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A SPACE-TIME VARIATIONAL FORMULATION FOR THE MANY-BODY ELECTRONIC SCHRÖDINGER EVOLUTION EQUATION

MI-SONG DUPUY*, VIRGINIE EHRLACHER†, AND CLÉMENT GUILLOT‡

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Abstract. We prove in this paper that the solution to the time-dependent Schrödinger equation can be expressed as the solution of a global space-time quadratic minimization problem that is amenable to Galerkin time-space discretization schemes, using an appropriate least-square formulation. The present analysis can be applied to the electronic many-body time-dependent Schrödinger equation with an arbitrary number of electrons and interaction potentials with Coulomb singularities. We motivate the interest of the present approach with two goals: first, the design of Galerkin space-time discretization methods; second, the definition of dynamical low-rank approximations following a variational principle different from the classical Dirac-Frenkel principle, and for which it is possible to prove the global-in-time existence of solutions.

Key words. Schrödinger equation, Space-time variational formulation

MSC codes. 35A15, 35Q41, 35L15, 65M15

1. Introduction. The aim of this paper is to introduce a new global space-time variational formulation of the linear evolution Schrödinger equation

$$(1.1) \quad \begin{cases} (i\partial_t - H - B(t))u^*(t) = f(t), & t \in I, \\ u^*(0) = u_0, \end{cases}$$

where H is a self-adjoint operator on a separable Hilbert space \mathcal{H} with domain $D(H)$, $I = (0, T)$ for some $T > 0$ and $B : \bar{I} \ni t \mapsto B(t)$ is a strongly continuous family of bounded self-adjoint operators on \mathcal{H} , and $f \in L^2(I, \mathcal{H})$. Throughout the paper, the equation will often be studied first without the time dependent part of the operator (i.e. with $B(t) = 0$) before extending the result to the case of nonzero B ’s, in which case we will refer to

$$(1.2) \quad \begin{cases} (i\partial_t - H)u^{*,0}(t) = f(t), & t \in I \\ u^{*,0}(0) = u_0. \end{cases}$$

which is only a particular case of (1.1).

The general setting above includes the case of the time-dependent Schrödinger equation defined on the whole space (in arbitrary large dimension) and with interaction potential with Coulomb singularities. This includes in particular the case of the time-dependent Schrödinger evolution equation associated to the many-body electronic Hamiltonian for molecules. The latter concerns the following case: consider a system of $N \in \mathbb{N}^*$ electrons in a molecule with $M \in \mathbb{N}^*$ nuclei in the Born-Oppenheimer approximation [4, 7]. Let us assume that the positions and electric charges of the nuclei are given respectively as $R_1, \dots, R_M \in \mathbb{R}^3$ and $Z_1, \dots, Z_M > 0$. Then, $\mathcal{H} = L^2(\mathbb{R}^{3N})$ (or, for fermions, $\mathcal{H} = \bigwedge_{i=1}^N L^2(\mathbb{R}^3)$ the set of antisymmetric functions of $L^2(\mathbb{R}^{3N})$) and

$$(1.3) \quad H = -\Delta - \sum_{k=1}^M \sum_{i=1}^N \frac{Z_k}{|x_i - R_k|} + \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|},$$

the quantity $|\cdot|$ denoting the euclidean norm in \mathbb{R}^3 .

The outline of this paper is as follows. In Section 2, we introduce the space of solutions (as defined in Definition 2.1) to (1.2):

$$(1.4) \quad \mathcal{X}_H = \{u^{*,0} \in L^2(I, \mathcal{H}) : \exists (u_0, f) \in \mathcal{H} \times L^2(I, \mathcal{H}) \text{ such that } u^{*,0} \text{ solves (1.2)}\}.$$

We prove that a solution to (1.1) belongs to \mathcal{X}_H , and that u^* solution to (1.1) can also be characterized as follows:

$$(1.5) \quad \text{Find } u^* \in \mathcal{X}_H \text{ such that } u^* = \underset{u \in \mathcal{X}_H}{\operatorname{argmin}} E(u),$$

*Laboratoire Jacques-Louis Lions, Paris, France (mi-song.dupuy@sorbonne-universite.fr, <https://msdupuy.github.io/>).

†École Nationale des Ponts et Chaussées, Champs-sur-Marne, France (virginie.ehrlacher@enpc.fr, <https://team.inria.fr/materials/team-members/virginie-ehrlacher-galland/>).

‡École Nationale des Ponts et Chaussées, Champs-sur-Marne, France (clement.guilLOT@enpc.fr, <https://team.inria.fr/materials/team-members/clement-guilLOT/>).

where

$$(1.6) \quad \forall u \in \mathcal{X}_H, \quad E(u) = |u(0) - u_0|^2 + T \|(i\partial_t - H - B(t))u - f\|_{L^2(I, \mathcal{H})}^2.$$

In Section 3, we state our main results: first, in Theorem 3.7, we will prove that when $H = H_0 + A$ with H_0 a “well known” operator and A a “perturbation”, we actually have the equality $\mathcal{X}_H = \mathcal{X}_{H_0}$.

We then state in Corollary 3.8 that this result, combined with (2.9), leads to another space-time formulation of (1.1):

$$(1.7) \quad \text{Find } v^* \in H^1(I, \mathcal{H}) \text{ such that } v^* = \underset{v \in H^1(I, \mathcal{H})}{\operatorname{argmin}} F(v),$$

where

$$(1.8) \quad \forall v \in H^1(I, \mathcal{H}), \quad F(v) = |v(0) - u_0|^2 + T \|(i\partial_t - e^{itH_0}(A + B(t))e^{-itH_0})v - e^{itH_0}f\|_{L^2(I, \mathcal{H})}^2.$$

Since the functionals E and F are quadratic, both (1.5) and (1.7) can be associated to a Lax-Milgram variational problem of the form

$$\forall u \in \mathcal{X}_H, \quad a(u^*, u) = l(u), \quad (\text{resp. } \forall v \in H^1(I, \mathcal{H}), \quad b(v^*, v) = m(v))$$

where $a : \mathcal{X}_H \times \mathcal{X}_H \rightarrow \mathbb{C}$ (resp. $b : H^1(I, \mathcal{H}) \times H^1(I, \mathcal{H}) \rightarrow \mathbb{C}$) is a continuous hermitian coercive sesquilinear form on $\mathcal{X}_H \times \mathcal{X}_H$ (resp. $H^1(I, \mathcal{H}) \times H^1(I, \mathcal{H})$) and $l : \mathcal{X}_H \rightarrow \mathbb{C}$ (resp. $m : H^1(I, \mathcal{H}) \rightarrow \mathbb{C}$) is a continuous linear form. More precisely, we introduce an appropriate least-square formulation [12] of the latter equation, satisfying the following wish list (under suitable assumptions on the Hamiltonian H):

- (i) the coercivity and continuity constants of the bilinear form a should not decrease (respectively increase) faster than some inverse of polynomial (respectively polynomial) with the value of the final time T ;
- (ii) it should yield practical Galerkin space-time numerical schemes;
- (iii) it should be useful to define new dynamical low-rank approximations using a different variational principle than the classical Dirac-Frenkel principle [1, 3, 13, 27, 28, 30]. The advantage of the proposed formulation is that it is possible then to prove the global-in-time existence of some dynamical low-rank approximations, without any restrictions on the data of the problem.

We would like to stress the fact that our present analysis covers the case of unbounded domains and interaction potentials with Coulomb singularities (see Subsection 3.4), which includes the case of the many-body electronic Schrödinger Hamiltonian introduced above. While our main motivation for the present work stems from the design of new global-in-time dynamical low-rank approximations, which is the object of another article [11], we present here some preliminary numerical results about global space-time Galerkin discretization schemes for the time-dependent Schrödinger equation associated to the variational formulation presented here.

Section 4 opens some perspectives about the usefulness of the proposed formulation for the definition of new dynamical low-rank approximations of the solution to the time-dependent Schrödinger equation, which can be proved to be well-posed globally in time without any restrictions on the data of the problem. As mentioned above, this line of research will be the object of a follow-up article [11].

Lastly, in Appendix A, we propose Galerkin space-time discretization methods associated with the formulations proposed in Section 3 and illustrate their numerical behavior.

Similar least-square formulations exist for parabolic problems [9], the wave equation [14, 20], and the Navier-Stokes equation [26]. Let us thus comment here about the state-of-the-art of global space-time discretization methods for the time-dependent Schrödinger equation. In [10], a spacetime discontinuous Petrov-Galerkin (DPG) method for the linear time-dependent Schrödinger equation is proposed. Two variational formulations are proved to be well posed: a strong formulation (with no relaxation of the original equation) and a weak formulation (also called the *ultra-weak formulation*, which transfers all derivatives onto test functions). However, the analysis is restricted to the case of an equation posed on a bounded domain and without an interaction potential. In [15] and [16], space-time discontinuous Galerkin methods for the linear Schrödinger equation are proposed, where the equations are posed on a bounded domain, and with potentials that are bounded. In these works, the focus is on setting the appropriate discontinuous Galerkin method for the Schrödinger evolution. In [18], the authors propose an ultra-weak global space-time formulation for the time-dependent Schrödinger operator with instationary Hamiltonian. An associated discretization scheme is proposed method as a Petrov-Galerkin global space-time discretization method. The scope of the latter work is however restricted to the case of bounded domains and bounded interaction potentials. Let us also mention here the works [22, 23] where continuous and discontinuous methods for the nonlinear cubic Schrödinger equation are analyzed. We stress here the fact that our present analysis is restricted to the case of linear time-dependent Schrödinger equations. However, some ideas and tools used in this paper also appear in the nonlinear Schrödinger literature [5].

2. Preliminaries. The aim of this section is twofold: (i) we introduce some notation which will be used throughout the article, together with the appropriate notion of weak solution for the time-dependent Schrödinger equations we consider in this work; (ii) we introduce a preliminary global time-space variational formulation of the time-dependent Schrödinger problem in the case when the Hamiltonian does not depend on time. However, we will see that this first variational formulation is not convenient to use in practice for numerical purposes, which motivates the main results we establish in the next section.

2.1. Notations and Weak Solutions. Throughout this paper, we fix some final time $T > 0$, and the interval $I = (0, T)$. We also fix $(\mathcal{H}, \langle \cdot, \cdot \rangle)$ a separable Hilbert space with the associated norm $|\cdot| = \sqrt{\langle \cdot, \cdot \rangle}$. For a bounded operator \mathfrak{B} defined on \mathcal{H} , we define its operator norm as

$$(2.1) \quad \|\mathfrak{B}\| = \sup_{x \in \mathcal{H} \setminus \{0\}} \frac{|\mathfrak{B}x|}{|x|}.$$

Unless stated otherwise, H is a self-adjoint operator on \mathcal{H} with domain $D(H) \subset \mathcal{H}$, and $B : \bar{I} \ni t \mapsto B(t)$ is a strongly continuous family of bounded self-adjoint operators on \mathcal{H} .

We consider the Bochner space $L^2(I, \mathcal{H})$, which is a Hilbert space when equipped with the inner product

$$(2.2) \quad \forall u, v \in L^2(I, \mathcal{H}), \quad (u|v)_{L^2(I, \mathcal{H})} = \int_I dt \langle u(t), v(t) \rangle.$$

The norm associated with the inner product (2.2) is denoted by $\|\cdot\|_{L^2(I, \mathcal{H})}$. See for example [21] for an introduction to Bochner spaces. For any normed space E , we also denote by $\mathcal{C}^k(I, E)$ (resp. $\mathcal{C}_c^k(I, E)$) the space of k -th times continuously differentiable functions (resp. with compact support $K \subset I$) from I to E .

We use a standard notion of weak solutions to (1.1) defined as follows. Although the paper mostly focuses on time intervals of the form $(0, T)$, it will be useful for us to state the definition for more general time intervals:

DEFINITION 2.1. *Let $J \subset \mathbb{R}$ be a (possibly unbounded) open time interval such that $0 \in \bar{J}$. Let $u_0 \in \mathcal{H}$ and $f \in L^2(J, \mathcal{H})$.*

An element $u \in L^2_{loc}(J, \mathcal{H})$ is said to be a weak solution to (1.2) if the following two conditions are satisfied:

(C1) *For any $\varphi \in \mathcal{C}_c^0(J, D(H)) \cap \mathcal{C}_c^1(J, \mathcal{H})$,*

$$(2.3) \quad (u|(i\partial_t - H)\varphi)_{L^2(J, \mathcal{H})} = (f|\varphi)_{L^2(J, \mathcal{H})}.$$

(C2) *The equality $u(0) = u_0$ holds in \mathcal{H} .*

Remark 2.2. By Proposition B.2, (C1) implies that $u \in \mathcal{C}^0(\bar{J}, \mathcal{H})$, hence $u(0)$ is well defined as an element of \mathcal{H} , and (C2) can be understood as a pointwise equality.

Remark 2.3. A consequence of Definition 2.1 is that, for $J = I = (0, T)$ and $u \in L^2(I, \mathcal{H})$, we say that u is a weak solution to (1.1) if:

(C1) For any $\varphi \in \mathcal{C}_c^0(J, D(H)) \cap \mathcal{C}_c^1(J, \mathcal{H})$,

$$(2.4) \quad (u|(i\partial_t - H - B(t))\varphi)_{L^2(I, \mathcal{H})} = (f|\varphi)_{L^2(I, \mathcal{H})}.$$

(C2) The equality $u(0) = u_0$ holds in \mathcal{H} .

2.2. Duhamel formula and functional space. Let us equip the space \mathcal{X}_H defined in (1.4) with the inner product

$$(2.5) \quad \forall u, v \in \mathcal{X}_H, \quad (u|v)_{\mathcal{X}_H} = \langle u(0), v(0) \rangle + T ((i\partial_t - H)u|(i\partial_t - H)v)_{L^2(I, \mathcal{H})}.$$

The associated norm is then denoted by $\|u\|_{\mathcal{X}_H} = \sqrt{(u|u)_{\mathcal{X}_H}}$. The factor T in (2.5) is introduced for homogeneity, ensuring that the estimates for the $\mathcal{C}^0(I, \mathcal{H})$ norm have constants independent of T (see Proposition 2.4). It is an arbitrary choice, and removing it will result in an equivalent norm (with equivalence constants that depend on T), and will also influence the constants in Theorem 3.7 and Corollary 3.8.

