k_x}\|f_2\|_{\mathcal{H}^k_x}, \quad \text{for a.a. } y \in \mathbb{R}^{d_2}, \\
&\left|\langle H_y^{\ell-1}[w(x,\cdot), H_y]g_1, g_2\rangle_{L^2_y}\right| + \left|\langle [w(x,\cdot), H_y]H_y^{\ell-1}g_1, g_2\rangle_{L^2_y}\right| \\
&\qquad\qquad \leq c_2\left(1 + V_1(x)\right)\|g_1\|_{\mathcal{H}^\ell_y}\|g_2\|_{\mathcal{H}^\ell_y}, \quad \text{for a.a. } x \in \mathbb{R}^{d_1}.
\end{aligned}$$

Assumption **(H3)**$_{\alpha,\beta}$ is made in order to generalize the framework of Example 3.5. The subsequent proofs do not use the special form of the Hamiltonians H_x, H_y, so that our result extends as soon as they are self-adjoint operators and assumptions **(H1)**, **(H2)**, **(H3)**$_{\alpha,\beta}$ are satisfied. This applies in particular for magnetic Schrödinger operators.

Remark 3.7. It is not necessary to assume that the potential w is smooth, $w \in C^\infty(\mathbb{R}^{d_1+d_2};\mathbb{R})$. We only need enough regularity in order to write assumption **(H3)**$_{\alpha,\beta}$ for the α and β that we consider (recalling that H_x^{k-1} and $H_y^{\ell-1}$ are self-adjoint). For example, if

$w \in C^2(\mathbb{R}^{d_1+d_2};\mathbb{R})$, then Theorem 3.11 holds with $\alpha = \beta = 2$. We make this regularity assumption for simplicity, as the most important properties are those discussed in this subsection.

Remark 3.8. Whenever $w(x,y)$ is a Coulomb potential as in Section 3.1, the assumptions $\mathbf{(H3)}_{\alpha,\beta}$ are not satisfied. One then needs to take advantage of the convolution feature of the coupling and of the properties of H_x and H_y such as the Strichartz estimates in Proposition B.2.

We next present sufficient conditions on the potentials guaranteeing that assumptions **(H2)** and $\mathbf{(H3)}_{2,2}$ hold.

Lemma 3.9 (Sufficient conditions)**.** *Let $V_1 \in C^\infty(\mathbb{R}^{d_1};\mathbb{R})$ and $V_2 \in C^\infty(\mathbb{R}^{d_2};\mathbb{R})$ such that $V_1, V_2 \geq 0$. The above assumptions* **(H2)** *and* $\mathbf{(H3)}_{2,2}$ *are satisfied provided that the following estimates hold:*

- *There exists $C > 0$ such that*

$$|\nabla V_1(x)| \leq C\left(1 + V_1(x)\right), \forall x \in \mathbb{R}^{d_1}; \quad |\nabla V_2(y)| \leq C\left(1 + V_2(y)\right), \forall y \in \mathbb{R}^{d_2}. \tag{3.2}$$

- *There exist $0 < c_0 < 1$ and $c > 0$ independent of $x \in \mathbb{R}^{d_1}$ and $y \in \mathbb{R}^{d_2}$ such that*

$$\begin{cases} |w(x,y)| \leq c_0(V_1(x) + V_2(y) + c), \\ |\nabla_x w(x,y)| \leq c(\sqrt{V_1(x)} + V_2(y) + 1), \\ |\nabla_y w(x,y)| \leq c(V_1(x) + \sqrt{V_2(y)} + 1), \\ |\Delta_x w(x,y)| + |\Delta_y w(x,y)| \leq c(V_1(x) + V_2(y) + 1). \end{cases} \tag{3.3}$$

The proof of this lemma is given in Section 7.

Remark 3.10. We note that Example 3.5 meets the requirements stated in Lemma 3.9, provided that $\|\chi\|_{L^\infty(\mathbb{R})} < \omega^2/2$. Thus it satisfies the assumptions of Theorem 3.11 below for $\alpha = \beta = 2$.

3.3. **Main result and comments.** Before stating our main result we informally summarize the previous assumptions on the potentials for the case of polynomial coupling:

(H1) : boundedness from below of the potentials $V_1(x)$ and $V_2(y)$;

(H2) : control of $w(x,y)$ in terms of $V_1(x) + V_2(y)$;

$\mathbf{(H3)}_{\alpha,\beta}$: control of commutators involving $w(x,y)$, in terms of H_x and H_y.

We have the following result on existence and uniqueness as well norm and energy conservation of the time-dependent Hartree approximation.

Theorem 3.11. *Let $d_1, d_2 \geq 1$, $\alpha, \beta \geq 2$ and $\phi_0^x \in \mathcal{H}_x^\alpha$, $\phi_0^y \in \mathcal{H}_y^\beta$. Suppose that* **(H1)**, **(H2)** *and* $\mathbf{(H3)}_{\alpha,\beta}$ *are satisfied.*

- (1.2) *possesses a unique, global solution in $\Phi \in C(\mathbb{R}_+; L^2 \times L^2) \cap \bigcap_{T>0} X_T^{\alpha,\beta}$.*

- Conservations: *the L^2-norms of ϕ^x and ϕ^y are independent of $t \geq 0$, hence in view of* (1.3),
$$\|\phi^x(t)\|_{L^2(\mathbb{R}^{d_1})} = \|\phi^y(t)\|_{L^2(\mathbb{R}^{d_2})} = 1, \quad \forall t \geq 0.$$
In addition, the following total energy is also independent of $t \geq 0$:
$$E(t) := \langle H_x \phi^x(t), \phi^x(t)\rangle_{L^2_x} + \langle H_y \phi^y(t), \phi^y(t)\rangle_{L^2_y} + \iint_{\mathbb{R}^{d_1}\times\mathbb{R}^{d_2}} w(x,y)|\phi^x(t,x)|^2|\phi^y(t,y)|^2 dxdy.$$

We will see that the assumption $c_0 < 1$ in **(H2)** arises in two steps of the proof of Theorem 3.11. First, to make sure that the approximating scheme (1.4) introduced below is well-defined, we invoke Kato–Rellich Theorem, to show essentially that $\langle w\rangle_y$ (or more precisely, $\langle w_n\rangle_y$) is H_x-bounded with relative bound smaller than one, and that the same holds when the roles of x and y are swapped. Second, the assumption $c_0 < 1$ guarantees that the conserved energy E, defined in Theorem 3.11, is a coercive functional, so the conservation of E provides uniform in times a priori estimates, which in turn allow to show that the local in time solutions are actually global in time solutions.

The property $\Phi \in C(\mathbb{R}_+; L^2 \times L^2) \cap \bigcap_{T>0} X_T^{\alpha,\beta}$ means that $t \mapsto \|\Phi(t)\|_{\alpha,\beta}$ is *locally* bounded on $\mathbb{R}_+$. The map $t \mapsto \|\Phi(t)\|_{1,1}$ is bounded on $\mathbb{R}_+$ in view of the conservation of the coercive energy E, but higher order norms may not be bounded as t goes to infinity (recall that Theorem 3.11 requires $\alpha, \beta \geq 2$).

4. Analysis of the iterative scheme: existence and uniform bounds

This section is devoted to the analysis of the system (1.4). For $n \in \mathbb{N}$, we denote by $\Phi_n = (\phi_n^x, \phi_n^y)$, the solution to the scheme (1.4) and we prove local in time uniform estimates. At this stage, we only need that $\phi_0^x \in \mathcal{H}_x^\alpha$, $\phi_0^y \in \mathcal{H}_y^\beta$ for integers $\alpha, \beta \geq 1$.

Lemma 4.1. *Let $\alpha, \beta \geq 1$. Assume that* **(H1)**, **(H2)** *and* **(H3)**$_{\alpha,\beta}$ *are satisfied. Assume $\phi_0^x \in \mathcal{H}_x^\alpha$, and $\phi_0^y \in \mathcal{H}_y^\beta$. Then, the sequence $(\Phi_n)_{n\in\mathbb{N}}$ solution to* (1.4) *is well-defined and there exists $T > 0$ such that for all $n \in \mathbb{N}$, the solution $\Phi_n \in X_T^{\alpha,\beta}$ of the scheme* (1.4) *satisfies*
$$\|\Phi_n\|_{X_T^{\alpha,\beta}} \leq 2\|\Phi_0\|_{\alpha,\beta}. \tag{4.1}$$

The proof of this lemma relies on the fact that the control of Φ_{n+1} involves terms which are linear in Φ_{n+1} and quadratic in Φ_n, and require the $X_T^{1,1}$-norm of Φ_n. For this reason, the Lemma holds as soon as $\alpha, \beta \geq 1$. However in Theorem 3.11 , we require at least an $X_T^{2,2}$ regularity. The reason will appear in Section 5, as we do need uniform (in n) estimates in $X_T^{2,2}$ to show that the sequence $(\Phi_n)_n$ converges in $X_T^{0,0} = L_T^\infty L^2$.

In Section 4.1, we address the construction of the family $(\Phi_n)_{n\in\mathbb{N}}$, which relies on a commutation lemma that we prove in Section 4.3. Section 4.2 is devoted to the proof of the uniform bound stated in Lemma 4.1.

4.1. **Well-posedness of the scheme.** Before entering into the proof of Lemma 4.1, let us discuss why the scheme is indeed well-defined: as Φ_{n+1} solves a decoupled system of linear Schrödinger equations, it suffices to study the properties of the time-dependent potentials $\langle w_n\rangle_y$ and $\langle w_n\rangle_x$. We fix $T>0$ arbitrary and take $\phi_0^x\in\mathcal{H}_x^\alpha$, and $\phi_0^y\in\mathcal{H}_y^\beta$, with $\alpha,\beta\geq 1$. For $n=0$, Φ_0 is obviously well-defined with $\Phi_0\in X_T^{\alpha,\beta}$, and

$$\|\phi_n^x(t)\|_{L_x^2}=\|\phi_n^y(t)\|_{L_y^2}=1,\quad \forall t\in\mathbb{R}, \tag{4.2}$$

holds for $n=0$. We argue by induction. If $\Phi_n\in X_T^{1,1}$ satisfies (4.2), then in view of **(H2)**, $\langle w_n\rangle_y(t,x)$ and $\langle w_n\rangle_x(t,y)$ are well-defined. In addition, for $t\in[0,T]$, **(H2)** yields

$$\begin{aligned}|\langle w_n\rangle_y(t,x)|&\leq c_0V_1(x)\|\phi_n^y(t)\|_{L^2}^2+C\|\phi_n^y(t)\|_{\mathcal{H}_y^1}^2,\quad \text{a.e. } x,\\ |\langle w_n\rangle_x(t,y)|&\leq c_0V_2(y)\|\phi_n^x(t)\|_{L^2}^2+C\|\phi_n^x(t)\|_{\mathcal{H}_x^1}^2,\quad \text{a.e. } y,\end{aligned} \tag{4.3}$$

for some constant C whose value is irrelevant here, unlike the fact that we assume $c_0<1$. Indeed, together with (4.2), this implies that $\langle w_n\rangle_y$ is H_x-bounded with relative bound at most c_0. By Kato–Rellich Theorem (see e.g. [18, Theorem X.12]), $\Phi_{n+1}\in X_T^{0,0}$ is well-defined (see e.g. [19, Section VIII.4]), and (4.2) holds at level $n+1$. Next, we prove that $\Phi_{n+1}\in X_T^{1,1}$. Applying the operator H_x to the first equation in (1.4), we find

$$(i\partial_t-H_x)(H_x\phi_{n+1}^x)=\langle w_n\rangle_y(t)(H_x\phi_{n+1}^x)+[H_x,\langle w_n\rangle_y(t)]\phi_{n+1}^x. \tag{4.4}$$

Since H_x is self-adjoint, we deduce

$$\begin{aligned}\|H_x^{1/2}\phi_{n+1}^x(t)\|_{L_x^2}^2&=\mathrm{Re}\langle H_x\phi_{n+1}^x(t),\phi_{n+1}^x(t)\rangle_{L_x^2}\\ &=\|H_x^{1/2}\phi_0^x\|_{L_x^2}^2+\mathrm{Re}\left(\int_0^t\frac{d}{ds}\langle H_x\phi_{n+1}^x(s),\phi_{n+1}^x(s)\rangle_{L_x^2}ds\right)\\ &=\|H_x^{1/2}\phi_0^x\|_{L_x^2}^2-\mathrm{Re}\left(\int_0^t\langle i[H_x,\langle w_n\rangle_y]\phi_{n+1}^x(s),\phi_{n+1}^x(s)\rangle_{L_x^2}ds\right).\end{aligned}$$

Minkowski inequality yields, in view of $\mathbf{(H3)}_{1,1}$,

$$\left|\langle[H_x,\langle w_n\rangle_y(t)]f_1,f_2\rangle_{L_x^2}\right|\lesssim\|\phi_n^y\|_{L_T^\infty\mathcal{H}_y^1}^2\|f_1\|_{\mathcal{H}_x^1}\|f_2\|_{\mathcal{H}_x^1}. \tag{4.5}$$

We infer the existence of a universal constant $C>0$ such that

$$\|H_x^{1/2}\phi_{n+1}^x(t)\|_{L_x^2}^2\leq\|H_x^{1/2}\phi_0^x\|_{L_x^2}^2+C\|\Phi_n\|_{X_T^{1,1}}^2\int_0^t\|\phi_{n+1}^x(s)\|_{\mathcal{H}_x^1}^2ds.$$

We deduce

$$\sup_{t\in[0,T]}\|\phi_{n+1}^x(t)\|_{\mathcal{H}_x^1}^2\lesssim\|\phi_0^x\|_{\mathcal{H}_x^1}^2+C\|\Phi_n\|_{X_T^{1,1}}^2\int_0^t\|\phi_{n+1}^x(s)\|_{\mathcal{H}_x^1}^2ds, \tag{4.6}$$

We have a similar estimate for $\|H_y^{1/2}\phi_{n+1}^y(t)\|_{L_x^2}^2$:

$$\sup_{t\in[0,T]}\|\phi_{n+1}^y(t)\|_{\mathcal{H}_y^1}^2\lesssim\|\phi_0^y\|_{\mathcal{H}_y^1}^2+C\|\Phi_n\|_{X_T^{1,1}}^2\int_0^t\|\phi_{n+1}^y(s)\|_{\mathcal{H}_y^1}^2ds, \tag{4.7}$$

and so Gronwall lemma and the inductive assumption yields $\Phi_{n+1} \in X_T^{1,1}$ and completes the construction of the sequence $(\Phi_n)_{n\in\mathbb{N}}$.

4.2. **Uniform bounds.** We conclude the proof of Lemma 4.1 in analyzing the regularity of the solutions.

Proof of Lemma 4.1. In view of the definition of the scheme and of the conservations

$$\frac{d}{dt}\|\phi_n^x\|_{L^2}^2 = \frac{d}{dt}\|\phi_n^y\|_{L^2}^2 = 0,$$

we need now consider $H_x^\alpha \phi_n^x$ and $H_y^\beta \phi_n^y$ for $\alpha, \beta \geq 1$. Let

$$R = 2\|\Phi_0\|_{\alpha,\beta},$$

and introduce

$$B_{R,T} = \{\Phi \in X_T^{\alpha,\beta},\ \|\Phi\|_{X_T^{\alpha,\beta}} \leq R\}.$$

We distinguish two cases for the ease of presentation.

First case: $\alpha = \beta = 1$**.** In that case, if $\Phi_n \in B_{R,T}$, then estimates (4.6) and (4.7) imply

$$\|\Phi_{n+1}(t)\|_{X_T^{1,1}}^2 \leq \|\Phi_0\|_{1,1}^2 + CTR^2\|\Phi_{n+1}(t)\|_{X_T^{1,1}}^2.$$

We infer that choosing $T > 0$ sufficiently small in terms of R, but independently of n, $\Phi_n \in B_{R,T}$ implies $\Phi_{n+1} \in B_{R,T}$.

Higher regularity: The control of higher order regularity is obtained by a similar recursive argument which uses an iterated commutator estimate. Let $\alpha, \beta \geq 1$. We have

$$\begin{cases} i\partial_t H_x^k \phi_{n+1}^x = (H_x + \langle w_n\rangle_y) H_x^k \phi_{n+1}^x + [H_x^k, \langle w_n\rangle_y]\phi_{n+1}^x, \quad H_x^k \phi_{n+1|t=0}^x = H_x^k \phi_0^x, \\ i\partial_t H_y^\ell \phi_{n+1}^y = (H_y + \langle w_n\rangle_x) H_y^\beta \phi_{n+1}^y + [H_y^\ell, \langle w_n\rangle_x]\phi_{n+1}^y, \quad H_y^\ell \phi_{n+1|t=0}^y = H_y^\ell \phi_0^y. \end{cases} \tag{4.8}$$

The next lemma allows to control the commutators.