The essential properties of the space \mathcal{X}_H are summarized in the following result, the proof of which only requires to carefully work with Definition 2.1 and can be found in Appendix B:

PROPOSITION 2.4. *The space \mathcal{X}_H equipped with the inner product $(\cdot|\cdot)_{\mathcal{X}_H}$ defined in (2.5) is a Hilbert space, and the application*

$$(2.6) \quad \begin{cases} L^2(I, \mathcal{H}) & \longrightarrow & L^2(I, \mathcal{H}) \\ u & \longmapsto & (I \ni t \mapsto e^{itH} u(t)) \end{cases}$$

defines an isomorphism between \mathcal{X}_H and $H^1(I, \mathcal{H})$. In particular, \mathcal{X}_H is continuously embedded into $\mathcal{C}^0(I, \mathcal{H})$, and we have the estimate

$$(2.7) \quad \forall u \in \mathcal{X}_H, \quad \|u\|_{\mathcal{C}^0(I, \mathcal{H})} \leq \sqrt{2} \|u\|_{\mathcal{X}_H}.$$

Furthermore, for any $f \in L^2(I, \mathcal{H})$, $u_0 \in \mathcal{H}$ and $B : \bar{I} \ni t \mapsto B(t)$ a strongly continuous family of bounded self-adjoint operators acting on \mathcal{H} , there exists a unique solution $u^* \in L^2(I, \mathcal{H})$ to (1.1) in the sense of Definition 2.1. Moreover, u^* belongs to \mathcal{X}_H and satisfies

$$(2.8) \quad \forall t \in I, \quad u^*(t) = e^{-itH} u_0 - i \int_0^t ds e^{-i(t-s)H} (f(s) - B(s)u^*(s)).$$

In other words, the first part of Proposition 2.4 states that the set \mathcal{X}_H can be equivalently characterized as follows:

$$(2.9) \quad \mathcal{X}_H = \{I \ni t \mapsto e^{-itH} v(t) : v \in H^1(I, \mathcal{H})\}.$$

Remark 2.5. It is easy to check that, whenever H is bounded, we simply have $\mathcal{X}_H = H^1(I, \mathcal{H})$, and the norms $\|\cdot\|_{\mathcal{X}_H}$ and $\|\cdot\|_{H^1(I, \mathcal{H})}$ are equivalent. However, this equality does not hold when H is an unbounded operator: let $\varphi \in \mathcal{H} \setminus D(H)$, and define $\psi : I \ni t \mapsto \varphi$. It is clear that $\psi \in H^1(I, \mathcal{H}) \setminus \mathcal{X}_H$. Conversely, the function $\eta : I \ni t \mapsto e^{-itH} \varphi$ belongs to $\mathcal{X}_H \setminus H^1(I, \mathcal{H})$.

Remark 2.6. We do not include the time dependent part $B(t)$ in the definition (1.4) because, as we will prove in Theorem 3.7, this would yield the same space with a different norm

$$(2.10) \quad \forall u \in \mathcal{X}_H, \quad N(u) = \left(|u(0)|^2 + T \|(i\partial_t - H - B(t))u\|_{L^2(I, \mathcal{H})}^2 \right)^{\frac{1}{2}},$$

which turns out to be equivalent to $\|\cdot\|_{\mathcal{X}_H}$.

Thanks to Proposition 2.4, one can reformulate the solution $u^{*,0}$ of the evolution equation (1.2) (in the sense of Definition 2.1) as follows: since

$$(2.11) \quad \forall u \in \mathcal{X}_H, \quad \|u - u^{*,0}\|_{\mathcal{X}_H}^2 = |u(0) - u_0|^2 + T \|(i\partial_t - H)u - f\|_{L^2(I, \mathcal{H})}^2,$$

the solution $u^{*,0}$ of (1.2) is equivalently the unique solution to the minimization problem

$$(2.12) \quad u^{*,0} = \operatorname{argmin}_{u \in \mathcal{X}_H} \left(|u(0) - u_0|^2 + T \|(i\partial_t - H)u - f\|_{L^2(I, \mathcal{H})}^2 \right).$$

Although this problem is well-posed and seemingly simple, this formulation is unsatisfactory, since the only explicit characterization given for \mathcal{X}_H at this point involves the evolution group e^{-itH} (as can be seen from equation (2.9)). In particular, finding an orthonormal basis (or a Riesz basis) of \mathcal{X}_H is not a trivial task. Theorem 3.7 will provide a more satisfying characterization of \mathcal{X}_H under some assumptions.

In our analysis, we will need the following property of the space \mathcal{X}_H . Let us define the space

$$(2.13) \quad \mathcal{W}_H^\infty = \bigcap_{k \in \mathbb{N}} \mathcal{C}^\infty(\bar{I}, D(H^k)).$$

The spaces $D(H^k)$ are defined recursively by $D(H^k) := \{\varphi \in D(H^{k-1}) : H^{k-1}\varphi \in D(H)\}$ and endowed with the graph norm of H^k . The following density result then holds.

PROPOSITION 2.7. *The space \mathcal{W}_H^∞ defined in (2.13) is a dense subspace of \mathcal{X}_H , and for any $u, v \in \mathcal{X}_H$ we have*

$$(2.14) \quad \int_I dt \langle (i\partial_t - H)u(t), v(t) \rangle = -i(\langle u(T), v(T) \rangle - \langle u(0), v(0) \rangle) + \int_I dt \langle u, (i\partial_t - H)v \rangle.$$

Proof. We first prove that $\mathcal{C}^\infty(\bar{I}, \mathcal{H})$ is a dense subset of \mathcal{X}_H . Subsequently, we demonstrate that \mathcal{W}_H^∞ is also a dense subset of \mathcal{X}_H .

Let $u^{*,0} \in \mathcal{X}_H$, $f = (i\partial_t - H)u^{*,0}$ and $u_0 = u^{*,0}(0) \in \mathcal{H}$. Define for any $t \in \mathbb{R}$

$$\tilde{u}(t) = e^{-itH} u_0 - i \int_0^t ds e^{-i(t-s)H} \mathbf{1}_I(s) f(s),$$

where $\mathbf{1}_I$ is the characteristic function of the interval I . As in Corollary B.3, it can be checked that $\tilde{u} \in L^2_{\text{loc}}(\mathbb{R}, \mathcal{H})$ is the unique solution to the evolution problem

$$\begin{cases} (i\partial_t - H)\tilde{u} = \mathbf{1}_I f, & t \in \mathbb{R} \\ \tilde{u}(0) = u_0, \end{cases}$$

in the sense of Definition 2.1. In particular, the uniqueness of weak solutions implies that $\tilde{u}|_I = u^{*,0}$. Now, for all $n \geq 0$, let $\rho_n : \mathbb{R} \rightarrow \mathbb{R}$ be such that $(\rho_n)_{n \geq 0}$ is a family of mollifiers (for the t variable) and

$$\forall t \in \mathbb{R}, \quad u_n(t) = \rho_n * \tilde{u}(t) = \int_{\mathbb{R}} ds \rho_n(s) \tilde{u}(t-s).$$

The usual properties of mollifiers imply

$$\begin{cases} u_n \in \mathcal{C}^\infty(\bar{I}, \mathcal{H}), \\ u_n \xrightarrow[n \rightarrow \infty]{} \tilde{u} \quad \text{in } L^2(I, \mathcal{H}), \\ f_n = (i\partial_t - H)u_n = \rho_n * (\mathbf{1}_I f) \xrightarrow[n \rightarrow \infty]{} f \quad \text{in } L^2(I, \mathcal{H}). \end{cases}$$

To check the last equality, take $\varphi \in \mathcal{C}_c^0(I, D(H)) \cap \mathcal{C}_c^1(I, \mathcal{H})$ and compute

$$\begin{aligned} (u_n | (i\partial_t - H)\varphi) &= \int_{\mathbb{R}} ds \rho_n(s) (\tilde{u}(\cdot - s) | (i\partial_t - H)\varphi) \\ &= \int_{\mathbb{R}} ds \rho_n(s) (f(\cdot - s) | \varphi) \\ &= (\rho_n * f | \varphi). \end{aligned}$$

We have thus proved that $\|u_n|_I - u\|_{\mathcal{X}_H} \rightarrow 0$. This proves that $\mathcal{C}^\infty(\bar{I}, \mathcal{H})$ is a dense subspace of \mathcal{X}_H .

Now let $u \in \mathcal{C}^\infty(\bar{I}, \mathcal{H})$. Let $n \geq 0$ and $\pi_{(-n, n)}(H)$ be the spectral projector on $(-n, n)$ associated with the self-adjoint operator H . We then define $v_n(t) = \pi_{(-n, n)}(H)u(t)$ for all $t \in I$. We easily check that for all $n \geq 0$,

$$\begin{cases} v_n \in \mathcal{W}_H^\infty, \\ v_n \xrightarrow[n \rightarrow \infty]{} u \quad \text{in } L^2(I, \mathcal{H}), \\ f_n = (i\partial_t - H)v_n = \pi_{(-n, n)}(H)f \xrightarrow[n \rightarrow \infty]{} f \quad \text{in } L^2(I, \mathcal{H}), \end{cases}$$

which implies that $\|v_n - u\|_{\mathcal{X}_H} \rightarrow 0$, and it follows that \mathcal{W}_H^∞ is a dense subspace of \mathcal{X}_H .

To prove (2.14), we simply integrate by part for any $u, v \in \mathcal{W}_H^\infty$ and conclude by density since both sides are continuous with respect to $\|\cdot\|_{\mathcal{X}_H}$. \square

3. Space-time variational formulation for the Schrödinger equation. In this section, after stating some preliminary results and definitions in Section 3.1, we state an abstract condition on operators H and H_0 which guarantees the equality $\mathcal{X}_H = \mathcal{X}_{H_0}$. Section 3.3 contains the proof of this characterization. In Section 3.4, we consider the case of the electronic many-body hamiltonian (1.3), and prove that the characterization of the previous sections holds for $H_0 = -\Delta$. In Section 3.5, we also focus on the electronic Schrödinger equation to obtain some additional time regularity for the solution under the assumption that the electronic potential is smooth. Lastly, in Section 3.6, we make some additional comments on an alternative formulation which relies on the use of the Duhamel formula and draw the link between the proposed formulation and previous works in the literature.

3.1. Preliminary results from Kato smoothing theory. Our analysis requires some tools from Kato smoothing theory. For the sake of completeness, we gather here all the definitions and results needed for the next sections. Most of them can be found in [29] or can be directly derived from it.

Throughout this section, H_0 is a self-adjoint operator on \mathcal{H} with domain $D(H_0)$, and A is a symmetric closed operator on \mathcal{H} .

LEMMA 3.1 (Plancherel identity). *Let $\varphi \in L^1(\mathbb{R}, \mathcal{H})$. Define for all $p \in \mathbb{R}$,*

$$(3.1) \quad \widehat{\varphi}(p) = (2\pi)^{-\frac{1}{2}} \int_{\mathbb{R}} dt e^{-ipt} \varphi(t).$$

Then

$$(3.2) \quad \int_{\mathbb{R}} dt |A\varphi(t)|^2 = \int_{\mathbb{R}} dp |A\widehat{\varphi}(p)|^2,$$

where the integrals are set equal to ∞ if we do not have that $\varphi(t)$ (resp. $\widehat{\varphi}(p)$) is in $D(A)$ for almost all $t \in \mathbb{R}$.

Proof. See [29], Chapter XIII, Section 3, Lemma 1, p. 142. □

PROPOSITION 3.2. *The two following properties are equivalent*

(i) *It holds that*

$$c_1 = \sup_{\varphi \in \mathcal{H}, |\varphi|=1} \frac{1}{2\pi} \int_{\mathbb{R}} dt |A e^{-itH_0} \varphi|^2 < \infty.$$

(ii) *It holds that $D(H_0) \subset D(A)$, and*

$$c_2 = \frac{1}{\pi} \sup_{\mu \in \mathbb{C} \setminus \mathbb{R}, \varphi \in \mathcal{H}, |\varphi|=1} |A(H_0 - \mu)^{-1} \varphi|^2 |\Im \mu| < \infty,$$

where $\Im \mu$ denotes the imaginary part of μ .

Moreover, when (i) and (ii) hold, then $c_1 = c_2$.

Proof. See [29], Chapter XIII, Section 3, Theorem XIII.25, p. 146. □

DEFINITION 3.3. *If A satisfies the properties (i) and (ii) from Proposition 3.2, we say that A is H_0 -smooth. Additionally, the common value of $\sqrt{c_1}$ and $\sqrt{c_2}$ is denoted by $\|A\|_{H_0}$.*

From the proof of Proposition 3.2, we also extract the following lemma.

LEMMA 3.4. *Let H_0 be a self-adjoint operator and A a closed operator. For any $\varepsilon > 0$ we have*

$$\sup_{\varphi \in \mathcal{H}, |\varphi|=1} \frac{1}{2} \int_{\mathbb{R}} dt e^{-2\varepsilon|t|} |A e^{-itH_0} \varphi|^2 \leq \sup_{\lambda \in \mathbb{R}, \varphi \in \mathcal{H}, |\varphi|=1} \varepsilon |A(H_0 - \lambda \pm i\varepsilon)^{-1} \varphi|^2.$$

Proof. The following proof is just an extract of the proof of Proposition 3.2. Since it is instructive, we recall it here for the sake of completeness.