Lemma 4.2. *Let $\Phi_n \in X_T^{1,1}$ for some $T > 0$, and $k, \ell \geq 1$ be integers. Suppose that* **(H3)**$_{k,\ell}$ *is satisfied. For all $t \in [0, T]$,*

$$\left|\langle [H_x^k, \langle w_n\rangle_y(t)] f_1, f_2\rangle_{L_x^2}\right| \lesssim \|\phi_n^y\|_{L_T^\infty \mathcal{H}_y^1}^2 \|f_1\|_{\mathcal{H}_x^k}\|f_2\|_{\mathcal{H}_x^k}, \qquad \forall f_1, f_2 \in \mathcal{H}_x^k$$

$$\left|\langle [H_y^\ell, \langle w_n\rangle_x(t)] g_1, g_2\rangle_{L_y^2}\right| \lesssim \|\phi_n^x\|_{L_T^\infty \mathcal{H}_x^1}^2 \|g_1\|_{\mathcal{H}_y^\ell}\|g_2\|_{\mathcal{H}_y^\ell}, \qquad \forall g_1, g_2 \in \mathcal{H}_y^\ell.$$

Taking the lemma for granted, (4.8) implies, since H_x is self-adjoint,

$$\begin{aligned} \|\phi_{n+1}^x(t)\|_{\mathcal{H}_x^\alpha}^2 &= \mathrm{Re}\langle H_x^\alpha \phi_{n+1}^x(t), \phi_{n+1}^x(t)\rangle_{L_x^2} \\ &= \|H_x^{\alpha/2}\phi_0^x\|_{L_x^2}^2 + \mathrm{Re}\left(\int_0^t \frac{d}{ds}\langle H_x^\alpha \phi_{n+1}^x(s), \phi_{n+1}^x(s)\rangle_{L_x^2} ds\right) \\ &= \|H_x^{\alpha/2}\phi_0^x\|_{L_x^2}^2 - \mathrm{Re}\left(\int_0^t \langle i[H_x^\alpha, \langle w_n\rangle_y]\phi_{n+1}^x(s), \phi_{n+1}^x(s)\rangle_{L_x^2} ds\right) \\ &\leq \|H_x^{\alpha/2}\phi_0^x\|_{L_x^2}^2 + CT\|\phi_n^y\|_{L_T^\infty \mathcal{H}_y^1}^2 \sup_{t\in[0,T]} \|\phi_{n+1}^x(t)\|_{\mathcal{H}_x^\alpha}^2. \end{aligned}$$

We have a similar estimate for $\|H_y^{\beta/2}\phi_{n+1}^y(t)\|_{L_x^2}^2$, and so if $\Phi_n \in B_{R,T}$, then equations (4.6) and (4.7) imply

$$\|\Phi_{n+1}(t)\|_{X_T^{\alpha,\beta}}^2 \leq \|\Phi_0\|_{\alpha,\beta}^2 + CTR^2\|\Phi_{n+1}(t)\|_{X_T^{\alpha,\beta}}^2.$$

We infer that choosing $T > 0$ sufficiently small in terms of R, but independently of n, $\Phi_n \in B_{R,T}$ implies $\Phi_{n+1} \in B_{R,T}$. It thus remains to prove the lemma, which is the subject of the next subsection. □

Remark 4.3. Lemma 4.1 holds as soon as $\alpha, \beta \geq 1$, but this is not enough in order to conclude that the sequence $(\Phi_n)_{n\in\mathbb{N}}$ converges to some solution of (1.2). Indeed, the mere boundedness in $X_T^{1,1}$ only implies the convergence of a subsequence in the weak-* topology: this is not enough to pass to the limit in (1.4), both because the subsequence need not retain consecutive indices, and because the topology considered is too large to pass to the limit in nonlinear terms. These issues are overcome by requiring $\alpha, \beta \geq 2$ in Sections 5 and 6.

4.3. **Proof of Lemma 4.2.** Of course, (4.5) implies the result when $k = 1$. Take $k \geq 1$ and assume that the result holds for all $m \leq k$. We write

$$\begin{aligned}[H_x^{k+1}, \langle w_n\rangle_y(t)] &= H_x^k[H_x, \langle w_n\rangle_y(t)] + [H_x^k, \langle w_n\rangle_y(t)]H_x \\ &= H_x[H^{k-1}, \langle w_n\rangle_y(t)]H_x + H_x^k[H_x, \langle w_n\rangle_y(t)] + [H_x, \langle w_n\rangle_y(t)]H_x^k.\end{aligned}$$

We deduce from (4.5) and the recursive assumption that for $f_1, f_2 \in \mathcal{S}(\mathbb{R}^{d_1})$, we have

$$\begin{aligned}\left|\langle [H_x^{k+1}, \langle w_n\rangle_y(t)]f_1, f_2\rangle_{L_x^2}\right| &\leq \left|\langle [H_x^{k-1}, \langle w_n\rangle_y(t)]H_xf_1, H_xf_2\rangle_{L_x^2}\right| \\ &\quad + \left|\langle H_x^k[H_x, \langle w_n\rangle_y(t)]f_1, f_2\rangle_{L_x^2}\right| + \left|\langle [H_x, \langle w_n\rangle_y(t)]H_x^kf, g\rangle_{L_x^2}\right|.\end{aligned}$$

By the recursive assumption

$$\begin{aligned}\left|\langle [H_x^{k-1}, \langle w_n\rangle_y(t)]H_xf_1, H_xf_2\rangle_{L_x^2}\right| &\lesssim \|\phi_n^y\|_{L_T^\infty\mathcal{H}_y^1}^2\|H_xf_1\|_{\mathcal{H}_x^{k-1}}\|H_xf_2\|_{\mathcal{H}_x^{k-1}} \\ &\lesssim \|\phi_n^y\|_{L_T^\infty\mathcal{H}_y^1}^2\|f_1\|_{\mathcal{H}_x^{k+1}}\|f_2\|_{\mathcal{H}_x^{k+1}}.\end{aligned}$$

Finally, in view of $\mathbf{(H3)}_{k,\ell}$ and Minkowski inequality, we have

$$\begin{aligned}\left|\langle H_x^k[H_x, \langle w_n\rangle_y(t)]f_1, f_2\rangle_{L_x^2}\right| &\lesssim \|\phi_n^y\|_{L_T^\infty\mathcal{H}_y^1}^2\|f_1\|_{\mathcal{H}_x^{k+1}}\|f_2\|_{\mathcal{H}_x^{k+1}}, \\ \left|\langle [H_x, \langle w_n\rangle_y(t)]H_x^kf_1, f_2\rangle_{L_x^2}\right| &\lesssim \|\phi_n^y\|_{L_T^\infty\mathcal{H}_y^1}^2\|f_1\|_{\mathcal{H}_x^{k+1}}\|f_2\|_{\mathcal{H}_x^{k+1}},\end{aligned}$$

which concludes the proof, after arguing similarly with H_y.

5. Convergence in small norms

The second step of the proof of Theorem 3.11 consists in passing to the limit $n \to +\infty$ and prove the existence of a limit to the sequence $(\Phi_n)_{n\in\mathbb{N}}$ of solutions to (1.4). The main result in this section is:

Lemma 5.1. *Assume that there exist $T>0$ and $R>0$ such that*

$$\sup_{n\in\mathbb{N}} \|\Phi_n\|_{X_T^{2,2}} \leq R.$$

Then there exist $T_1 \in]0,T]$ and $\Phi \in X_{T_1}^{2,2}$ such that

$$\sup_{0\leq t\leq T_1} \|\Phi_n(t)-\Phi(t)\|_{L^2_x\times L^2_y} = \|\Phi_n-\Phi\|_{X_{T_1}^{0,0}} \underset{n\to\infty}{\longrightarrow} 0. \tag{5.1}$$

If in addition $(\Phi_n)_n$ is bounded in $X_T^{\alpha,\beta}$ for some integers $\alpha,\beta\geq 2$, then $\Phi\in X_{T_1}^{\alpha,\beta}$.

Proof. Consider (1.4) at steps $n+1$ and n, respectively, and subtract the corresponding equations. We find, for $n\geq 1$,

$$\begin{aligned}(i\partial_t - H_x)\left(\phi_{n+1}^x-\phi_n^x\right) &= \langle w_n\rangle_y \phi_{n+1}^x - \langle w_{n-1}\rangle_y \phi_n^x\\ &= \langle w_n\rangle_y \left(\phi_{n+1}^x-\phi_n^x\right) + \Big(\langle w_n\rangle_y - \langle w_{n-1}\rangle_y\Big)\phi_n^x,\end{aligned}$$

and energy estimates yield, for $T_1\in]0,T]$, since $\Phi_{n+1|t=0}=\Phi_{n|t=0}$,

$$\|\phi_{n+1}^x-\phi_n^x\|_{L^\infty_{T_1}L^2_x} \leq \int_0^{T_1} \left\|\Big(\langle w_n(s)\rangle_y - \langle w_{n-1}(s)\rangle_y\Big)\phi_n^x(s)\right\|_{L^2_x} ds. \tag{5.2}$$

In view of **(H2)**, the key term is estimated by

$$\Big|\langle w_n(t)\rangle_y - \langle w_{n-1}(t)\rangle_y\Big| \lesssim \int_{\mathbb{R}^{d_2}} (V_1(x)+V_2(y)+1)\left||\phi_n^y(t,y)|^2-|\phi_{n-1}^y(t,y)|^2\right| dy.$$

Writing $|\phi_n^y|^2-|\phi_{n-1}^y|^2 = \mathrm{Re}\Big((\phi_n^y-\phi_{n-1}^y)(\overline{\phi_n^y}+\overline{\phi_{n-1}^y})\Big)$, and using Cauchy-Schwarz inequality,

$$\begin{aligned}\Big|\langle w_n(t)\rangle_y - \langle w_{n-1}(t)\rangle_y\Big| &\lesssim (V_1(x)+1)\left(\|\phi_n^y\|_{L^2_y}+\|\phi_{n-1}^y\|_{L^2_y}\right)\|\phi_n^y-\phi_{n-1}^y\|_{L^2_y}\\ &\quad + \left(\|V_2\phi_n^y\|_{L^2_y}+\|V_2\phi_{n-1}^y\|_{L^2_y}\right)\|\phi_n^y-\phi_{n-1}^y\|_{L^2_y}\\ &\lesssim (V_1(x)+1))\sup_{k\in\mathbb{N}}\|\Phi_k\|_{X_T^{2,2}}\|\phi_n^y-\phi_{n-1}^y\|_{L^2_y}.\end{aligned} \tag{5.3}$$

Plugging this estimate into (5.2), we infer, thanks to Minkowski inequality,

$$\begin{aligned}\|\phi_{n+1}^x-\phi_n^x\|_{L^\infty_{T_1}L^2_x} &\lesssim \sup_{k\in\mathbb{N}}\|\Phi_k\|_{X_T^{2,2}}\int_0^{T_1}\|(V_1+1))\,\phi_n^x(s)\|_{L^2_x}\,\|\phi_n^y(s)-\phi_{n-1}^y(s)\|_{L^2_y}ds\\ &\lesssim \sup_{k\in\mathbb{N}}\|\Phi_k\|^2_{X_T^{2,2}}\int_0^{T_1}\|\phi_n^y(s)-\phi_{n-1}^y(s)\|_{L^2_y}ds\\ &\lesssim R^2T_1\sup_{t\in[0,T_1]}\|\phi_n^y(t)-\phi_{n-1}^y(t)\|_{L^2_y}.\end{aligned}$$

We obtain a similar estimate by exchanging the roles of x and y, and so

$$\|\Phi_{n+1}-\Phi_n\|_{X_{T_1}^{0,0}} \lesssim R^2T_1\|\Phi_n-\Phi_{n-1}\|_{X_{T_1}^{0,0}}. \tag{5.4}$$

Fixing $T_1 \in]0,T]$ sufficiently small, the series

$$\sum_{n\in\mathbb{N}} \|\Phi_{n+1}-\Phi_n\|_{X^{0,0}_{T_1}}$$

converges geometrically, and Φ_n converges in $X^{0,0}_{T_1}$, to some $\Phi \in X^{0,0}_{T_1}$.

On the other hand, the boundedness of $(\Phi_n)_n$ in $X^{2,2}_T$ implies that a subsequence is converging in the weak-* topology of $X^{2,2}_T$. By uniqueness of limits in the sense of distributions, we infer $\Phi \in X^{2,2}_{T_1}$. The same holds when $X^{2,2}_T$ is replaced by $X^{\alpha,\beta}_T$ for $\alpha,\beta \geq 2$. □

6. Passing to the limit in the equation

We now have all the elements in hands for proving Theorem 3.11 by showing that the limit function Φ constructed in Lemma 5.1 is a solution to equation (1.2) with the properties stated in Theorem 3.11.

6.1. **Existence of a local solution.** Combining Lemmas 4.1 and 5.1, we infer that under the assumptions of Theorem 3.11, there exists $T_1 > 0$ such that $\Phi_n \to \Phi$ in $X^{0,0}_{T_1}$. By uniqueness of the limit, we also have $\Phi_n \rightharpoonup \Phi$ in $X^{\alpha,\beta}_{T_1}$ (and no extraction of a subsequence is needed). Resuming the estimates from the proof of Lemma 5.1, we observe that for $n,m \in \mathbb{N}$, $t \in [0,T_1]$ and $x \in \mathbb{R}^{d_1}$,

$$\begin{aligned}|\langle w_n(t)\rangle_y - \langle w_m(t)\rangle_y| &= \left|\int_{\mathbb{R}^{d_2}} w(x,y)\left(|\phi^y_n(t,y)|^2 - |\phi^y_m(t,y)|^2\right)dy\right| \\ &\lesssim (V_1(x)+1)\sup_{k\in\mathbb{N}}\|\Phi_k\|_{X^{2,2}_T}\|\phi^y_n(t)-\phi^y_m(t)\|_{L^2_y}.\end{aligned}$$

Passing to the limit $m \to +\infty$, we obtain that for $n \in \mathbb{N}$, $t \in [0,T_1]$ and $x \in \mathbb{R}^{d_1}$,

$$|\langle w_n(t)\rangle_y - \langle w(t)\rangle_y| \lesssim (V_1(x)+1)\sup_{k\in\mathbb{N}}\|\Phi_k\|_{X^{2,2}_T}\|\phi^y_n(t)-\phi^y(t)\|_{L^2_y}.$$

Therefore, keeping the same notation R as from Lemma 5.1,

$$\begin{aligned}\left\|\langle w_n(t)\rangle_y\phi^x_{n+1}(t) - \langle w(t)\rangle_y\phi^x(t)\right\|_{L^2_x} &\lesssim \left\|\left(\langle w_n(t)\rangle_y - \langle w(t)\rangle_y\right)\phi^x_{n+1}(t)\right\|_{L^2_x} \\ &\quad + \left\|\langle w(t)\rangle_y\left(\phi^x_{n+1}(t)-\phi^x(t)\right)\right\|_{L^2_x} \\ &\lesssim R\|\phi^y_n(t)-\phi^y(t)\|_{L^2_y}\left\|(V_1+1)\phi^x_{n+1}(t)\right\|_{L^2_x} \\ &\quad + \left\|\left(V_1+1+\|\phi^y\|^2_{L^\infty_{T_1}\mathcal{H}^1_y}\right)\left(\phi^x_{n+1}(t)-\phi^x(t)\right)\right\|_{L^2_x},\end{aligned}$$

where we have used (4.3) and the normalization (1.3). The first term on the right hand side goes to zero as $n \to \infty$, uniformly in $t \in [0,T_1]$. So does the last one in the case $\alpha,\beta \geq 3$, since by interpolation Φ_n then converges to Φ strongly in $X^{2,2}_T$. In the case where α or β is equal to 2, we can only claim a weak convergence,

$$\langle w_n\rangle_y\phi^x_{n+1} \underset{n\to\infty}{\rightharpoonup} \langle w\rangle_y\phi^x \quad \text{in } L^\infty([0,T_1];L^2_x) \text{ weak-}*.$$

Similarly,

$$\langle w_n\rangle_x \phi^y_{n+1} \underset{n\to\infty}{\rightharpoonup} \langle w\rangle_x \phi^y \quad \text{in } L^\infty([0,T_1];L^2_y) \text{ weak-}*,$$

and Φ solves (1.2) for $t\in[0,T_1]$, in the sense of distributions. In view of the regularity $\Phi\in X^{\alpha,\beta}_{T_1}$, Duhamel's formula,

$$\phi^x(t) = e^{-itH_x}\phi^x_0 - i\int_0^t e^{-i(t-s)H_x}\left(\langle w\rangle_y \phi_x\right)(s)ds,$$
$$\phi^y(t) = e^{-itH_y}\phi^y_0 - i\int_0^t e^{-i(t-s)H_y}\left(\langle w\rangle_x \phi_y\right)(s)ds,$$

then shows the continuity in time $\Phi\in C([0,T_1];L^2_x\times L^2_y)$.

6.2. **Uniqueness.** At this stage, it is rather clear that uniqueness holds in $X^{2,2}_T$, no matter how large α and β are. Suppose that $\tilde\Phi\in X^{2,2}_T$ is another solution to (1.2) for $T>0$: the system satisfied by $\Phi-\tilde\Phi$ is similar to the one satisfied by $\Phi_{n+1}-\Phi_n$, and considered in the proof of Lemma 5.1. Since $\Phi,\tilde\Phi\in X^{2,2}_T$, there exists $R>0$ such that

$$\|\Phi\|_{X^{2,2}_T} + \|\tilde\Phi\|_{X^{2,2}_T} \le R,$$

and repeating the computations presented in the proof of Lemma 5.1, we obtain, for any $T_1\in]0,T]$,

$$\|\Phi-\tilde\Phi\|_{X^{0,0}_{T_1}} \le CT_1R\|\Phi-\tilde\Phi\|_{X^{0,0}_{T_1}}.$$

Picking $T_1>0$ such that $CT_1R<1$ shows that $\Phi\equiv\tilde\Phi$ for $t\in[0,T_1]$, and we infer that $\Phi\equiv\tilde\Phi$ on $[0,T]$ by covering $[0,T]$ by finitely many intervals of length at most T_1.

6.3. **Conservations.** We now address the second point in Theorem 3.11: we assume that (1.2) has a unique solution $\Phi\in X^{2,2}_T$ for some $T>0$. This implies in particular, in view of (1.2), that $\partial_t\phi^x\in L^\infty([0,T];L^2_x)$ and $\partial_t\phi^y\in L^\infty([0,T];L^2_y)$, and the multiplier techniques evoked below are justified without using regularizing argument as in e.g. [10].