We first notice that, for a bounded operator C on \mathcal{H} , we have

$$\forall \psi_1 \in D(A^*), \forall \psi_2 \in \mathcal{H}, \quad (C^* A^* \psi_1 | \psi_2) = (A^* \psi_1 | C \psi_2),$$

from which we conclude that, the following statements are equivalent :

- a) $\text{Ran } C \subset D(A)$ and $\|AC\| < \infty$
- b) It holds

$$\sup_{\varphi \in D(A^*), |\varphi|=1} |C^* A^* \varphi| < \infty.$$

Moreover, whenever a) and b) hold, we have the following equality:

$$\sup_{\varphi \in D(A^*), |\varphi|=1} |C^* A^* \varphi| = \|AC\|.$$

Therefore, taking $C = (H_0 - \lambda - i\varepsilon)^{-1}$, we obtain

$$\begin{aligned} c_\varepsilon &:= \sup_{\lambda \in \mathbb{R}, \varphi \in \mathcal{H}, |\varphi|=1} \varepsilon |A(H_0 - \lambda - i\varepsilon)^{-1} \varphi|^2 \\ &= \sup_{\substack{\lambda \in \mathbb{R} \\ \varphi \in D(A^*), |\varphi|=1}} \varepsilon |(H_0 - \lambda + i\varepsilon)^{-1} A^* \varphi|^2 \\ &= \sup_{\substack{\lambda \in \mathbb{R} \\ \varphi \in D(A^*), |\varphi|=1}} (\varepsilon (H_0 - \lambda - i\varepsilon)^{-1} (H_0 - \lambda + i\varepsilon)^{-1} A^* \varphi | A^* \varphi). \end{aligned}$$

The operator $\varepsilon (H_0 - \lambda - i\varepsilon)^{-1} (H_0 - \lambda + i\varepsilon)^{-1} = (2i)^{-1} ((H_0 - \lambda - i\varepsilon)^{-1} - (H_0 - \lambda + i\varepsilon)^{-1})$ being bounded, self-adjoint and positive, we can consider its square root $K_\varepsilon(\lambda)$, and the previous equality is equivalent to

$$\sup_{\substack{\lambda \in \mathbb{R} \\ \varphi \in D(A^*), |\varphi|=1}} |K_\varepsilon(\lambda) A^* \varphi|^2 = \sup_{\lambda \in \mathbb{R}, \varphi \in \mathcal{H}, |\varphi|=1} \varepsilon |A(H_0 - \lambda - i\varepsilon)^{-1} \varphi|^2 = c_\varepsilon^2,$$

hence, for any $\lambda \in \mathbb{R}$ $\text{Ran } K_\varepsilon(\lambda) \subset D(A)$ and

$$\|AK_\varepsilon(\lambda)\| = c_\varepsilon$$

We now observe that

$$-i(H_0 - \lambda - i\varepsilon)^{-1} = \int_0^\infty dt e^{-\varepsilon t} e^{i\lambda t} e^{-itH_0}.$$

Using a similar identity for $(H_0 - \lambda + i\varepsilon)^{-1}$ and applying Lemma 3.1 and the resolvent identity, we obtain, for all $\varphi \in \mathcal{H}$,

$$\begin{aligned} \int_{\mathbb{R}} dt e^{-2\varepsilon|t|} |A e^{-itH_0} \varphi|^2 &= (2\pi)^{-1} \int_{\mathbb{R}} d\lambda |A((H_0 - \lambda - i\varepsilon)^{-1} - (H_0 - \lambda + i\varepsilon)^{-1})\varphi|^2 \\ &= \frac{2}{\pi} \int_{\mathbb{R}} d\lambda |AK_\varepsilon(\lambda)^2 \varphi|^2 \\ &\leq \frac{2}{\pi} c_\varepsilon^2 \int_{\mathbb{R}} d\lambda |K_\varepsilon(\lambda)\varphi|^2 \\ &\leq \frac{2}{\pi} \frac{c_\varepsilon^2}{2i} \int_{\mathbb{R}} d\lambda (((H_0 - \lambda - i\varepsilon)^{-1} - (H_0 - \lambda + i\varepsilon)^{-1})\varphi|\varphi). \end{aligned}$$

Denoting by $d\mu_\varphi$ the spectral measure of φ for H , we have

$$\begin{aligned} &\frac{2}{\pi} \frac{1}{2i} \int_{\mathbb{R}} d\lambda (((H_0 - \lambda - i\varepsilon)^{-1} - (H_0 - \lambda + i\varepsilon)^{-1})\varphi|\varphi) \\ &= \frac{2}{\pi} \int_{\mathbb{R}} d\lambda \int_{\mathbb{R}} d\mu_\varphi(x) \frac{\varepsilon}{(x - \lambda)^2 + \varepsilon^2} \\ &= \frac{2}{\pi} \int_{\mathbb{R}} d\mu_\varphi(x) \int_{\mathbb{R}} d\lambda \frac{\varepsilon}{(x - \lambda)^2 + \varepsilon^2} \\ &= 2 \int_{\mathbb{R}} d\mu_\varphi(x) = 2|\varphi|^2, \end{aligned}$$

and the result follows. \square

3.2. Global space-time formulation in $H^1(I, \mathcal{H})$. The following theorem states an abstract condition on a couple of operators H_0 and A on \mathcal{H} which ensures that $\mathcal{X}_{H_0+A} = \mathcal{X}_{H_0}$. The proof is postponed to Subsection 3.3.

More precisely, we make the following set of assumptions on the operators H_0 and A .

Assumptions (A):

- (A1) The operator H_0 is a self-adjoint operator on \mathcal{H} .
- (A2) The operator A is a closed symmetric operator on \mathcal{H} such that $D(H_0) \subset D(A)$.
- (A3) There exists some $\varepsilon > 0$ such that

$$(3.3) \quad \sup_{\lambda \in \mathbb{R}} \|A(H_0 - \lambda \pm i\varepsilon)^{-1}\| < 1.$$

LEMMA 3.5. *Let H_0 and A be operators on \mathcal{H} satisfying (A), and $B : \bar{I} \ni t \mapsto B(t)$ be a strongly continuous family of bounded self-adjoint operator on \mathcal{H} . Then, for any $t \in \bar{I}$, $H(t) = H_0 + A + B(t)$ defined on $D(H(t)) := D(H_0)$ is self-adjoint.*

Proof. By (A3), we have $a = \|A(H_0 + i\varepsilon)^{-1}\| < 1$. Let $\varphi \in D(H_0)$, then we have

$$\begin{aligned} |A\varphi| &= |A(H_0 + i\varepsilon)^{-1}(H_0 + i\varepsilon)\varphi| \leq a|(H_0 + i\varepsilon)\varphi| \\ &\leq a|H_0\varphi| + a|\varepsilon||\varphi|, \end{aligned}$$

i.e. A is H_0 -bounded with relative bound strictly smaller than 1. Since, by (A2), A is symmetric, the Kato-Rellich theorem implies that $H_0 + A$ is self-adjoint on $D(H_0)$. Since $B(t)$ is a bounded self-adjoint operator, the same statement holds for $H(t)$. \square

Remark 3.6. If H_0 is such that assumption (A1) is satisfied, we can already identify two cases for which assumptions (A2) and (A3) are satisfied:

- i) the operator A is a bounded self-adjoint operator: as we have $D(H_0) \subset \mathcal{H} = D(A)$ and

$$\sup_{\lambda \in \mathbb{R}} \|A(H_0 - \lambda \pm i\varepsilon)^{-1}\| \leq \|A\| \| (H_0 - \lambda \pm i\varepsilon)^{-1} \| \leq \frac{\|A\|}{|\varepsilon|} \xrightarrow{|\varepsilon| \rightarrow \infty} 0;$$

- ii) the operator A is closed symmetric and H_0 -smooth (in the sense of Definition 3.3): as these properties ensure that $D(H_0) \subset D(A)$ (see Proposition 3.2) and

$$\sup_{\lambda \in \mathbb{R}} \|A(H_0 - \lambda \pm i\varepsilon)^{-1}\| \leq \sqrt{\frac{c_2}{\varepsilon}} \xrightarrow{|\varepsilon| \rightarrow \infty} 0,$$

where c_2 is the constant appearing in Proposition 3.2.

We then have the following theorem, which is one of our key results:

THEOREM 3.7. *Let H_0 and A be operators on \mathcal{H} satisfying (A). Set $H = H_0 + A$.*

(i) **Time-independent operator case:** *It holds that $\mathcal{X}_H = \mathcal{X}_{H_0}$ and there exist constants $\alpha, C > 0$ independent of T such that*

$$(3.4) \quad \forall u \in \mathcal{X}_{H_0}, \quad \frac{\alpha}{1+T} \|u\|_{\mathcal{X}_{H_0}} \leq \|u\|_{\mathcal{X}_H} \leq C(1+T) \|u\|_{\mathcal{X}_{H_0}}.$$

(ii) **Time-dependent operator case:** *Let $B : t \in \bar{I} \mapsto B(t)$ be a strongly continuous family of bounded self-adjoint operators on \mathcal{H} . The map $N : \mathcal{X}_{H_0} \rightarrow \mathbb{R}_+$ defined by*

$$(3.5) \quad \forall u \in \mathcal{X}_{H_0}, \quad N(u) = \left(|u(0)|^2 + T \|(i\partial_t - H - B(t))u\|_{L^2(I, \mathcal{H})}^2 \right)^{\frac{1}{2}},$$

defines a norm on \mathcal{X}_{H_0} , and there exist constants $\alpha, C > 0$ independent of T such that

$$(3.6) \quad \forall u \in \mathcal{X}_{H_0}, \quad \frac{\alpha}{(1+T)^2} \|u\|_{\mathcal{X}_{H_0}} \leq N(u) \leq C(1+T) \|u\|_{\mathcal{X}_{H_0}}.$$

Proof. See Subsection 3.3.1. □

The main advantage of Theorem 3.7 is that the space \mathcal{X}_{H_0} can be characterized by the evolution group e^{-itH_0} . As a corollary, it is possible to use this property to reformulate a global space-time formulation for the time-dependent Schrödinger operator defined on the Hilbert space $H^1(I, \mathcal{H})$.

COROLLARY 3.8. *Let H_0 and A be operators on \mathcal{H} satisfying (A). Set $H = H_0 + A$. Let $B : t \in \bar{I} \mapsto B(t)$ be a strongly continuous family of bounded self-adjoint operators on \mathcal{H} . Let $u_0 \in \mathcal{H}$ and $f \in L^2(I, \mathcal{H})$. Let $u^* \in \mathcal{X}_{H_0}$ be the solution to (1.1) (in the sense of Definition 2.1), and $v^* : t \in I \mapsto e^{itH_0} u^*(t)$.*

Then, the functional F defined in (1.8) is well-defined and quadratic. Furthermore, there exist constants $C, \alpha > 0$ independent of T such that

$$(3.7) \quad \forall v \in H^1(I, \mathcal{H}), \quad \frac{\alpha}{(1+T)^\gamma} \|v - v^*\|_{H^1(I, \mathcal{H})} \leq \sqrt{F(v)} \leq C(1+T) \|v - v^*\|_{H^1(I, \mathcal{H})},$$

with $\gamma = 1$ if $B = 0$, and $\gamma = 2$ otherwise.

In particular, it follows that $v^ \in H^1(I, \mathcal{H})$ is the unique solution to the minimization problem (1.7).*

Proof. See Subsection 3.3.2 □

Remark 3.9. In physics, the function v^* corresponds to the *interaction picture* or *Dirac picture* as opposed to u^* which is called the *Schrödinger picture*. In our case, the motivation behind the introduction of this v^* lies in the particular dynamics that it follows, which can be understood as the dynamics of the real solution u^* preconditionned by the “well-known” free dynamics associated with H_0 , and allows us to work with $H^1(I, \mathcal{H})$ instead of the space of mixed regularity \mathcal{X}_H . Similar reasons motivate the introduction of the minimization problem (1.7) in place of (1.5), the price to pay being that the operator $H + B(t)$ is replaced by the “skewed” operator $e^{itH_0}(A + B(t))e^{-itH_0}$.

The global space-time numerical scheme we propose is simply a Galerkin method which consists in computing an approximation $v^{*,n} \in V_n \subset H^1(I, \mathcal{H})$ of v^* solution to

$$v^{*,n} = \operatorname{argmin}_{v_n \in V_n} F(v_n).$$

Using C ea’s lemma and Corollary 3.8, we then easily obtain that

$$\|v^* - v^{*,n}\|_{H^1(I, \mathcal{H})} \leq \frac{C(1+T)^{\gamma+1}}{\alpha} \inf_{v_n \in V_n} \|v^* - v_n\|_{H^1(I, \mathcal{H})},$$

which in turn implies that

$$\|u^* - u^{*,n}\|_{\mathcal{X}_{H_0}} \leq \frac{C(1+T)^{\gamma+1}}{\alpha} \inf_{u_n \in U_n} \|u^* - u_n\|_{\mathcal{X}_{H_0}},$$

where $u^{*,n} = e^{-itH_0} v^{*,n}$ and $U_n = e^{-itH_0} V_n$. For this numerical scheme to be practical, it is important to choose V_n so that elements of the form $e^{itH_0} v_n$ could be efficiently computed for any $v_n \in V_n$. We will give some examples of practical choices of discretization spaces V_n in the following sections.

Some remarks are in order here.

Remark 3.10. One can prove directly, as a consequence of estimate (B.3) in Proposition B.4, that

$$(3.8) \quad \forall v \in H^1(I, \mathcal{H}), \quad \|v - v^*\|_{C^0(I, \mathcal{H})} \leq \sqrt{2F(v)}.$$

This estimate is actually better than the “naive” estimate

$$\|v - v^*\|_{C^0(I, \mathcal{H})} \leq \sqrt{2} \|v - v^*\|_{H^1(I, \mathcal{H})} \leq \frac{(1+T)}{\alpha} \sqrt{2F(v)},$$

and can be used to compute a posteriori error estimates.

Remark 3.11. Given a set $\Sigma \subset \mathcal{H}$, and \tilde{v} the solution to the problem

$$\tilde{v} \in \underset{v \in H^1(I, \Sigma)}{\operatorname{argmin}} F(v),$$

it follows from (3.7) that \tilde{v} satisfies the “Céa-type” estimate

$$\|\tilde{v} - v^*\|_{H^1(I, \mathcal{H})} \leq \frac{C(1+T)^{\gamma+1}}{\alpha} \min_{v \in H^1(I, \Sigma)} \|v - v^*\|_{H^1(I, \mathcal{H})}.$$

For instance, if Σ is a low-rank subset (or any other approximation subset), then \tilde{v} is a quasi-optimal approximation of v^* in $H^1(I, \Sigma)$, and the dependency of the quasi-optimality constants on T is polynomial. This should be compared with the error estimates that typically arise for this kind of approximation. For instance, time-stepping procedures on low-rank manifolds only yield results that are provably quasi-optimal, with a constant that grows exponentially in time [2, Theorem 27], [25, Theorem 5.1].

If we make the additional assumption that A is H_0 -smooth in the sense of Definition 3.3, we have the following result which is a slight improvement of estimate (3.4).

THEOREM 3.12. *Assume that H_0 and A satisfy the set of assumptions (A). Let us assume in addition that A is H_0 -smooth. Then the operator $H = H_0 + A$ on \mathcal{H} is self-adjoint with $D(H) = D(H_0)$ and we have $\mathcal{X}_H = \mathcal{X}_{H_0}$. Besides, there exist constants $\alpha, C > 0$ such that*

$$(3.9) \quad \forall u \in \mathcal{X}_{H_0}, \quad \frac{\alpha}{1+T} \|u\|_{\mathcal{X}_{H_0}} \leq \|u\|_{\mathcal{X}_H} \leq C\sqrt{1+T} \|u\|_{\mathcal{X}_{H_0}}.$$

Proof. See Subsection 3.3.3. □

3.3. Proofs of theoretical results of Section 3.2. We first state a proposition that we will use in the proofs of the results of the previous section.