For the conservation of the L^2-norms, multiply the first equation in (1.2) by $\overline{\phi^x}$, integrate in space on $\mathbb{R}^{d_1}$, and consider the imaginary part: we readily obtain

$$\frac{d}{dt}\|\phi^x(t)\|^2_{L^2_x} = 0.$$

We proceed similarly for ϕ^y, and the conservation of the L^2-norms follows.

For the energy, consider the multiplier $\partial_t\overline{\phi^x}$ in the equation for ϕ^x: as evoked above, all the products are well-defined, in the worst possible case as products of two L^2 functions. Integrate in space and consider the real part: we obtain

$$\frac{d}{dt}E(t) = 0.$$

6.4. **Globalization.** In view of Lemmas 4.1 and 5.1, it suffices to prove a priori estimates on $\|\Phi\|_{X_T^{2,2}}$, showing that this quantity is locally bounded in T, to infer that $\Phi \in X_T^{2,2}$ for all $T > 0$, and then globalize the solution by the standard ODE alternative.

We use the conservation of the total energy, whose expression we develop:

$$\begin{aligned} E(t) &= (H_x\phi^x(t), \phi^x(t))_{L^2_x} + (H_y\phi^y(t), \phi^y(t))_{L^2_y} \\ &\quad + \iint_{\mathbb{R}^{d_1}\times\mathbb{R}^{d_2}} w(x,y)|\phi^x(t,x)|^2|\phi^y(t,y)|^2 dxdy \\ &= \frac{1}{2}\|\nabla_x\phi^x(t)\|^2_{L^2(\mathbb{R}^{d_1})} + \int_{\mathbb{R}^{d_1}} V_1(x)|\phi^x(t,x)|^2dx + \frac{1}{2}\|\nabla_y\phi^y(t)\|^2_{L^2(\mathbb{R}^{d_2})} \\ &\quad + \int_{\mathbb{R}^{d_2}} V_2(y)|\phi^y(t,y)|^2dy + \iint_{\mathbb{R}^{d_1}\times\mathbb{R}^{d_2}} w(x,y)|\phi^x(t,x)|^2|\phi^y(t,y)|^2dxdy. \end{aligned}$$

Since $c_0 < 1$ in **(H2)**, we infer

$$\begin{aligned} E(t) \geq \frac{1}{2}\|\nabla_x\phi^x(t)\|^2_{L^2(\mathbb{R}^{d_1})} + \frac{1}{2}\|\nabla_y\phi^y(t)\|^2_{L^2(\mathbb{R}^{d_2})} + (1-c_0)\int_{\mathbb{R}^{d_1}} V_1(x)|\phi^x(t,x)|^2dx \\ + (1-c_0)\int_{\mathbb{R}^{d_2}} V_2(y)|\phi^y(t,y)|^2dy - c_0C\int_{\mathbb{R}^{d_1}} |\phi^x(t,x)|^2dx - c_0C\int_{\mathbb{R}^{d_2}} |\phi^y(t,y)|^2dy. \end{aligned}$$

The conservations established above yield

$$\begin{aligned} \frac{1}{2}\|\nabla_x\phi^x(t)\|^2_{L^2(\mathbb{R}^{d_1})} + \frac{1}{2}\|\nabla_y\phi^y(t)\|^2_{L^2(\mathbb{R}^{d_2})} + (1-c_0)\int_{\mathbb{R}^{d_1}} V_1(x)|\phi^x(t,x)|^2dx \\ + (1-c_0)\int_{\mathbb{R}^{d_2}} V_2(y)|\phi^y(t,y)|^2dy \leq E(0) + 2c_0C. \end{aligned}$$

This is the coercivity property announced in the introduction, showing that there exists M depending only on $\|\Phi_0\|_{1,1}$ such that

$$\|\Phi\|_{X_T^{1,1}} \leq M,$$

for any interval $[0,T]$ on which the solution is well-defined. Proceeding like in the proof of Lemma 4.1, we have

$$\sup_{t\in[0,T]} \|H_x\phi^x(t)\|^2_{L^2_x} \leq \|H_x\phi^x_0\|^2_{L^2_x} + 2\int_0^T \left|([H_x, \langle w\rangle_y(t)]\phi^x(t), H_x\phi^x(t))_{L^2_x}\right| dt. \tag{6.1}$$

In view of Lemma 4.2 with $k = 1$, $f = \phi^x$ and $g = H_x\phi^x$, we infer

$$\begin{aligned} \sup_{t\in[0,T]} \|H_x\phi^x(t)\|^2_{L^2_x} &\leq \|H_x\phi^x_0\|^2_{L^2_x} + C\|\phi^y\|^2_{L^\infty_T\mathcal{H}^1_y}\int_0^T \|\phi^x(t)\|_{\mathcal{H}^2_x}\|H_x\phi^x(t)\|_{L^2_x}dt \\ &\leq \|H_x\phi^x_0\|^2_{L^2_x} + CM^2\int_0^T \|\phi^x(t)\|^2_{\mathcal{H}^2_x}dt. \end{aligned}$$

The conservation of the L^2-norm of ϕ^x implies

$$\sup_{t\in[0,T]} \|\phi^x(t)\|^2_{\mathcal{H}^2_x} \leq \|\phi^x\|^2_{\mathcal{H}^2_x} + CM^2 \int_0^T \|\phi^x(t)\|^2_{\mathcal{H}^2_x} dt,$$

hence an exponential a priori control of the $\mathcal{H}^2_x$-norm of $\phi^x(t)$ by Gronwall lemma. The same holds for $\phi^y(t)$, hence the conclusion of Theorem 3.11.

7. Proof of Lemma 3.9

We briefly explain why (3.3) implies $\mathbf{(H3)}_{2,2}$, thanks to an integration by parts, in view of (3.2). Typically, for $f_1, f_2 \in \mathcal{S}(\mathbb{R}^{d_1})$,

$$\langle [w(x,y), H_x] f_1, f_2\rangle_{L^2_x} = \frac{1}{2}\langle \Delta_x w(\cdot,y) f_1, f_2\rangle_{L^2_x} + \langle \nabla_x w(\cdot,y)\cdot\nabla f_1, f_2\rangle_{L^2_x}.$$

Therefore, for almost all $y \in \mathbb{R}^{d_2}$, Cauchy-Schwarz inequality yields

$$\begin{aligned}\left|\langle [w(x,y), H_x] f_1, f_2\rangle_{L^2_x}\right| \leq \frac{1}{2}\||\Delta_x w(\cdot,y)|^{1/2} f_1\|_{L^2_x}\||\Delta_x w(\cdot,y)|^{1/2} f_2\|_{L^2_x} \\ + \|\nabla_x f_1\|_{L^2_x}\|\nabla_x w(\cdot,y) f_2\|_{L^2_x}.\end{aligned}$$

Using (3.3),

$$\begin{aligned}\||\Delta_x w(\cdot,y)|^{1/2} f\|^2_{L^2_x} \lesssim \|\sqrt{V_1} f\|^2_{L^2_x} + (1+V_2(y))\|f\|^2_{L^2_x} \lesssim \|f\|^2_{\mathcal{H}^1_x} + (1+V_2(y))\|f\|^2_{L^2_x}, \\ \|\nabla_x w(\cdot,y) f\|_{L^2_x} \lesssim \|(\sqrt{V_1} + V_2(y) + 1) f\|_{L^2_x} \lesssim \|f\|_{\mathcal{H}^1_x} + (1+V_2(y))\|f\|_{L^2_x}.\end{aligned}$$

We deduce the expected relation for $k = \ell = 1$:

$$\left|\langle [w(x,y), H_x] f_1, f_2\rangle_{L^2_x}\right| \lesssim (1+V_2(y))\|f_1\|_{\mathcal{H}^1_x}\|f_2\|_{\mathcal{H}^1_x}.$$