PROPOSITION 3.13. *Assume that H_0 and A satisfy the set of assumptions (A). Then, the operator $H = A + H_0$ is self-adjoint on \mathcal{H} with domain $D(H) = D(H_0)$, and there exists $C \geq 0$ such that*

$$(3.10) \quad \forall T > 0, \quad \forall \varphi \in \mathcal{H}, \quad \int_{-T}^T dt |A e^{-itH_0} \varphi|^2 \leq C(1+T) |\varphi|^2,$$

$$(3.11) \quad \forall T > 0, \quad \forall \varphi \in \mathcal{H}, \quad \int_{-T}^T dt |A e^{-itH} \varphi|^2 \leq C(1+T) |\varphi|^2.$$

Proof. Let us introduce

$$(3.12) \quad c_\varepsilon := \sup_{\lambda \in \mathbb{R}} \|A(H_0 - \lambda \pm i\varepsilon)^{-1}\| < 1,$$

for some $\varepsilon > 0$ such that (A3) is satisfied.

First, let us prove that $H_0 + A$ is self-adjoint on \mathcal{H} with domain $D(H_0)$. Using (3.12), we obtain for all $\psi \in D(H_0)$,

$$|A\psi| = |A(H_0 - i\varepsilon)^{-1}(H_0 - i\varepsilon)\psi| \leq c_\varepsilon |(H_0 - i\varepsilon)\psi| \leq c_\varepsilon |H_0\psi| + c_\varepsilon \varepsilon |\psi|.$$

This proves that A is H_0 -bounded with relative bound lower than 1. Since we assumed A symmetric, the self-adjointness of $H_0 + A$ is a consequence of the Kato-Rellich theorem.

We now need to prove the estimates. We only prove the second one, since the proof for the first one is similar. For any $\lambda \in \mathbb{R}$,

$$(H - \lambda - i\varepsilon)^{-1} = ((1 + A(H_0 - \lambda - i\varepsilon)^{-1})(H_0 - \lambda - i\varepsilon))^{-1} = (H_0 - \lambda - i\varepsilon)^{-1}(1 + A(H_0 - \lambda - i\varepsilon)^{-1})^{-1},$$

hence it follows from Neumann's inversion formula

$$|A(H - \lambda - i\varepsilon)^{-1}| = |A(H_0 - \lambda - i\varepsilon)^{-1}(1 + A(H_0 - \lambda - i\varepsilon)^{-1})^{-1}| \leq \frac{c_\varepsilon}{1 - c_\varepsilon}.$$

We can therefore apply Lemma 3.4, which shows that there exists a constant $C_\varepsilon \geq 0$ (which may vary along the calculations) such that

$$\forall \varphi \in \mathcal{H}, \quad \int_{\mathbb{R}} dt e^{-2\varepsilon|t|} |A e^{-itH} \varphi|^2 \leq C_\varepsilon |\varphi|^2.$$

Reducing the integration domain to $[0, \frac{1}{\varepsilon}]$, we obtain

$$\forall \varphi \in \mathcal{H}, \quad \int_0^{\frac{1}{\varepsilon}} dt |A e^{-itH} \varphi|^2 \leq C_\varepsilon |\varphi|^2.$$

Now, taking any integer $n \geq 1$ and $\varphi \in \mathcal{H}$, we have

$$\begin{aligned} \int_0^{\frac{n}{\varepsilon}} dt |A e^{-itH} \varphi|^2 &= \sum_{k=0}^{n-1} \int_{\frac{k}{\varepsilon}}^{\frac{k+1}{\varepsilon}} dt |A e^{-itH} \varphi|^2 \\ &= \sum_{k=0}^{n-1} \int_0^{\frac{1}{\varepsilon}} dt |A e^{-itH} (e^{-i\frac{k}{\varepsilon}H} \varphi)|^2 \\ &\leq C_\varepsilon \sum_{k=0}^{n-1} |e^{-i\frac{k}{\varepsilon}H} \varphi|^2 = C_\varepsilon n |\varphi|^2. \end{aligned}$$

Applying the same process for negative times, and writing any $T \geq 0$ as $T = \frac{n}{\varepsilon} + \tau$, $0 \leq \tau < \frac{1}{\varepsilon}$, the estimate is proved. \square

3.3.1. Proof of Theorem 3.7.

Proof of Theorem 3.7. Case (i): Assume that $H = H_0 + A$. Let $u \in \mathcal{X}_{H_0}$. By Proposition 2.4, there exists $v \in H^1(I, \mathcal{H})$ such that $u = e^{-itH_0} v$ and $\|(i\partial_t - H_0)u\|_{L^2(I, \mathcal{H})} = \|\partial_t v\|_{L^2(I, \mathcal{H})}$. Therefore,

$$\begin{aligned} \|Au\|_{L^2(I, \mathcal{H})} &= \left\| A e^{-itH_0} \left(u(0) + \int_0^t ds \partial_t v(s) \right) \right\|_{L^2(I, \mathcal{H})} \\ &\leq \|A e^{-itH_0} v(0)\|_{L^2(I, \mathcal{H})} + \int_0^T ds \|\mathbf{1}_{s \leq t} A e^{-itH_0} \partial_t v(s)\|_{L^2(I, \mathcal{H})}. \end{aligned}$$

Proposition 3.13 shows the existence of a constant $C > 0$ such that

$$\begin{aligned} \|Au\|_{L^2(I, \mathcal{H})} &\leq C\sqrt{1+T} |v(0)| + C\sqrt{1+T} \int_0^T ds |\partial_t v(s)| \\ (3.13) \quad &\leq C\sqrt{1+T} |v(0)| + C\sqrt{1+T}\sqrt{T} \|\partial_t v\|_{L^2(I, \mathcal{H})} \\ &\leq C\sqrt{1+T} \left(|u(0)|^2 + T \|(i\partial_t - H_0)u\|_{L^2(I, \mathcal{H})}^2 \right)^{\frac{1}{2}} \\ &\leq C\sqrt{1+T} \|u\|_{\mathcal{X}_{H_0}}. \end{aligned}$$

Thus, $(i\partial_t - H)u = (i\partial_t - H_0)u - Au \in L^2(I, \mathcal{H})$, that is, $u \in \mathcal{X}_H$ and

$$\begin{aligned} \|u\|_{\mathcal{X}_H} &\leq |u(0)| + \sqrt{T} \|(i\partial_t - H_0 - A)u\|_{L^2(I, \mathcal{H})} \\ (3.14) \quad &\leq |u(0)| + \sqrt{T} \|(i\partial_t - H_0)u\|_{L^2(I, \mathcal{H})} + \sqrt{T} \|Au\|_{L^2(I, \mathcal{H})} \\ &\leq C(\|u\|_{\mathcal{X}_{H_0}} + \sqrt{T}\sqrt{1+T} \|u\|_{\mathcal{X}_{H_0}}) \\ &\leq C(1+T) \|u\|_{\mathcal{X}_{H_0}}. \end{aligned}$$

This proves the right inequality in (3.4).

We now turn to the left inequality in (3.4). Let $u \in \mathcal{X}_H$. Applying Proposition 3.13, we obtain the existence of a $C > 0$ such that

$$\forall \varphi \in \mathcal{H}, \quad \|A e^{-itH} \varphi\|_{L^2(I, \mathcal{H})} \leq C\sqrt{1+T} |\varphi|.$$

The rest of the proof can be carried out without change, simply by permuting H_0 and H .

Case (ii): We now turn to the case $H(t) = H_0 + A + B(t)$.

Let $u \in \mathcal{X}_{H_0}$, then

$$\begin{aligned} N(u)^2 &= |u(0)|^2 + T \|(i\partial_t - H_0 - A - B(t))u(t)\|_{L^2(I, \mathcal{H})}^2 \\ &\leq |u(0)|^2 + 2T \|(i\partial_t - H_0 - A)u(t)\|_{L^2(I, \mathcal{H})}^2 + 2TM^2 \|u\|_{L^2(I, \mathcal{H})}^2. \end{aligned}$$

The sum of the two first terms can be estimated by the first part of Theorem 3.7 as follows,

$$|u(0)|^2 + 2T \|(i\partial_t - H_0 - A)u(t)\|_{L^2(I, \mathcal{H})}^2 \leq C(1+T)^2 \|u\|_{\mathcal{X}_{H_0}}^2$$

and for the third term we write

$$\|u\|_{L^2(I, \mathcal{H})} \leq \sqrt{T} \|u\|_{C^0(I, \mathcal{H})} \leq \sqrt{2T} \|u\|_{\mathcal{X}_{H_0}}.$$

Therefore,

$$N(u)^2 \leq C(1+T)^2 \|u\|_{\mathcal{X}_{H_0}}^2,$$

which is the right-hand estimate of (3.6).

Conversely, let $u \in \mathcal{X}_{H_0}$ and write $u_0 = u(0)$ and $f(t) = (i\partial_t - H_0 - A - B(t))u(t)$. Then it follows from the continuity estimate in Proposition B.4 that

$$\|u\|_{L^2(I, \mathcal{H})}^2 \leq T \|u\|_{C^0(I, \mathcal{H})}^2 \leq 2T(|u(0)|^2 + T \|f\|_{L^2(I, \mathcal{H})}^2) = 2TN(u)^2,$$

therefore,

$$\begin{aligned} \|u\|_{\mathcal{X}_H}^2 &\leq 2(N(u)^2 + M^2T \|u\|_{L^2(I, \mathcal{H})}^2) \\ &\leq C(1+T^2)N(u)^2. \end{aligned}$$

Using the first part of the proof, we finally obtain

$$\|u\|_{\mathcal{X}_{H_0}} \leq C(1+T) \|u\|_{\mathcal{X}_H} \leq C(1+T)^2 N(u),$$

which concludes the proof. \square

3.3.2. Proof of Corollary 3.8.

Proof of Corollary 3.8. Let $v = e^{itH_0} u \in H^1(I, \mathcal{H})$, then

$$\begin{aligned} (i\partial_t - e^{itH_0} A e^{-itH_0})v - e^{itH_0} f &= i\partial_t e^{itH_0} u - e^{itH_0} Au - e^{itH_0} f \\ &= e^{itH_0} (i\partial_t - H_0)u - e^{itH_0} Au - e^{itH_0} (i\partial_t - H)u^* \\ &= e^{itH_0} (i\partial_t - H)(u - u^*). \end{aligned}$$

It immediately follows that

$$F(v) = \|u - u^*\|_{\mathcal{X}_H}^2,$$

and the result is a consequence of (3.4) and the fact that $\|u - u^*\|_{\mathcal{X}_{H_0}} = \|v - v^*\|_{H^1(I, \mathcal{H})}$. \square

3.3.3. Proof of Theorem 3.12.

Proof of Theorem 3.12. To prove Theorem 3.12, notice that if A is H_0 -smooth, then (3.13) in the proof above can be replaced by

$$\|Au\|_{L^2(I, \mathcal{H})} \leq C \|u\|_{\mathcal{X}_{H_0}}.$$

The result is proved by adapting (3.14). \square

3.4. Application to electronic many-body Schrödinger operators. In this section, we show that the variational formulation proposed in the previous section can also be applied to electronic many-body Schrödinger operators of the form (1.3).

More precisely, let $H_0 = -\Delta$, and let $A = V$ denote the multiplication by the electronic potential

$$(3.15) \quad \forall x_1, \dots, x_N \in \mathbb{R}^3, \quad V(x_1, \dots, x_N) = \sum_{k=1}^M \sum_{\ell=1}^N \frac{-Z_k}{|x_\ell - X_k|} + \sum_{1 \leq k < \ell \leq N} \frac{1}{|x_k - x_\ell|},$$

where the $Z_k > 0$ denote the charges of the nuclei.

The fundamental result needed here concerns the one-body case ($N = 1$), and is proven in [6, 24]:

PROPOSITION 3.14. *For any $\varphi \in L^2(\mathbb{R}^3)$, we have:*

$$(3.16) \quad \left\| \frac{1}{|x|} e^{it\Delta} \varphi \right\|_{L^2(\mathbb{R}_t \times \mathbb{R}_x^3)} \leq 2\sqrt{\frac{2}{\pi}} \|\varphi\|_{L^2(\mathbb{R}^3)}.$$

In other words, the multiplication operator by $\frac{1}{|x|}$ is $-\Delta$ -smooth.

Using this result, we can obtain a similar one for the many-body case:

PROPOSITION 3.15. *For any $\varphi \in L^2(\mathbb{R}^{3N})$*

$$(3.17) \quad \|V e^{it\Delta} \varphi\|_{L^2(\mathbb{R}_t \times \mathbb{R}_x^{3N})} \leq 2\sqrt{\frac{2}{\pi}} \left(N \sum_{k=1}^M |Z_k| + \frac{N(N-1)}{2\sqrt{2}} \right) \|\varphi\|_{L^2(\mathbb{R}^{3N})},$$

where V is defined in (3.15). In other words, the multiplication operator by V is $-\Delta$ -smooth in the sense of Definition 3.3.