For $k = 2$, write

$$\begin{aligned}\left|\langle H_x[w(x,y), H_x] f_1, f_2\rangle_{L^2_x}\right| &= \left|\langle [w(x,y), H_x] f_1, H_x f_2\rangle_{L^2_x}\right| \\ &\leq \frac{1}{2}\left|\langle \Delta_x w(\cdot,y) f_1, H_x f_2\rangle_{L^2_x}\right| + \left|\langle \nabla_x w(\cdot,y)\cdot\nabla f_1, H_x f_2\rangle_{L^2_x}\right| \\ &\lesssim \|\left(1+V_1+V_2(y)\right) f_1\|_{L^2_x}\|H_x f_2\|_{L^2_x} \\ &\quad + \|\nabla_x w(\cdot,y)\cdot\nabla f_1\|_{L^2_x}\|H_x f_2\|_{L^2_x} \\ &\lesssim \|f_1\|_{\mathcal{H}^2_x}\|f_2\|_{\mathcal{H}^2_x} + V_2(y)\|f_1\|_{L^2_x}\|f_2\|_{\mathcal{H}^2_x} \\ &\quad + \|\nabla_x w(\cdot,y)\cdot\nabla f_1\|_{L^2_x}\|f_2\|_{\mathcal{H}^2_x},\end{aligned}$$

where we have used the estimate $\|H_x f\|_{L^2_x} \leq \|f\|_{\mathcal{H}^2_x}$. For the last term, (3.3) yields

$$\begin{aligned}\|\nabla_x w(\cdot,y)\cdot\nabla f_1\|_{L^2_x} &\lesssim \left\|\left(\sqrt{V_1}+V_2(y)+1\right)\nabla f_1\right\|_{L^2_x}\\ &\lesssim \left\|\sqrt{V_1}\nabla f_1\right\|_{L^2_x} + (V_2(y)+1)\|\nabla f_1\|_{L^2_x}\\ &\lesssim \left\|\sqrt{V_1}\nabla f_1\right\|_{L^2_x} + (V_2(y)+1)\|f\|^{1/2}_{L^2_x}\|\Delta f\|^{1/2}_{L^2_x}\\ &\lesssim \left\|\sqrt{V_1}\nabla f_1\right\|_{L^2_x} + (V_2(y)+1)\|f_1\|_{\mathcal{H}^2_x}.\end{aligned}$$

For the first term on the last right hand side, we use an integration by parts:

$$\begin{aligned}\left\|\sqrt{V_1}\nabla f_1\right\|^2_{L^2_x} &= \int_{\mathbb{R}^{d_1}} V_1(x)\nabla f_1(x)\cdot\nabla f_1(x)dx\\ &= -\int_{\mathbb{R}^{d_1}} V_1(x)f_1(x)\Delta f_1(x)dx - \int_{\mathbb{R}^{d_1}} f_1(x)\nabla V_1(x)\cdot\nabla f_1(x)dx.\end{aligned}$$

By Cauchy-Schwarz inequality, the first term on the right hand side is estimated by

$$\|V_1 f_1\|_{L^2_x}\|\Delta f_1\|_{L^2_x} \leq 2\|H_x f_1\|^2_{L^2_x}.$$

Invoking (3.2), and using Cauchy-Schwarz inequality again,

$$\begin{aligned}\left|\int_{\mathbb{R}^{d_1}} f(x)\nabla V_1(x)\cdot\nabla f(x)dx\right| &\lesssim \int_{\mathbb{R}^{d_1}}(1+V_1(x))|f(x)||\nabla f(x)|dx \lesssim \|(1+V_1)f\|_{L^2_x}\|\nabla f\|_{L^2_x}\\ &\lesssim \left(\|f\|_{L^2_x}+\|H_x f\|_{L^2_x}\right)\|f\|^{1/2}_{L^2_x}\|\Delta f\|^{1/2}_{L^2_x}\\ &\lesssim \|H_x f\|^{1/2}_{L^2_x}\|f\|^{3/2}_{L^2_x} + \|H_x f\|^{3/2}_{L^2_x}\|f\|^{1/2}_{L^2_x} \lesssim \|f\|^2_{L^2_x} + \|H_x f\|^2_{L^2_x},\end{aligned}$$

where we have used Young inequality for the last estimate.

$$|\langle [w(x,y),H_x]H_x f_1, f_2\rangle| = |\langle H_x f_1, [w(x,y),H_x]f_2\rangle| \leq \|H_x f_1\|_{L^2_x}\|\Delta_x w(\cdot,y)f_2\|_{L^2_x}.$$

To estimate $\langle [w(\cdot,y),H_x]H_x f_1, f_2\rangle_{L^2_x}$, we use the self-adjointness of H_x and write

$$\langle [w(\cdot,y),H_x]H_x f_1, f_2\rangle_{L^2_x} = \langle H_x f_1, [w(\cdot,y),H_x]f_2\rangle_{L^2_x}.$$

We use the above estimate, where the roles of f_1 and f_2 have been swapped, to conclude that the first inequality in $\mathbf{(H3)}_{2,2}$ holds. The proof of the second one is similar.

Appendix A. Tangent space

For completeness, we give the elementary considerations for determining the tangent spaces of the Hartree manifold, Lemma 2.1.

Proof. We consider a curve $\Gamma(s) = \varphi^x(s)\otimes\varphi^y(s) \in \mathcal{M}$ with $\Gamma(0) = u$. Then,

$$\dot{\Gamma}(0) = \dot{\varphi}^x(0)\otimes\varphi^y + \varphi^x\otimes\dot{\varphi}^y(0),$$

which verifies the claimed representation of any tangent function as

$$v = v^x\otimes\varphi^y + \varphi^x\otimes v^y.$$

Let us consider $a = (a^x, a^y) \in \mathbb{C}^2$ with $a^x + a^y = 0$. We set $w^x = v^x + a^x\varphi^x$ and $w^y = v^y + a^y\varphi^y$. Then, $w = w^x \otimes \varphi^y + \varphi^x \otimes w^y$ satisfies

$$w = v^x \otimes \varphi^y + \varphi^x \otimes v^y + (a^x + a^y)\varphi^x \otimes \varphi^y = v.$$

Choosing $a^x = -\langle \varphi^x, v^x\rangle / \langle \varphi^x, \varphi^x\rangle$ and $a^y = -a^x$, we obtain a representation of v satisfying the claimed gauge condition. We verify that this condition implies uniqueness. We assume that $v = v^x \otimes \varphi^y + \varphi^x \otimes v^y = \tilde{v}^x \otimes \varphi^y + \varphi^x \otimes \tilde{v}^y$ with $\langle \varphi^x, v^x\rangle = \langle \varphi^x, \tilde{v}^x\rangle = 0$. Then, for any $\vartheta^y \in L^2_y$,

$$\langle \varphi^x \otimes \vartheta^y, v\rangle = \langle \varphi^x, \varphi^x\rangle\langle \vartheta^y, v^y\rangle = \langle \varphi^x, \varphi^x\rangle\langle \vartheta^y, \tilde{v}^y\rangle,$$

which implies $v^y = \tilde{v}^y$. Then, for any $\vartheta^x \in L^2_y$,

$$\begin{aligned}\langle \vartheta^x \otimes \varphi^y, v\rangle_{L^2_{x,y}} &= \langle \vartheta^x, v^x\rangle_{L^2_x}\langle \varphi^y, \varphi^y\rangle_{L^2_y} + \langle \vartheta^x, \varphi^x\rangle_{L^2_x}\langle \varphi^y, v^y\rangle_{L^2_y}\\ &= \langle \vartheta^x, \tilde{v}^x\rangle_{L^2_x}\langle \varphi^y, \varphi^y\rangle_{L^2_y} + \langle \vartheta^x, \varphi^x\rangle_{L^2_x}\langle \varphi^y, \tilde{v}^y\rangle_{L^2_y},\end{aligned}$$

which implies $v^x = \tilde{v}^x$. Choosing $v^x = 0$ and $v^y = \varphi^y$, we have $v = u$ so that $u \in \mathcal{T}_u\mathcal{M}$. □

Appendix B. Coulombic type coupling

We recall standard definition and results.

Definition B.1 (Admissible pairs in $\mathbb{R}^3$)**.** *A pair (q, r) is admissible if $q, r \geq 2$, and*

$$\frac{2}{q} = 3\left(\frac{1}{2} - \frac{1}{r}\right).$$

As the range allowed for (q, r) is compact, we set, for $I \subset \mathbb{R}$ a time interval,

$$\|u\|_{S(I)} = \sup_{(q,r) \text{ admissible}} \|u\|_{L^q(I;L^r(\mathbb{R}^3))}.$$

In view of [11] and [13], we have:

Proposition B.2. *Let $d = 3$ and $\mathbf{V} \in \mathcal{Q}$. Denote $\mathbf{H} = -\frac{1}{2}\Delta + \mathbf{V}$.*
(1) *There exists C_{hom} such that for all interval I such that $|I| \leq 1$,*

$$\|e^{-it\mathbf{H}}\varphi\|_{S(I)} \leq C_{\text{hom}}\|\varphi\|_{L^2}, \quad \forall \varphi \in L^2(\mathbb{R}^3).$$

(2) *Denote*

$$D(F)(t, x) = \int_0^t e^{-i(t-\tau)\mathbf{H}} F(\tau, x)\mathrm{d}\tau.$$

There exists C_{inhom} such that for all interval $I \ni 0$ such that $|I| \leq 1$,

$$\|D(F)\|_{S(I)} \leq C_{\text{inhom}} \|F\|_{S(I)^*}.$$

The existence of (local in time) Strichartz estimates of Proposition B.2 is the main ingredient of the proof of Theorem 3.1. Actually, as soon as such estimates are available for the operators $\mathbf{H}_x$ and $\mathbf{H}_y$, then Theorem 3.1 remains valid. As mentioned in the introduction, such cases can be found in e.g. [20] or [5]. On the other hand, we emphasize that for superquadratic potentials, like V_1 in Example 3.5, Strichartz estimates suffer a loss of regularity; see [16, 21].

Remark B.3. The case of a harmonic potential, $\mathbf{V}(x) = |x|^2$, shows that $\mathbf{H}$ may have eigenvalues, and explains why the above time intervals I are required to have finite length.

Remark B.4. The potential $\mathbf{V}$ may also be time dependent, in view the original framework of [11]: $\mathbf{V} \in L^\infty_{\mathrm{loc}}(\mathbb{R}_t \times \mathbb{R}^3_x)$ is real-valued, and smooth with respect to the space variable: for (almost) all $t \in \mathbb{R}$, $x \mapsto \mathbf{V}(t,x)$ is a C^∞ map. Moreover, it is at most quadratic in space:

$$\forall T > 0, \quad \forall \alpha \in \mathbb{N}^d,\ |\alpha| \geq 2, \quad \partial_x^\alpha \mathbf{V} \in L^\infty([-T,T] \times \mathbb{R}^3_x).$$

Under these assumptions, suitable modifications of Proposition B.2 are needed, but they do not alter the conclusion of Theorem 3.1 (see [8]). See also [20] for another class of time dependent potentials.

Proof of Theorem 3.1. We give the main technical steps of the proof, and refer to [10] for details. By Duhamel's formula, we write (1.2) as

$$\begin{aligned}
\phi^x(t) &= e^{-it\mathbf{H}_x}\phi_0^x - i\int_0^t e^{-i(t-\tau)\mathbf{H}_x}\left(v_1\phi^x + \left(W * |\phi^y|^2\right)\phi^x\right)(\tau)d\tau =: F_1(\phi^x,\phi^y),\\
\phi^y(t) &= e^{-it\mathbf{H}_y}\phi_0^y - i\int_0^t e^{-i(t-\tau)\mathbf{H}_y}\left(v_2\phi^y + \left(W * |\phi^x|^2\right)\phi^y\right)(\tau)d\tau =: F_2(\phi^x,\phi^y).
\end{aligned}$$

Theorem 3.1 follows from a standard fixed point argument based on Strichartz estimates. For $0 < T \leq 1$, we introduce

$$\begin{aligned}
Y(T) = \{(\phi^x,\phi^y) \in C([0,T];L^2(\mathbb{R}^3))^2 :\quad & \|\phi^x\|_{S([0,T])} \leq 2C_{\mathrm{hom}}\|\phi_0^x\|_{L^2},\\
& \|\phi^y\|_{S([0,T])} \leq 2C_{\mathrm{hom}}\|\phi_0^y\|_{L^2}\},
\end{aligned}$$

and the distance

$$d(\phi_1,\phi_2) = \|\phi_1 - \phi_2\|_{S([0,T]},$$

where C_{hom} stems from Proposition B.2. Then $(Y(T),d)$ is a complete metric space.

By using Strichartz estimates and Hölder inequality, we have:

$$\|F_1(\phi^x,\phi^y)\|_{S([0,T])} \leq C_{\mathrm{hom}}\|\phi_0^x\|_{L^2} + C_{\mathrm{inhom}}\left(\|v_1\phi^x\|_{S([0,T])^*} + \left\|\left(W * |\phi^y|^2\right)\phi^x\right\|_{S([0,T])^*}\right),$$

for any $(\phi^x,\phi^y) \in Y(T)$. By assumption (see Theorem 3.1), we may write

$$v_1 = v_1^p + v_1^\infty, \quad v_2 = v_2^p + v_2^\infty, \quad W = W^p + W^\infty, \quad v_1^q, v_2^q, W^q \in L^q(\mathbb{R}^3),$$

and the value p can obviously be the same for the three potentials, by taking the minimum between the three p's if needed. Regarding $\|v_1\phi^x\|_{S([0,T])^*}$, we write

$$\begin{aligned}
\|v_1^\infty\phi^x\|_{S([0,T])^*} &\leq \|v_1^\infty\phi^x\|_{L^1([0,T];L^2)} \leq \|v_1^\infty\|_{L^\infty}\|\phi^x\|_{L^1([0,T];L^2)}\\
&\leq T\|v_1^\infty\|_{L^\infty}\|\phi^x\|_{L^\infty\leq([0,T];L^2)} \leq T\|v_1^\infty\|_{L^\infty}\|\phi^x\|_{S([0,T])}.
\end{aligned}$$

Let r be such that

$$\frac{1}{r'} = \frac{1}{r} + \frac{1}{p} \Longleftrightarrow 1 = \frac{2}{r} + \frac{1}{p}.$$

Note that this exponent is the one introduced in the statement of Theorem 3.1. The assumption $p > 3/2$ implies $2 \le r < 6$. Let q be such that (q, r) is admissible: $r < 6$ implies $q > 2$. Hölder inequality yields

$$\begin{aligned}\|v_1^p \phi^x\|_{S([0,T])^*} &\le \|v_1^p \phi^x\|_{L^{q'}([0,T];L^{r'})} \le \|v_1^p\|_{L^p} \|\phi^x\|_{L^{q'}([0,T];L^r)} \\ &\le T^{1/\theta} \|v_1^p\|_{L^p} \|\phi^x\|_{L^q([0,T];L^r)} \le T^{1/\theta} \|v_1^p\|_{L^p} \|\phi^x\|_{S([0,T])},\end{aligned}$$

where θ is such that

$$\frac{1}{q'} = \frac{1}{q} + \frac{1}{\theta}.$$

Note that θ is finite, as $q > 2$

For the convolution term, first write

$$\begin{aligned}\left\|\left(W^\infty * |\phi^y|^2\right)\phi^x\right\|_{S([0,T])^*} &\le \left\|\left(W^\infty * |\phi^y|^2\right)\phi^x\right\|_{L^1([0,T];L^2)} \\ &\le \left\|W^\infty * |\phi^y|^2\right\|_{L^1([0,T];L^\infty)} \|\phi^x\|_{L^\infty([0,T];L^2)} \\ &\le T\|W^\infty\|_{L^\infty} \|\phi^y\|^2_{L^\infty([0,T];L^2)} \|\phi^x\|_{L^\infty([0,T];L^2)} \\ &\le T\|W^\infty\|_{L^\infty} \|\phi^y\|^2_{S([0,T])} \|\phi^x\|_{S([0,T])}.\end{aligned}$$

Introduce r_1 such that

$$\frac{1}{r_1'} = \frac{1}{r_1} + \frac{1}{2p} \Longleftrightarrow 2 = \frac{4}{r_1} + \frac{1}{p} \Longleftrightarrow 1 + \frac{1}{2p} = \frac{1}{p} + \frac{2}{r_1}. \tag{B.1}$$

The assumption $p > 3/2$ implies $2 \le r_1 < 3$. Let q_1 be such that (q_1, r_1) is admissible: $q_1 > 4$. Hölder inequality yields

$$\begin{aligned}\left\|\left(W^p * |\phi^y|^2\right)\phi^x\right\|_{S([0,T])^*} &\le \left\|\left(W^p * |\phi^y|^2\right)\phi^x\right\|_{L^{q_1'}([0,T];L^{r_1'})} \\ &\le \left\|W^p * |\phi^y|^2\right\|_{L^k([0,T];L^{2p})} \|\phi^x\|_{L^{q_1}([0,T];L^{r_1})} \\ &\le \left\|W^p * |\phi^y|^2\right\|_{L^k([0,T];L^{2p})} \|\phi^x\|_{S([0,T])},\end{aligned}$$

where k is such that

$$\frac{1}{q_1'} = \frac{1}{q_1} + \frac{1}{k} \Longleftrightarrow 1 = \frac{2}{q_1} + \frac{1}{k}.$$

Note that since $q_1 > 4$, we have $q_1 > 2k$. In view of (B.1), Young inequality yields

$$\begin{aligned}\left\|W^p * |\phi^y|^2\right\|_{L^k([0,T];L^{2p})} &\le \|W^p\|_{L^p} \left\||\phi^y|^2\right\|_{L^k([0,T];L^{r_1/2})} = \|W^p\|_{L^p} \|\phi^y\|^2_{L^{2k}([0,T];L^{r_1})} \\ &\le T^\eta \|W^p\|_{L^p} \|\phi^y\|^2_{L^{q_1}([0,T];L^{r_1})} \le T^\eta \|W^p\|_{L^p} \|\phi^y\|^2_{S([0,T])},\end{aligned}$$

where $\eta > 0$ is given by $\eta = 1/(2k) - 1/q_1$.

The same inequalities obviously holds by switching x and y, and so for $T > 0$ sufficiently small, $\Phi := (\phi^x, \phi^y) \mapsto (F_1(\phi^x, \phi^y), F_2(\phi^x, \phi^y)) =: \mathbf{F}(\Phi)$ leaves $Y(T)$ invariant.