Proof. We first consider the case $V = \frac{1}{|x_1|}$. Let $\varphi \in L^2(\mathbb{R}^{3N})$. Using the fact that $L^2(\mathbb{R}^{3N}) = L^2(\mathbb{R}^3) \otimes L^2(\mathbb{R}^{3(N-1)})$, introducing the singular value decomposition of φ , there exist two orthogonal sequences $(v_k)_{k \geq 1} \subset L^2(\mathbb{R}^3)$, $(w_k)_{k \geq 1} \subset L^2(\mathbb{R}^{3(N-1)})$ such that for almost all $x_1 \in \mathbb{R}^3$ and $X = (x_2, \dots, x_N) \in \mathbb{R}^{3(N-1)}$

$$\varphi(x_1, X) = \sum_{k \geq 1} v_k(x_1) w_k(X),$$

the sum above being possibly infinite. Therefore,

$$\begin{aligned} \left\| \frac{e^{it\Delta} \varphi}{|x_1|} \right\|_{L^2(\mathbb{R} \times \mathbb{R}^{3N})}^2 &= \left\| \sum_{k \geq 1} \left(\frac{e^{it\Delta_{x_1}} v_k}{|x_1|} \right) \otimes (e^{it\Delta_X} w_k) \right\|_{L^2(\mathbb{R} \times \mathbb{R}^{3N})}^2 \\ &= \sum_{k \geq 1} \left\| \left(\frac{e^{it\Delta_{x_1}} v_k}{|x_1|} \right) \otimes (e^{it\Delta_X} w_k) \right\|_{L^2(\mathbb{R} \times \mathbb{R}^{3N})}^2, \end{aligned}$$

where we used the fact that, for each t , $(e^{it\Delta_X} w_k)_k$ is an orthogonal family of $L^2(\mathbb{R}^{3N})$. Thus,

$$\begin{aligned} \left\| \frac{e^{it\Delta} \varphi}{|x_1|} \right\|_{L^2(\mathbb{R} \times \mathbb{R}^{3N})}^2 &= \sum_{k \geq 1} \int_{\mathbb{R}} dt \left\| \frac{e^{it\Delta_{x_1}} v_k}{|x_1|} \right\|_{L^2(\mathbb{R}^3)}^2 \|e^{it\Delta_X} w_k\|_{L^2(\mathbb{R}^{3(N-1)})}^2 \\ &\leq \sum_{k \geq 1} \left(2\sqrt{\frac{2}{\pi}} \right)^2 \|v_k\|_{L^2(\mathbb{R}^3)}^2 \|w_k\|_{L^2(\mathbb{R}^{3(N-1)})}^2 \\ &= \left(2\sqrt{\frac{2}{\pi}} \right)^2 \|\varphi\|_{L^2(\mathbb{R}^{3N})}^2. \end{aligned}$$

For the general case, we consider each term of the sum (3.15) separately:

- for the terms $\frac{-Z_k}{|x_\ell - X_k|}$, we perform the change of variables $y_\ell = x_\ell - X_k$, and replace x_1 by y_ℓ in the computation above;
- for the terms $\frac{1}{|x_k - x_\ell|}$, we use the change of variables $y_k = \frac{x_k - x_\ell}{\sqrt{2}}$ and $y_\ell = \frac{x_k + x_\ell}{\sqrt{2}}$, and replace x_1 by y_k in the computation above.

The inequality (3.17) then follows by applying the triangle inequality and combining the inequalities obtained for each term. \square

For any $u_0 \in L^2(\mathbb{R}^{3N})$ and any $f \in L^2(I, L^2(\mathbb{R}^{3N}))$, we can therefore reformulate the solution to the evolution problem

$$(3.18) \quad \begin{cases} i\partial_t u^* = (-\Delta + V)u^* + f, \\ u(0) = u_0, \end{cases}$$

as in the previous section (Theorem 3.12):

THEOREM 3.16. *Let $u_0 \in L^2(\mathbb{R}^{3N})$ and $f \in L^2(I, L^2(\mathbb{R}^{3N}))$. Let u^* be the solution to (3.18), and $v^* := e^{-it\Delta} u^*$.*

Define for any $v \in H^1(I, L^2(\mathbb{R}^{3N}))$ the functional

$$(3.19) \quad F(v) = \|v(0) - u_0\|_{L^2(\mathbb{R}^{3N})}^2 + T \|(i\partial_t - e^{-it\Delta} V e^{it\Delta})v - e^{-it\Delta} f\|_{L^2(I, L^2(\mathbb{R}^{3N}))}^2.$$

Then, there exist constants $C, \alpha > 0$ such that for any $v \in H^1(I, L^2(\mathbb{R}^{3N}))$,

$$(3.20) \quad \frac{\alpha}{1+T} \|v - v^*\|_{H^1(I, L^2(\mathbb{R}^{3N}))} \leq \sqrt{F(v)} \leq C\sqrt{1+T} \|v - v^*\|_{H^1(I, L^2(\mathbb{R}^{3N}))}.$$

Remark 3.17. Let us consider the one-body case $N = 1$. In practice, the Coulomb potential may be regularized for valence electrons calculations, taking into account the frozen core orbitals. This is the effective core potential approach [19] similar to pseudopotentials in solid state physics. Schematically, at a rough level it may be described as follows: let $\rho \in L^1(\mathbb{R}^3)$ be a smooth and rapidly decaying function, and define $V_\delta = \rho_\delta * \frac{1}{|x|}$, where $\rho_\delta(x) = \delta^{-d}\rho(\frac{x}{\delta})$ represents a smeared charge distribution with a regularization parameter δ . Here, $V_\delta \in L^\infty(\mathbb{R}^3)$, therefore Corollary 3.8 can still be applied. However, we then have $\|V_\delta\|_{L^\infty} \rightarrow \infty$ as $\delta \rightarrow 0$, hence the constants C, α in Corollary 3.8 will degenerate.

An alternative approach can be derived by observing that, for any $\varphi \in L^2(\mathbb{R}^3)$, one has (taking advantage of the translation invariance of Δ)

$$\begin{aligned} \frac{1}{\sqrt{2\pi}} \|V_\delta e^{it\Delta} \varphi\|_{L^2(\mathbb{R}_t \times \mathbb{R}_x^3)} &= \frac{1}{\sqrt{2\pi}} \left\| \int_{\mathbb{R}^3} dy \rho_\delta(y) \frac{1}{|x-y|} (e^{it\Delta} \varphi)(x) \right\|_{L^2(\mathbb{R}_t \times \mathbb{R}_x^3)} \\ &\leq \int_{\mathbb{R}^3} dy |\rho_\delta(y)| \frac{1}{\sqrt{2\pi}} \left\| \frac{1}{|x-y|} (e^{it\Delta} \varphi)(x) \right\|_{L^2(\mathbb{R}_t \times \mathbb{R}_x^3)} \\ &\leq \int_{\mathbb{R}^3} dy |\rho_\delta(y)| \left\| \frac{1}{|x|} \right\|_{\Delta} \|\varphi\|_{L^2} \\ &\leq \|\rho_\delta\|_{L^1} \left\| \frac{1}{|x|} \right\|_{\Delta} \|\varphi\|_{L^2} = \|\rho\|_{L^1} \left\| \frac{1}{|x|} \right\|_{\Delta} \|\varphi\|_{L^2}. \end{aligned}$$

We recall here that $\|\cdot\|_{\Delta}$ is a special case of Definition 3.3 with $H_0 = \Delta$. It follows that V_δ is $-\Delta$ -smooth, and the value of $\|V_\delta\|_{\Delta}$ is bounded uniformly with respect to δ . Hence, the constants C, α in Corollary 3.8 can in fact be taken independent of δ .

This shows that, even for bounded potentials, the machinery developed in Subsection 3.1, Subsection 3.2, and Proposition 3.15 may provide some improvement compared to the more elementary approach used for bounded operators. The same argument can be applied to the many-body case.

Remark 3.18. To the knowledge of the authors, the arguments developed to prove Theorem 3.7 do not extend to the case of unbounded time dependent potentials. For instance, the important case of an ultrashort laser pulse modeled by a time-dependent potential of the form $B(t) = -x \cdot E(t)$ is not covered by the results of the present paper.

3.5. Time regularity of the solution. In this section, we study the regularity of the function v^* defined in Corollary 3.8 with respect to the time variable. We consider the case $H_0 = -\Delta$, $A = 0$ and $B(t) = V(t)$ a smooth potential, but assumptions could be replaced by more abstract assumptions regarding the commutators $[-\Delta, V(t)]$, $[-\Delta, [-\Delta, V(t)]]$, ...

THEOREM 3.19. *Let $k \in \mathbb{N}$. Assume $V = V(t, x) \in C^\infty(\mathbb{R} \times \mathbb{R}^d)$ is real-valued and*

$$(3.21) \quad \mu_k := \sup_{\substack{0 \leq l \leq k \\ 0 \leq |\alpha| \leq 2k}} \sup_{(t,x) \in \mathbb{R} \times \mathbb{R}^d} |\partial_t^l \partial_x^\alpha V(t, x)| < \infty.$$

Let $u_0 \in H^k(\mathbb{R}^d)$, and $u^* \in \mathcal{X}_{-\Delta}$ be the solution to

$$(3.22) \quad \begin{cases} i\partial_t u^* = (-\Delta + V)u^*, \\ u^*(0) = u_0, \end{cases}$$

in the sense of Definition 2.1 (with $J = \mathbb{R}$), and define $v^* := e^{-it\Delta} u^*$. Then $v^* \in C^{k+1}(\mathbb{R}, L^2(\mathbb{R}^d))$, and there exists a constant C_k , that only depends on μ_k such that

$$(3.23) \quad \forall t \in \mathbb{R}, \|(i\partial_t)^{k+1} v^*\|_{C^0(\mathbb{R}, L^2(\mathbb{R}^d))} \leq C_k (1 + |t|^{\frac{k}{2}}) \|u_0\|_{H^k(\mathbb{R}^d)}.$$

The proof of Theorem 3.19 is based upon the following observation: if V satisfies (3.21), then for any given $t \in \mathbb{R}$ and $k \geq 1$, the form domains $Q((-\Delta + V(t))^k)$ and $Q((-\Delta)^k) = H^k(\mathbb{R}^d)$ coincide, and the associated norms are equivalent, that is, there exist constants $a_k, M_k > 0$ such that

$$(3.24) \quad \forall \varphi \in H^k(\mathbb{R}^d), \quad \frac{1}{M_k} \|\varphi\|_{H^k(\mathbb{R}^d)}^2 \leq \langle (-\Delta + V(t))^k \varphi, \varphi \rangle + a_k \|\varphi\|_{L^2(\mathbb{R}^d)}^2 \leq M_k \|\varphi\|_{H^k(\mathbb{R}^d)}^2.$$

Moreover, the constants a_k, M_k only depend on $\sup_{x \in \mathbb{R}^d} |\partial_x^\alpha V(t, x)|$ for $|\alpha| \leq k$, hence can be chosen independent of t according to (3.21).

Proof of Theorem 3.19. First assume that $u_0 \in \bigcap_{s \geq 0} H^s(\mathbb{R}^d)$, which ensures that we only manipulate strong derivatives.

We prove the following result by induction : for any $k \geq 0$ there exists a family of differential operators differential operator $P_k(t) = \sum_{|\alpha| \leq k} a_\alpha^k(t, x) \partial_x^\alpha$ whose coefficients are smooth functions with bounded derivatives that only depend on the $\partial_t^j \partial_x^\alpha V$ for $j \leq k$ and $|\alpha| \leq 2k$ such that

$$\forall t \in \mathbb{R}, (i\partial_t)^{k+1}v(t) = e^{-it\Delta} P_k(t)u(t),$$

and there exists a constant C_k that only depends on k and V such that

$$\forall t \in \mathbb{R}, \|u(t)\|_{H^k(\mathbb{R}^d)} \leq C_k(1 + |t|^{\frac{k}{2}}) \|u_0\|_{H^k(\mathbb{R}^d)}.$$

- For $k = 0$ just take $P_0(t) = V(t)$, and use the fact that $\|u(t)\|_{L^2(\mathbb{R}^d)}$ is constant.
- Assume the result holds for $k - 1$. Then

$$\begin{aligned} (i\partial_t)^{k+1}v &= (i\partial_t)(e^{-it\Delta} P_{k-1} e^{it\Delta} v) \\ &= e^{-it\Delta} [\Delta, P_{k-1}] e^{it\Delta} v + e^{-it\Delta} (i\partial_t P_{k-1}) e^{it\Delta} v(t) + e^{-it\Delta} P_{k-1} e^{it\Delta} i\partial_t v \\ &= e^{-it\Delta} [\Delta, P_{k-1}] u + e^{-it\Delta} (i\partial_t P_{k-1}) u + e^{-it\Delta} P_{k-1} V u, \end{aligned}$$

and $P_k(t) = [\Delta, P_{k-1}(t)] + i\partial_t P_{k-1}(t) + P_{k-1}(t)V(t)$ is as stated.

Now we compute

$$\begin{aligned} &\frac{d}{dt} \langle (-\Delta + V(t))^k u(t), u(t) \rangle \\ &= 2 \underbrace{\Re \langle (-\Delta + V(t))^k u(t), \partial_t u(t) \rangle}_{=0} + \Re \left\langle \sum_{j=1}^k (-\Delta + V(t))^{j-1} \partial_t V(t) (-\Delta + V(t))^{j-k} u(t), u(t) \right\rangle, \end{aligned}$$

which implies

$$\forall t \in \mathbb{R}, \quad \frac{d}{dt} \langle (-\Delta + V(t))^k u(t), u(t) \rangle \leq C_k \|u(t)\|_{H^{k-1}(\mathbb{R}^d)}^2 \leq C_k(1 + |t|^{k-1}) \|u_0\|_{H^{k-1}(\mathbb{R}^d)}^2.$$

Integrating with respect to the time variable between 0 and t , we obtain

$$\forall t \in \mathbb{R}, \quad |\langle (-\Delta + V(t))^k u(t), u(t) \rangle| \leq C_k(1 + |t|^k) \|u_0\|_{H^k(\mathbb{R}^d)}^2.$$

The conclusion follows from (3.24).

We extend the result to all $u_0 \in H^k(\mathbb{R}^d)$ by regularization: let $\chi \in C_c^\infty(\mathbb{R}^d)$ be such that $0 \leq \chi \leq 1$, and $\chi = 1$ near 0 and for all $n \in \mathbb{N}$, set $u_0^n = \chi(\frac{\cdot}{n})u_0 = \mathcal{F}^{-1} \left(\chi(\frac{\xi}{n}) \widehat{u_0} \right)$ (that is $\chi(\frac{\cdot}{n})$ is used as a cut-off in the Fourier domain) and u^n the solution to

$$\begin{cases} i\partial_t u^n = (-\Delta + V(t))u^n, \\ u^n(0) = u_0^n, \end{cases}$$

as well as $v^n = e^{-it\Delta} u^n$. Then

$$u_0^n \xrightarrow[n \rightarrow \infty]{H^k(\mathbb{R}^d)} u_0,$$

and

$$\sup_{t \in \mathbb{R}} \|v^*(t) - v^n(t)\|_{L^2(\mathbb{R}^d)} = \|u_0 - u_0^n\|_{L^2(\mathbb{R}^d)} \xrightarrow[n \rightarrow \infty]{} 0,$$

so in particular we have convergence in the weak sense.

Additionally, it follows from what we proved earlier that $(i\partial_t)^{k+1}v^n$ is continuous with respect to t and that for any $A > 0$,

$$\forall m, n \in \mathbb{N}, \quad \|(i\partial_t)^{k+1}v^m - (i\partial_t)^{k+1}v^n\|_{C^0([-A, A], L^2(\mathbb{R}^d))} \leq C_k(1 + A^{\frac{k}{2}}) \|u_0^m - u_0^n\|_{H^k(\mathbb{R}^d)}.$$

Therefore, $((i\partial_t)^{k+1}v^n)_n$ is a Cauchy sequence in the complete space $C^0([-A, A], L^2(\mathbb{R}^d))$, and there exists a $w \in C^0([-A, A], L^2(\mathbb{R}^d))$ such that

$$(i\partial_t)^{k+1}v^n \xrightarrow[n \rightarrow \infty]{} w \quad \text{strongly in } C^0([-A, A], L^2(\mathbb{R}^d)).$$

We infer, by identifying weak limits, that $(i\partial_t)^{k+1}v^* = w$, and

$$|(i\partial_t)^{k+1}v^*(t)| = \lim_{n \rightarrow \infty} |(i\partial_t)^{k+1}v^n(t)| \leq C_k(1 + |t|^{\frac{k}{2}}) \lim_{n \rightarrow \infty} \|v_0^n\|_{H^k(\mathbb{R}^d)} = C_k(1 + |t|^{\frac{k}{2}}) \|v_0\|_{H^k(\mathbb{R}^d)}$$

for any $t \in [-A, A]$. Since A is arbitrary, the result is proved. \square

3.6. Dual formulation. The aim of this section is to comment on an alternative formulation and highlight the link between our work and the approach presented in [18].

In all this section we will assume, as in Theorem 3.7, that the operators H_0 and A satisfy the set of assumptions (A), $H = H_0 + A$, and $B : t \in \bar{I} \mapsto B(t)$ is a strongly continuous family of bounded self-adjoint operators on \mathcal{H} .

Using some ideas from [18], a different formulation on the less regular space $L^2(I, \mathcal{H})$ can be obtained. Let us first recall here the principle of the approach of [18]. The idea of this method is to consider the Hilbert space

$$(3.25) \quad \mathcal{Y}_H = \{u \in \mathcal{X}_H : u(T) = 0\},$$

equipped with the inner product

$$(3.26) \quad \forall u_1, u_2 \in \mathcal{Y}_H, \quad \langle u_1, u_2 \rangle_{\mathcal{Y}_H} = ((i\partial_t - H)u_1 | (i\partial_t - H)u_2)_{L^2(I, \mathcal{H})}$$

and the associated norm

$$(3.27) \quad \forall u \in \mathcal{Y}_H, \quad \|u\|_{\mathcal{Y}_H} = \|(i\partial_t - H)u\|_{L^2(I, \mathcal{H})}.$$

Similarly, let us consider the space \mathcal{Y}_{H_0} defined by (3.25) with $H = H_0$.

We then consider the antidual space

$$(3.28) \quad \mathcal{Y}_H^\dagger = \left\{ \ell : \mathcal{Y}_H \rightarrow \mathbb{C} : \begin{array}{l} \ell \text{ is continuous and} \\ \forall u_1, u_2 \in \mathcal{Y}_H, \forall \lambda \in \mathbb{C}, \ell(u_1 + \lambda u_2) = \ell(u_1) + \bar{\lambda} \ell(u_2) \end{array} \right\},$$

that is, the space of continuous antilinear forms on \mathcal{Y}_H . We denote by $\langle \cdot, \cdot \rangle_{\mathcal{Y}_H \times \mathcal{Y}_H^\dagger}$ the antidual pairing $\mathcal{Y}_H \times \mathcal{Y}_H^\dagger$, antilinear (resp. linear) with respect to the first (resp. second) variable. In particular, the Riesz representation theorem states that, for any $l \in \mathcal{Y}_H^\dagger$, there exists a $u_l \in \mathcal{Y}_H$ such that

$$\forall u \in \mathcal{Y}_H, \quad \langle u, l \rangle_{\mathcal{Y}_H \times \mathcal{Y}_H^\dagger} = \langle u, u_l \rangle_{\mathcal{Y}_H}.$$

In [18], a variational formulation for (1.1) is proposed by means of a continuous bilinear form defined on $L^2(I; \mathcal{H} \times \mathcal{Y}_H)$ which can be proved to satisfy classical inf-sup conditions. The conditioning of this formulation is proved to be optimal. However, one drawback is that there is no explicit characterization of the set \mathcal{Y}_H . Our aim here is to provide an alternative formulation exploiting the fact that we can, in the present perturbative setting, give an explicit characterization of \mathcal{Y}_H . We then have the following result, which is proved analogously to Theorem 3.7, simply by taking the integrals from T to t instead of 0 to t . Let us point out that this result is an extension of Theorem 2.4 of [18], which enables us to treat unbounded potentials and Schrödinger equations defined on unbounded domains.

PROPOSITION 3.20. *Let H_0 and A be operators satisfying the set of assumptions (A), and $B : t \in \bar{I} \mapsto B(t)$ be a strongly continuous family of bounded self-adjoint operators on \mathcal{H} . Set $H = H_0 + A$. It holds that $\mathcal{Y}_H = \mathcal{Y}_{H_0}$. Moreover, the map $L : \mathcal{Y}_{H_0} \rightarrow \mathbb{R}_+$ defined by*

$$(3.29) \quad \forall u \in \mathcal{Y}_{H_0}, \quad L(u) = \|(i\partial_t - H - B(t))u\|_{L^2(I, \mathcal{H})},$$

defines a norm on \mathcal{Y}_{H_0} , and there exist constants $\alpha, C > 0$ independent of T such that

$$(3.30) \quad \forall u \in \mathcal{Y}_{H_0}, \quad \frac{\alpha}{(1+T)^2} \|u\|_{\mathcal{Y}_{H_0}} \leq L(u) \leq C(1+T) \|u\|_{\mathcal{Y}_{H_0}}.$$

Now consider the operator $S^* : L^2(I, \mathcal{H}) \mapsto \mathcal{Y}_{H_0}^\dagger$ defined by

$$(3.31) \quad \forall w \in L^2(I, \mathcal{H}), \quad \forall u \in \mathcal{Y}_{H_0} \quad \langle u, S^*w \rangle_{\mathcal{Y}_{H_0} \times \mathcal{Y}_{H_0}^\dagger} = ((i\partial_t - H - B(t))u | w)_{L^2(I, \mathcal{H})},$$

and similarly the operator $S_0^* : L^2(I, \mathcal{H}) \mapsto \mathcal{Y}_{H_0}^\dagger$ defined by

$$(3.32) \quad \forall w \in L^2(I, \mathcal{H}), \quad \forall u \in \mathcal{Y}_{H_0} \quad \langle S_0^*w, u \rangle_{\mathcal{Y}_{H_0} \times \mathcal{Y}_{H_0}^\dagger} = (w | (i\partial_t - H_0)u)_{L^2(I, \mathcal{H})}.$$

LEMMA 3.21. *We have the following estimates :*

$$(3.33) \quad \forall w \in L^2(I, \mathcal{H}), \quad \frac{\alpha}{(1+T)^2} \|w\|_{L^2(I, \mathcal{H})} \leq \|S^*w\|_{\mathcal{Y}_0^\dagger} \leq C(1+T) \|w\|_{L^2(I, \mathcal{H})}.$$

Proof. Both estimates follow from (3.30) by a classical inf-sup argument which we recall here. For all $w \in L^2(I, \mathcal{H})$, one has with (3.29)

$$\begin{aligned} \|S^* w\|_{\mathcal{Y}_0^\dagger} &= \sup_{\|u\|_{\mathcal{Y}_{H_0}}=1} \langle (i\partial_t - H - B(t))u, w \rangle_{\mathcal{Y}_{H_0} \times \mathcal{Y}_{H_0}^\dagger} \leq \sup_{\|u\|_{\mathcal{Y}_{H_0}}=1} \|w\|_{L^2(I, \mathcal{H})} L(u) \\ &\leq C(1+T) \|w\|_{L^2(I, \mathcal{H})}, \end{aligned}$$

which proves the second inequality in (3.33).

For the first inequality, define u_w as the unique element of \mathcal{Y}_{H_0} such that $(i\partial_t - H - B(t))u_w = w$ (in particular $L(u_w) = \|w\|_{L^2(I, \mathcal{H})}$), then by (3.30)

$$\begin{aligned} \|S^* w\|_{\mathcal{Y}_{H_0}^\dagger} &\geq \frac{\langle w, (i\partial_t - H - B(t))u_w \rangle_{\mathcal{Y}_{H_0} \times \mathcal{Y}_{H_0}^\dagger}}{\|u_w\|_{\mathcal{Y}_{H_0}}} = \frac{\|w\|_{L^2(I, \mathcal{H})}^2}{\|u_w\|_{\mathcal{Y}_{H_0}}} = \|w\|_{L^2(I, \mathcal{H})} \frac{L(u_w)}{\|u_w\|_{\mathcal{Y}_{H_0}}} \\ &\geq \frac{\alpha}{(1+T)^2} \|w\|_{L^2(I, \mathcal{H})}, \end{aligned}$$

which yields the desired result. \square

For $u_0 \in \mathcal{H}$ and $f \in L^2(I, \mathcal{H})$, we denote by $i\delta_{t=0} \otimes u_0 + f$ the element of $\mathcal{Y}_{H_0}^\dagger$ defined by

$$(3.34) \quad \forall u \in \mathcal{Y}_{H_0}, \quad \langle u, i\delta_{t=0} \otimes u_0 + f \rangle_{\mathcal{Y}_{H_0} \times \mathcal{Y}_{H_0}^\dagger} = i\langle u(0), u_0 \rangle + (u|f)_{L^2(I, \mathcal{H})}$$

We have the following proposition which connects the Schrödinger evolution equation and the operators S^* and S_0^* .

PROPOSITION 3.22. (i) *The function $u \in L^2(I, \mathcal{H})$ solves (1.1) in the sense of Definition 2.1 if and only if*

$$S^* u = (S_0^* + A + B(t))u = i\delta_0 \otimes u_0 + f,$$

or equivalently

$$(\text{Id} + (S_0^*)^{-1}(A + B(t)))u = (S_0^*)^{-1}(i\delta_0 \otimes u_0 + f).$$

(ii) *For any $u_0 \in \mathcal{H}$ and $f \in L^2(I, \mathcal{H})$, we have*

$$(3.35) \quad (S_0^*)^{-1}(i\delta_0 \otimes u_0 + f)(t, x) = e^{-itH_0} u_0 - i \int_0^t ds e^{-i(t-s)H_0} f(s).$$

Proof. Assume u solves (1.1). Then $u \in \mathcal{X}_H$ and we have for any $v \in \mathcal{Y}_{H_0}$ (using the “integration by part” formula (2.14))

$$\begin{aligned} \langle v, S^* u \rangle_{\mathcal{Y}_{H_0} \times \mathcal{Y}_{H_0}^\dagger} &= \langle (i\partial_t - H - B(t))v, u \rangle_{L^2(I, \mathcal{H})} = \int_I dt \langle (i\partial_t - H - B(t))v, u \rangle \\ &= \langle v(0), \underbrace{i u(0)}_{=u_0} \rangle + \langle v, \underbrace{(i\partial_t - H - B(t))u}_{=f} \rangle_{L^2(I, \mathcal{H})} \\ &= \langle v, i\delta_{t=0} \otimes u_0 + f \rangle_{\mathcal{Y}_{H_0} \times \mathcal{Y}_{H_0}^\dagger}. \end{aligned}$$

Conversely, assume $S^* u = i\delta_{t=0} \otimes u_0 + f$. Then, for any $w \in C_c^\infty(I, \mathcal{H}) \subset \mathcal{Y}_{H_0}$,

$$\begin{aligned} (i\partial_t w | e^{itH} u)_{L^2(I, \mathcal{H})} &= (e^{-itH} i\partial_t w | u)_{L^2(I, \mathcal{H})} = ((i\partial_t - H) e^{-itH} w | u)_{L^2(I, \mathcal{H})} \\ &= \langle e^{-itH} w, S^* u \rangle_{\mathcal{Y}_{H_0} \times \mathcal{Y}_{H_0}^\dagger} = \underbrace{\langle w(0), iu_0 \rangle}_{=0} + (e^{-itH} w | f)_{L^2(I, \mathcal{H})} \\ &= (w | e^{itH} f)_{L^2(I, \mathcal{H})}. \end{aligned}$$

This means that $e^{itH} u \in H^1(I, \mathcal{H})$ with $i\partial_t e^{itH} u = e^{itH} f$, hence $u \in \mathcal{X}_H$ and $(i\partial_t - H)u = f$. Therefore, for any $v \in \mathcal{Y}_{H_0}$,

$$(i\partial_t - H)v | u)_{L^2(I, \mathcal{H})} = \begin{cases} \langle v(0), iu_0 \rangle + (v|f)_{L^2(I, \mathcal{H})}, \\ \langle v(0), iu(0) \rangle + (v|(i\partial_t - H)u)_{L^2(I, \mathcal{H})} = \langle v(0), iu(0) \rangle + (v|f)_{L^2(I, \mathcal{H})}. \end{cases}$$

It follows that

$$\forall v \in \mathcal{Y}, \quad \langle iu(0), v(0) \rangle = \langle iu_0, v(0) \rangle,$$

and finally

$$u(0) = u_0.$$

The second part of the proposition is just the consequence of the first with $A = 0$ and $B(t) = 0$ for all $t \in \bar{I}$. \square

The following corollary gives an alternative variational formulation for the solution to the time-dependent Schrödinger equation.

COROLLARY 3.23. *Let $u_0 \in \mathcal{H}$, $f \in L^2(I, \mathcal{H})$. The functional*

$$(3.36) \quad E^*(u) = \left\| u(t) + i \int_0^t ds e^{-i(t-s)H_0} (Au) - \left(e^{-itH_0} u_0 - i \int_0^t ds e^{-i(t-s)H_0} f(s) \right) \right\|_{L^2(I, \mathcal{H})}^2$$

is a strongly convex quadratic functional defined on $L^2(I, \mathcal{H})$ which satisfies

$$(3.37) \quad \forall u \in L^2(I, \mathcal{H}), \quad \frac{\alpha}{(1+T)^2} \|u - u^*\|_{L^2(I, \mathcal{H})} \leq \sqrt{E^*(u)} \leq C(1+T) \|u - u^*\|_{L^2(I, \mathcal{H})}$$

where u^* is the solution to (1.1) in the sense of Definition 2.1.