Using similar estimates, again relying on Strichartz and Hölder inequalities involving the same Lebesgue exponents ($\mathbf{F}$ is the sum of a linear and a trilinear term in Φ), we infer that up to decreasing $T > 0$, $\mathbf{F}$ is a contraction on $Y(T)$, and so there exists a unique $\Phi \in Y(T)$

solving (1.2). The global existence of the solution for (1.2) follows from the conservation of the L^2-norms of ϕ^x and ϕ^y, respectively.

Uniqueness of such solutions follows once again from Strichartz and Hölder inequalities involving the same Lebesgue exponents as above, like for the contraction part of the argument. The main remark consists in noticing that the above Lebesgue indices satisfy $r > r_1$, hence $q < q_1$, and so $L^{q_1}_{\text{loc}} L^{r_1} \subset L^q_{\text{loc}} L^r \cap L^\infty L^2$. □

Remark B.5 (H^1-regularity). If in Theorem 3.1, we assume in addition that

$$\nabla v_1, \nabla v_2 \in L^p(\mathbb{R}^3) + L^\infty(\mathbb{R}^3) \quad \text{form some } p > 3/2,$$

then for $\phi_0^x, \phi_0^y \in H^1(\mathbb{R}^3)$ and $x\phi_0^x, y\phi_0^y \in L^2(\mathbb{R}^3)$ (this last assumption may be removed when $\nabla V_1, \nabla V_2 \in L^\infty(\mathbb{R}^3)$ – the minimal assumption to work at the H^1-level with $V_1, V_2 \in \mathcal{Q}$ is $\phi_0^x \nabla V_1, \phi_0^y \nabla V_2 \in L^2(\mathbb{R}^3)$, see [9]), the global solution constructed in Theorem 3.1 satisfies

$$(\phi^x, \phi^y) \in C(\mathbb{R}; H^1(\mathbb{R}^3))^2 \cap L^q_{\text{loc}}(\mathbb{R}; W^{1,r}(\mathbb{R}^3))^2, \quad (x\phi^x, y\phi^y) \in C(\mathbb{R}; L^2(\mathbb{R}^3)^3)^2.$$

To see this, it suffices to resume the above proof, and check that $\nabla_x F_1(\phi^x, \phi^y)$ and $\nabla_y F_2(\phi^x, \phi^y)$ satisfy essentially the same estimates as $F_1(\phi^x, \phi^y), F_2(\phi^x, \phi^y)$ in $S([0,T])$. One first has to commute the gradient with $e^{-it\mathbf{H}_x}$ or $e^{-it\mathbf{H}_y}$. Typically,

$$\begin{aligned}\nabla_x F_1(\phi^x, \phi^y) = e^{-it\mathbf{H}_x} \nabla_x \phi_0^x - i \int_0^t e^{-i(t-\tau)\mathbf{H}_x} \nabla_x \left(v_1 \phi^x + \left(W * |\phi^y|^2 \right) \phi^x \right)(\tau) d\tau \\ - i \int_0^t e^{-i(t-\tau)\mathbf{H}_x} F_1(\phi^x, \phi^y)(\tau) \nabla_x V_1 d\tau,\end{aligned}$$

where the last factor accounts for the possible lack of commutation between $\mathbf{H}_x$ and ∇_x, $[-i\partial_t - \mathbf{H}_x, \nabla_x] = \nabla_x V_1$. Since V_1 is at most quadratic, ∇V_1 is at most linear, and we obtain a closed system of estimates by considering

$$\begin{aligned}xF_1(\phi^x, \phi^y) = e^{-it\mathbf{H}_x}(x\phi_0^x) - i \int_0^t e^{-i(t-\tau)\mathbf{H}_x} \left(x \left(v_1 \phi^x + \left(W * |\phi^y|^2 \right) \phi^x \right) \right)(\tau) d\tau \\ + i \int_0^t e^{-i(t-\tau)\mathbf{H}_x} \nabla_x F_1(\phi^x, \phi^y)(\tau) d\tau,\end{aligned}$$

where we have used $[-i\partial_t - \mathbf{H}_x, x] = -\nabla_x$. We omit the details, and refer to [10] (see also [8]). As pointed in Remark 3.3, the energy

$$\begin{aligned}E(t) = (H_x \phi^x(t), \phi^x(t))_{L^2_x} + (H_y \phi^y(t), \phi^y(t))_{L^2_y} \\ + \iint_{\mathbb{R}^3 \times \mathbb{R}^3} W(x-y) |\phi^x(t,x)|^2 |\phi^y(t,y)|^2 dx dy,\end{aligned}$$

which is well defined with the above regularity, is independent of time. Formally, this can be seen by multiplying the first equation in (1.2) by $\partial_t \phi^x$, the second by $\partial_t \phi^y$, integrating in space, considering the real part, and summing the two identities. To make the argument rigorous (we may not have enough regularity to be allowed to proceed as described), one

may use a regularization procedure as in [10], or rely on a clever use of the regularity provided by Strichartz estimates, as in [17].

References

[1] S. Alinhac and P. Gérard. *Pseudo-differential operators and the Nash-Moser theorem*, volume 82 of *Graduate Studies in Mathematics*. American Mathematical Society, Providence, RI, 2007. Translated from the 1991 French original by Stephen S. Wilson.

[2] L. Baudouin. Existence and regularity of the solution of a time dependent Hartree-Fock equation coupled with a classical nuclear dynamics. *Rev. Mat. Complut.*, 18(2):285–314, 2005.

[3] I. Burghardt, R. Carles, C. Fermanian Kammerer, B. Lasorne, and C. Lasser. Separation of scales: Dynamical approximations for composite quantum systems. *J. Phys. A*, 54(41):414002, 2021.

[4] I. Burghardt, R. Carles, C. Fermanian Kammerer, B. Lasorne, and C. Lasser. Dynamical approximations for composite quantum systems: assessment of error estimates for a separable ansatz. *J. Phys. A*, 55(22):224010, 2022.

[5] N. Burq, F. Planchon, J. G. Stalker, and A. S. Tahvildar-Zadeh. Strichartz estimates for the wave and Schrödinger equations with potentials of critical decay. *Indiana Univ. Math. J.*, 53(6):1665–1680, 2004.

[6] F. Cacciafesta, A.-S. de Suzzoni, and D. Noja. A Dirac field interacting with point nuclear dynamics. *Math. Ann.*, 376(3-4):1261–1301, 2020.

[7] E. Cancès and C. Le Bris. On the time-dependent Hartree-Fock equations coupled with a classical nuclear dynamics. *Math. Models Methods Appl. Sci.*, 9(7):963–990, 1999.

[8] R. Carles. Nonlinear Schrödinger equation with time dependent potential. *Commun. Math. Sci.*, 9(4):937–964, 2011.

[9] R. Carles. Sharp weights in the Cauchy problem for nonlinear Schrödinger equations with potential. *Z. Angew. Math. Phys.*, 66(4):2087–2094, 2015.

[10] T. Cazenave. *Semilinear Schrödinger equations*, volume 10 of *Courant Lecture Notes in Mathematics*. New York University Courant Institute of Mathematical Sciences, New York, 2003.

[11] D. Fujiwara. Remarks on the convergence of the Feynman path integrals. *Duke Math. J.*, 47(3):559–600, 1980.

[12] S. Jin, C. Sparber, and Z. Zhou. On the classical limit of a time-dependent self-consistent field system: analysis and computation. *Kinet. Relat. Models*, 10(1):263–298, 2017.

[13] M. Keel and T. Tao. Endpoint Strichartz estimates. *Amer. J. Math.*, 120(5):955–980, 1998.

[14] C. Lasser and C. Su. Various variational approximations of quantum dynamics. *Journal of Mathematical Physics*, 63(7):072107, 2022.

[15] C. Lubich. *From quantum to classical molecular dynamics: reduced models and numerical analysis*. European Mathematical Society (EMS), Zürich, 2008.

[16] H. Mizutani. Strichartz estimates for Schrödinger equations with variable coefficients and unbounded potentials II. Superquadratic potentials. *Commun. Pure Appl. Anal.*, 13(6):2177–2210, 2014.

[17] T. Ozawa. Remarks on proofs of conservation laws for nonlinear Schrödinger equations. *Calc. Var. Partial Differ. Equ.*, 25(3):403–408, 2006.

[18] M. Reed and B. Simon. *Methods of modern mathematical physics. II. Fourier analysis, self-adjointness*. Academic Press [Harcourt Brace Jovanovich Publishers], New York, 1975.

[19] M. Reed and B. Simon. *Methods of modern mathematical physics. I Functional analysis*. Academic Press, Inc. [Harcourt Brace Jovanovich, Publishers], New York, second edition, 1980.

[20] I. Rodnianski and W. Schlag. Time decay for solutions of Schrödinger equations with rough and time-dependent potentials. *Invent. Math.*, 155(3):451–513, 2004.

[21] K. Yajima and G. Zhang. Local smoothing property and Strichartz inequality for Schrödinger equations with potentials superquadratic at infinity. *J. Differential Equations*, 202(1):81–110, 2004.

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