Proof of Corollary 3.23. Let u^* denote the solution to (1.1). It follows from Proposition 3.22 that

$$e^{-itH_0} u_0 - i \int_0^t ds e^{-i(t-s)H_0} f(s) = (S_0^*)^{-1}(\delta_0 \otimes u_0 + f) = (S_0^*)^{-1} S^* u^*,$$

and

$$u + i \int_0^t ds e^{-i(t-s)H_0} (Au) = u - (S_0^*)^{-1} Au = (S_0^*)^{-1} S^* u.$$

Therefore, since clearly S_0^* is an isometry between \mathcal{Y}_{H_0} and $\mathcal{Y}_{H_0}^\dagger$,

$$E^*(u) = \left\| (S_0^*)^{-1} S^*(u - u^*) \right\|_{L^2(I, \mathcal{H})}^2 = \|S^*(u - u^*)\|_{\mathcal{Y}_{H_0}^\dagger}^2,$$

and the desired estimate is a consequence of (3.33). \square

4. Conclusion and perspectives . In this work, we establish a space-time variational formulation for the Schrödinger evolution equation (1.1). This formulation encompasses the case of many-body electronic Coulomb interaction, or more general charge densities (see Remark 3.17), with a bounded time-dependent potential.

As mentioned in the introduction, this variational formulation was mainly developed to provide a numerically achievable way to compute low complexity approximations of the solution to (1.1). This will be the topic of a future work. We describe the main ideas here. One key ingredient is the following proposition:

PROPOSITION 4.1. *Let Σ be any non empty weakly closed subset of \mathcal{H} . Then the subset*

$$H^1(I, \Sigma) = \{u \in H^1(I, \mathcal{H}) : u(t) \in \Sigma \text{ for any } t \in I\}$$

is closed in $H^1(I, \mathcal{H})$ for the weak topology.

Proof. Since $H^1(I, \mathcal{H}) \hookrightarrow \mathcal{C}^0(I, \mathcal{H})$, for any $t \in I$ the linear application

$$T_t : \begin{cases} H^1(I, \mathcal{H}) & \longrightarrow \mathcal{H} \\ v & \longmapsto v(t) \end{cases}$$

is continuous.

Let $(v_n)_{n \geq 0} \subset H^1(I, \Sigma)$ be a sequence which weakly converges to some v in $H^1(I, \mathcal{H})$. Since any bounded linear operator between Banach spaces is also weakly continuous, this implies that for any $t \in I$,

$$v_n(t) = T_t v_n \xrightarrow{n \rightarrow +\infty} T_t v = v(t) \quad \text{in } \mathcal{H},$$

and the weak closedness of Σ implies $v(t) \in \Sigma$. \square

One possible interesting choice for the set Σ is some given set of functions which can be represented with low complexity, such as tensor formats, for instance the manifold of tensor trains with at most a given rank, or well-chosen neural network architectures. Proposition 4.1 implies that, for any value of the final time $T > 0$, there exists at least one minimizer to the minimization problem

$$(4.1) \quad u_\Sigma^* \in \underset{v \in H^1(I, \Sigma)}{\operatorname{argmin}} F(v)$$

where F is defined in (1.8).

As a consequence, for instance when Σ is given as some low-rank tensor format, the variational principle studied here enables to obtain the existence of a dynamical low-rank approximation of u^* whatever the value of

the final time T . This approximation is thus obtained through the variational principle (4.1) which is different from the classical Dirac-Frenkel one [8], for which, at least up to our knowledge, only local-in-time existence of solutions has been proved in the general case. However, we emphasize here that, while some quantities are preserved by the exact Schrödinger dynamics (1.1), these same quantities are not necessarily preserved for the solution to (4.1). The comparison of both types of dynamical low-rank approximations will be the object of a forthcoming article.

The alternative variational formulation presented in Section 3.6 also exhibits some interesting properties for dynamical low-rank approximations. Notably, it allows discontinuous functions in time, which is useful since the best low-rank tensor approximation of $u^*(t)$ is not always continuous in t . However, the existence of a global-in-time low-rank dynamical approximation of u^* using this formulation is not guaranteed in general, in contrast to the formulation presented in Section 3.2. More importantly, from a practical standpoint, it typically results in higher computational costs due to the presence of a time integral.

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Appendix A. Numerical implementation with spectral methods.

The aim of this section is to illustrate the interest of the proposed variational formulation for numerical purposes on some simple test cases. While our main motivation stems from the design of dynamical low-rank approximation schemes, we illustrate here the behaviour of Galerkin global-space time discretization schemes stemming from the variational formulation presented here. The latter mainly rely on the results of Section 3, and in particular Corollary 3.8. The code can be found at [17].

In Section 3.5, we prove a regularity result of the solutions with respect to the time variable for smooth interaction time-dependent potentials, which motivates the use of spectral methods in this simple case. We take advantage of this additional smoothness, coupled with the global space-time formulation obtained in Corollary 3.8, to apply spectral methods to the time variable.

In Section A.1, we begin with an elementary ordinary differential equation. Although simple, this first example is an opportunity to present the basic principles of the spectral discretization for the time variable in detail. We also give an example of a simple but efficient preconditioner which will also be useful for the next example.

In Section A.2, we present the numerical behaviour of the scheme applied to the simulation of the evolution of a 2D Schrödinger equation with periodic boundary conditions.

A.1. A first basic example. Consider the ordinary differential equation ($a, \omega \in \mathbb{R}$)

$$(A.1) \quad \begin{cases} i(u^*)'(t) = a(\cos \omega t)u^*(t), \\ u^*(0) = \eta_0 \in \mathbb{C}. \end{cases}$$

The solution admits the explicit expression $u^*(t) = z_0 e^{-ia \frac{\sin \omega t}{\omega}}$.

We will compute an approximation of this solution on the time interval $(-1, 1)$. We claim that the results established in the paper for $(0, T)$ extend straightforwardly to $(-T, T)$, due to the unitary nature of e^{-itH} when H is a self-adjoint operator. Corollary 3.8 (with $H_0 = A = 0$, and $B(t) = a(\cos \omega t)$) leads to the following problem:

$$(A.2) \quad \min_{u \in H^1(-1,1)} \left(|u(0) - \eta_0|^2 + \int_{-1}^1 dt |iu'(t) - a(\cos \omega t)u(t)|^2 \right).$$

However, in order to make the numerical computations easier, we will consider instead the minimization problem

$$(A.3) \quad \min_{u \in H_w^1(-1,1)} E_w(u), \quad \text{with } E_w(u) := |u(0) - \eta_0|^2 + \int_{-1}^1 dt w(t) |iu'(t) - a(\cos \omega t)u(t)|^2,$$

where $w(t) = \sqrt{1-t^2}$, and $u \in H_w^1(-1, 1)$ means that $\int_{-1}^1 dt w(t) (|u(t)|^2 + |u'(t)|^2) < \infty$. For convenience, we extended the problem to the whole time interval $(-1, 1)$, since it is the natural domain for the Chebyshev polynomials. The alternative would be to rescale the problem posed on $(0, 1)$ to obtain a new problem posed on $(-1, 1)$. In this case, the error estimate

$$\|u - u^*\|_{C^0(-1,1)} \leq \sqrt{2E_w(u)}$$

does not hold on $(-1, 1)$, but it can be replaced in this case by the similar estimate

$$(A.4) \quad \|u - u^*\|_{C^0((-1,1))} \leq \sqrt{2\pi E_w(u)}$$

obtained as follows : for any $u \in H_w^1(-1, 1)$, and any $0 \leq t < 1$,

$$\begin{aligned} |u(t)|^2 &= |u(0)|^2 + 2 \int_0^t ds \Im \left(\overline{(iu'(s) - a(\cos \omega s)u(s))} u(s) \right) \\ &\leq |u(0)|^2 + 2 \int_0^t ds |iu'(s) - a(\cos \omega s)u(s)| |u(s)| \\ &\leq |u(0)|^2 + 2 \left(\sup_{0 \leq s \leq t} |u(s)| \right) \left(\int_0^1 \frac{ds}{w(s)} \right)^{\frac{1}{2}} \left(\int_0^t ds w(s) |iu'(s) - a(\cos \omega s)u(s)|^2 \right)^{\frac{1}{2}} \\ &\leq |u(0)|^2 + \frac{1}{2} \sup_{0 \leq s \leq t} |u(s)|^2 + 2 \underbrace{\left(\int_0^1 \frac{ds}{w(s)} \right)}_{=\frac{\pi}{2}} \left(\int_0^t ds w(s) |iu'(s) - a(\cos \omega s)u(s)|^2 \right). \end{aligned}$$

Since a similar estimate can be obtained for $-1 < t \leq 0$, the result follows.

We introduce $(T_k)_{k \geq 0}$ and $(U_k)_{k \geq 0}$ the Chebyshev polynomials of the first and second kind respectively. We recall in particular the orthogonality relation:

$$(A.5) \quad \forall k, l, \quad \int_{-1}^1 dt w(t) U_k(t) U_\ell(t) = \delta_{k\ell} \frac{\pi}{2}$$

Fix some $K \geq 0$ and consider the discrete space

$$X^K = \left\{ u(t) = \sum_{k=0}^{K-1} u_k T_k(t) : \mathbf{u} := (u_k)_{k=0}^{K-1} \subset \mathbb{C} \right\} \subset H_w^1(-1, 1).$$

For any $u \in X^K$ and associated coordinates $\mathbf{u} = (u_k)_{k=0}^{K-1} \in \mathbb{C}^K$, we wish to compute $u(0)$ and an approximation of $iu'(t) - a(\cos \omega t)u(t)$ of the form $g(t) = \sum_{\ell=0}^{L-1} g_\ell U_\ell(t)$ for some $L \geq K$ and coefficients $(g_\ell)_{\ell=0}^{L-1} \in \mathbb{C}^L$.

- For $u(0)$, we can simply write

$$u(0) = \sum_{k=0}^{K-1} u_k T_k(0),$$

which motivates the introduction of the vector

$$(A.6) \quad \mathcal{J}^K = (T_0(0) \quad T_1(0) \quad \dots \quad T_{K-1}(0)) \in \mathbb{R}^{1 \times K},$$

so that $u(0) = \mathcal{J}^K \mathbf{u}$.

- Define

$$(A.7) \quad \mathcal{P}^{L,K} = \begin{pmatrix} I_K \\ 0_{(L-K) \times K} \end{pmatrix}$$

the extension operator where I_K is the $K \times K$ identity matrix, and $0_{(L-K) \times K}$ the $(L-K) \times K$ null matrix.

- The term $iu'(t)$ is easy to compute because of the identity $\forall k, T'_{k+1} = (k+1)U_k$. We define the corresponding matrix

$$(A.8) \quad \mathcal{D}^K = \begin{pmatrix} 0 & i & 0 & \dots & 0 \\ 0 & 0 & 2i & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & (K-1)i \\ 0 & 0 & 0 & \dots & 0 \end{pmatrix}.$$

- To approximate the term $a(\cos \omega t)u(t)$, we rely on the following method : let $\boldsymbol{\pi}^L : \mathbb{C}^L \mapsto \mathbb{C}^L$ be the ‘‘collocation operator with L points’’, that is,

$$(\boldsymbol{\pi}^L \mathbf{u})_\ell = \sum_{k=0}^{L-1} u_k T_k(x_\ell),$$

where $(x_\ell)_{\ell=0}^{L-1}$ are the Gauss-Chebyshev nodes. We know that there exist positive weights $(\mu_\ell)_{\ell=0}^{L-1}$ such that the quadrature formula

$$\int_{-1}^1 \frac{dt}{w(t)} P(t) \approx \sum_{\ell=0}^{L-1} \mu_\ell P(x_\ell),$$

is exact whenever P is a polynomial with degree $\leq 2L - 1$.

Let also \mathcal{A}^L be the operator $\mathbb{C}^L \rightarrow \mathbb{C}^L$ such that

$$\forall \mathbf{z} := (z_\ell)_{\ell=0}^{L-1}, \quad (\mathcal{A}^L \mathbf{z})_\ell = a(\cos \omega x_\ell) z_\ell$$

The last operation required is the transformation from the first-kind series to the second-kind series, which can be expressed in coordinates as follows thanks to the identities $\forall k \geq 2, T_k = \frac{U_k - U_{k-2}}{2}$, $T_1 = \frac{U_1}{2}$, and $T_0 = U_0$:

$$(A.9) \quad \mathbf{C}^L = \begin{pmatrix} 1 & 0 & -\frac{1}{2} & \dots & \dots & \dots & 0 \\ 0 & \frac{1}{2} & 0 & \ddots & & & 0 \\ 0 & 0 & \frac{1}{2} & \ddots & \ddots & & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & & \ddots & \ddots & -\frac{1}{2} \\ 0 & 0 & 0 & & & \ddots & 0 \\ 0 & 0 & 0 & \dots & \dots & \dots & \frac{1}{2} \end{pmatrix}.$$

The matrix of the quadratic part of (A.3) can therefore be written

$$(A.10) \quad \mathcal{Q}_{K,L} = \frac{\pi}{2} \left(\mathcal{P}^{L,K} \mathcal{D}^K - \mathbf{C}^L (\boldsymbol{\pi}^L)^{-1} \mathcal{A}^L \boldsymbol{\pi}^L \mathcal{P}^{K,L} \right)^* \left(\mathcal{P}^{L,K} \mathcal{D}^K - \mathbf{C}^L (\boldsymbol{\pi}^L)^{-1} \mathcal{A}^L \boldsymbol{\pi}^L \mathcal{P}^{K,L} \right) + (\mathcal{J}^K)^* \mathcal{J}^K$$

The only non explicit part of the above formula is the adjoint of $(\boldsymbol{\pi}^L)^{-1} \mathcal{A}^L \boldsymbol{\pi}^L$, which we compute as follows : Let $\mathbf{C} = \text{diag}(\frac{1}{2}, 1, \dots, 1) \in \mathbb{R}^{L \times L}$. Fix $\mathbf{u} = (u_\ell)_{\ell=0}^{L-1}$ and $\mathbf{v} = (v_\ell)_{\ell=0}^{L-1}$. Then

$$\begin{aligned} \sum_{\ell=0}^{L-1} \overline{((\boldsymbol{\pi}^L)^{-1} \mathcal{A}^L \boldsymbol{\pi}^L \mathbf{u})_\ell} v_\ell &= \frac{2}{\pi} \int \frac{dt}{w(t)} \overline{\left(\sum_{\ell=0}^{L-1} ((\boldsymbol{\pi}^L)^{-1} \mathcal{A}^L \boldsymbol{\pi}^L \mathbf{u})_\ell T_\ell(t) \right)} \left(\sum_{\ell=0}^{L-1} (\mathbf{C} \mathbf{v})_\ell T_\ell(t) \right) \\ &= \frac{2}{\pi} \sum_{\ell=0}^{L-1} \mu_\ell \overline{(\mathcal{A} \boldsymbol{\pi}^L \mathbf{u})_\ell} (\boldsymbol{\pi}^L \mathbf{C} \mathbf{v})_\ell = \frac{2}{\pi} \sum_{\ell=0}^{L-1} \mu_\ell a(\cos \omega x_\ell) \overline{(\boldsymbol{\pi}^L \mathbf{u})_\ell} (\boldsymbol{\pi}^L \mathbf{C} \mathbf{v})_\ell \\ &= \frac{2}{\pi} \sum_{\ell=0}^{L-1} \mu_\ell \overline{(\boldsymbol{\pi}^L \mathbf{u})_\ell} (\mathcal{A} \boldsymbol{\pi}^L \mathbf{C} \mathbf{v})_{T_k} \\ &= \frac{2}{\pi} \int \frac{dt}{w(t)} \overline{\left(\sum_{\ell=0}^{L-1} u_\ell T_\ell(t) \right)} \left(\sum_{\ell=0}^{L-1} ((\boldsymbol{\pi}^L)^{-1} \mathcal{A}^L \boldsymbol{\pi}^L \mathbf{C} \mathbf{v})_\ell T_\ell(t) \right) \\ &= \sum_{\ell=0}^{L-1} \overline{u_\ell} (\mathbf{C}^{-1} (\boldsymbol{\pi}^L)^{-1} \mathcal{A} \boldsymbol{\pi}^L \mathbf{C} \mathbf{v})_\ell, \end{aligned}$$

and the desired transpose is therefore $\mathbf{C}^{-1} (\boldsymbol{\pi}^L)^{-1} \mathcal{A} \boldsymbol{\pi}^L \mathbf{C}$. We therefore see that the minimization problem (A.3) is equivalent to the linear system

$$(A.11) \quad \mathcal{Q}_{K,L} \mathbf{u}_{K,L}^* = \eta_0 (\mathcal{J}^K)^*.$$

One may observe that computing $\mathcal{Q}_{K,L} \mathbf{u}$ using (A.10) only requires $\mathcal{O}(L \log L)$ operations, it is therefore tempting to try to solve (A.11) with an iterative method such as the conjugate gradient. However, it turns out that the matrix $\mathcal{Q}_{K,L}$ is in fact ill-conditioned, and the amount of iterations required to converge increases drastically with the size of K . This problem can be solved by introducing the matrix

$$(A.12) \quad \mathcal{Q}_K^0 = \frac{\pi}{2} (\mathcal{D}^K)^* \mathcal{D}^K + (\mathcal{J}^K)^* \mathcal{J}^K,$$

which is simply the matrix associated with the “free” quadratic form

$$|u(0)|^2 + \int_{-1}^1 dt w(t) |i\partial_t u|^2.$$

It turns out that the inverse of \mathcal{Q}_0 can be easily computed as follows : let $F \in \mathbb{R}^K$, then $\mathcal{Q}_0 u = F$ is equivalent to finding $u = \sum_{k=0}^K u_k T_k$ such that

$$\forall v = \sum_{k=0}^K v_k T_k, \quad \int_{-1}^1 dt w(t) (\overline{i\partial_t v})(i\partial_t u) + \overline{v(0)}u(0) = \langle v, F \rangle_{\mathbb{R}^{K+1}} = \sum_{k=0}^K \overline{v_k} F_k.$$

Taking $v = T_0$ yields $u(0) = F_0$, and then we obtain

$$\forall v = \sum_{k=0}^K k^2 v_k T_k, \quad \frac{\pi}{2} \sum_{k=1}^K \overline{v_k} u_k = \sum_{k=0}^K \overline{v_k} F_k - \left(\sum_{k=0}^K \overline{v_k} T_k(0) \right) F_0,$$

so we need to take

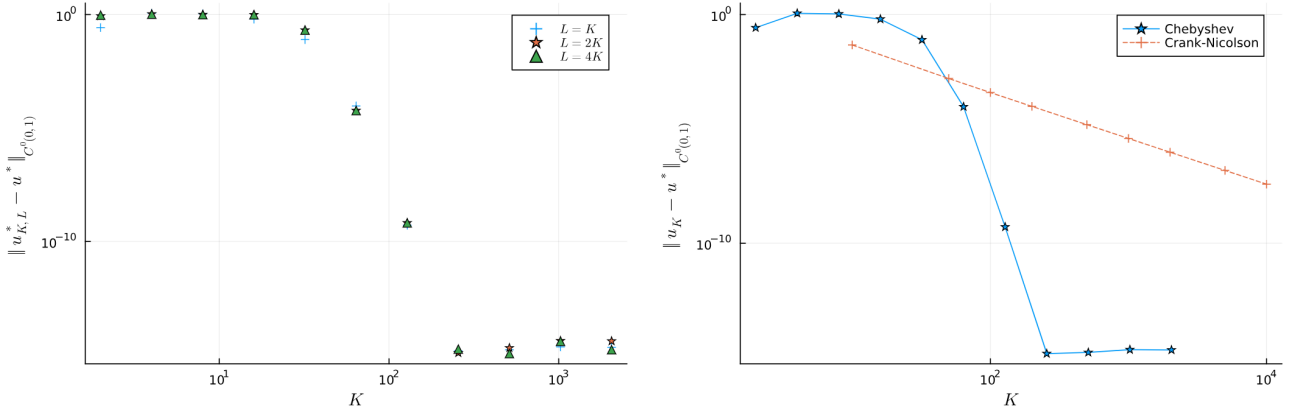
$$\forall 1 \leq k \leq K, \quad u_k = \frac{2}{\pi k^2} (F_k - T_k(0) F_0).$$

We then find u_0 thanks to the following equality :

$$F_0 = u(0) = \sum_{k=0}^K T_k(0) u_k.$$

Figure 1a shows $\|u_{K,L}^* - u^*\|_{C^0([0,1])}$, computed by sampling at 1000 uniformly distributed points as a function of K for different choices of L . Since taking $L > K$ does not seem to significantly improve the convergence, in what follows we always take $L = K$ and write $u_K^* := u_{K,K}^*$.

On Figure 1b, we display the difference with the exact solution computed at 1000 uniformly distributed points on the interval $[0, 1]$, and compare it with an order 2 Crank-Nicolson scheme as a function of K . For the the Crank-Nicolson scheme, K stands for the number of steps. As expected, the global in time Chebyshev approach exhibits spectral convergence, while the error evolves as K^{-2} (convergence of order 2) for the Crank-Nicolson scheme. A Crank-Nicolson scheme with K steps is cheaper than the procedure described above with K functions, therefore, a higher value of K does not necessarily mean that the computation is more expensive. The evolution of the computation time will be explored in the next example.



(a) $\|u_{K,L}^* - u^*\|_{C^0([0,1])}$ for different choices of L with $a = 5$ and $\omega = 20$

(b) $\|u_{K,L}^* - u^*\|_{C^0([0,1])}$ for a Crank-Nicolson scheme and the global in time Chebyshev approach

Fig. 1

A.2. Periodic Schrödinger equation. We consider the Schrödinger equation on the two-dimensional torus $\mathbb{T}^2 = (\mathbb{R}/\mathbb{Z})^2$, and on the time interval $(-\tau, \tau)$:

$$(A.13) \quad \begin{cases} i\partial_t u^* = (-\Delta_{x,y} + V(t))u^*, \\ u^*(0) = u_0, \end{cases}$$

where for all $t \in \mathbb{R}$ and $(x, y) \in \mathbb{T}^2$, $V(t, x, y) = \cos((2\pi(x - c_1t))) + \cos(2\pi(y - c_2t)) + \cos(2\pi(x - y))$. A simple rescaling of the time variable shows that we can instead solve the following equation on $(-1, 1)$

$$(A.14) \quad \begin{cases} i\partial_t u^* = \tau(-\Delta + V_\tau(t\tau))u^* \\ u^*(0) = u_0 \end{cases}$$

where $V_\tau(t, x, y) = V(t\tau, x, y)$.

The operator $-\Delta$ has a well-known diagonal structure with respect to the orthonormal system of Fourier modes $e_{k,l} = e^{2i\pi kx} e^{2i\pi ly}$, hence we will apply Theorem 3.7 and Corollary 3.8 with $H_0 = -\Delta$.

Define the discrete set

$$(A.15) \quad \Gamma_N = \text{span}\{e_{k,l}\}_{\substack{-N/2 \leq k < N/2 \\ -N/2 \leq l < N/2}} \subset L^2(\mathbb{T}^2),$$

and the orthogonal projector π_N on Γ_N . Since our goal here is to focus on the errors that arise from the time discretization, and not on the errors due to the truncation of the Fourier series, we will solve instead the “discrete” version of (A.13) that is well-posed in Γ_N ,

$$(A.16) \quad \begin{cases} i\partial_t u_N^* = \tau(-\Delta + \pi_N V_\tau \pi_N)u_N^*, \\ u_N^*(0) = \pi_N u_0 \in \Gamma_N. \end{cases}$$

Estimating the difference between the real solution u^* to (A.13) and the solution u_N^* to (A.16) is another problem that can be studied independently, but we do not consider it here.

We know from Corollary 3.8 that we can, instead of (A.16), solve the equivalent evolution equation

$$(A.17) \quad \begin{cases} i\partial_t v_N^* = \tau e^{-it\tau\Delta}(\pi_N V_\tau \pi_N) e^{it\tau\Delta} v_N^*, \\ v_N^*(0) = \pi_N u_0 \in \Gamma_N, \end{cases}$$

which is associated with the variational formulation

$$(A.18) \quad \min_{v \in H_w^1((-1,1), \Gamma_N)} \left(|v(0) - \pi_N u_0|^2 + \int_{-1}^1 dt w(t) |i\partial_t v - \tau e^{-it\tau\Delta}(\pi_N V_\tau \pi_N) e^{it\tau\Delta} v|^2 \right).$$

We define the discrete subspace

$$(A.19) \quad \Sigma_{K,N} := \left\{ \sum_{k=0}^{K-1} v_k U_k(t) : (v_k)_{k=0}^{K-1} \subset \Gamma_N \right\} \subset H_w^1((-1,1), L^2(\mathbb{T}^2)),$$

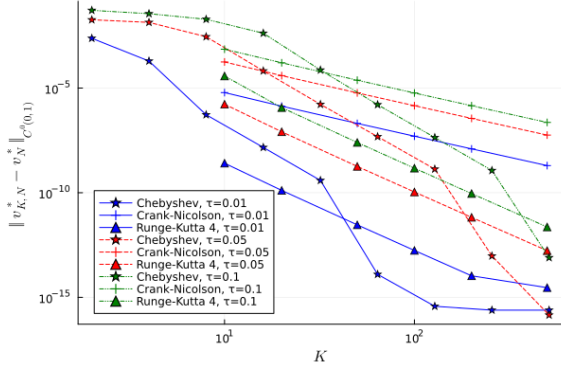
and the discrete solution $v_{K,N}^*$ as the unique solution to the restricted minimization problem

$$(A.20) \quad v_{K,N}^* = \underset{v \in \Sigma_{K,N}}{\text{argmin}} \left(|v(0) - \pi_N u_0|^2 + \int_{-1}^1 dt w(t) |i\partial_t v - \tau e^{-it\tau\Delta}(\pi_N V_\tau \pi_N) e^{it\tau\Delta} v|^2 \right).$$

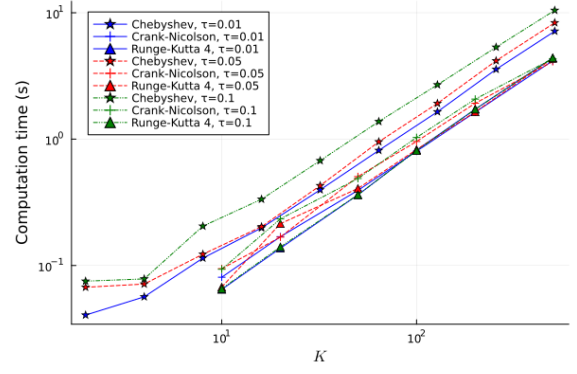
We employ a similar time discretization to that of Section A.1, and the matrix associated with the quadratic form is built similarly, except that it involves block entries instead of scalar entries. The difference between the computed solution $v_{K,N}^*$ and u_N^* is displayed in Figure 2a for several values of τ and $N = 64$. We compare it with an order 2 Crank-Nicolson scheme, and an order 4 Runge-Kutta scheme. As in the previous example, we observe a very fast convergence once K reaches a certain threshold. Although the global space-time Chebyshev approach does not necessarily outperform classical time stepping scheme, it seems more efficient to reach very high precision when enough regularity is available, which is an expected behavior for a spectral method. On Figure 2b, we display the computation time for several values of K . We observe that the computational cost of the Chebyshev for a given value of K has the same order of magnitude as the time-stepping schemes. The fact that it increases with τ is a consequence of the loss of quality of the preconditioner which leads to more iterations of the conjugate gradient algorithm used to solve the problem. Indeed, a smaller τ means that the equation is closer to the free dynamics that we use as a preconditioner. Finally, Figure 2c displays the errors of the different methods with respect to the computation cost. Since the computational cost of the different methods are very close, Figure 2c looks very much like Figure 1b with some corrections, and the same observations can be made.

Appendix B. Weak solutions to the Schrödinger equation.

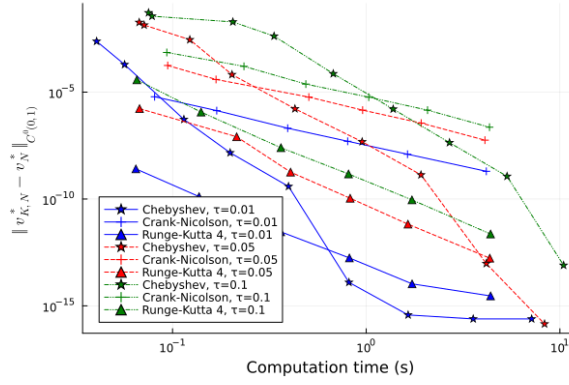
In this section we recall essential properties of weak solutions as defined in Definition 2.1. While the rest of the paper only mentioned the case of a time interval $I = (0, T)$, we consider here a general (possibly unbounded, unless stated otherwise) open time interval $J \subset \mathbb{R}$ and we assume that $0 \in \bar{J}$. We recall the definition of weak solutions in this context (see also Definition 2.1):



(a) $\|v_{K,N}^* - v_N^*\|_{C^0((-1,1))}$ for a Crank-Nicolson scheme, an order 4 Runge-Kutta scheme, and the global in time Chebyshev approach, for $N = 64$



(b) Computation time for a Crank-Nicolson scheme, an order 4 Runge-Kutta scheme, and the global in time Chebyshev approach, for $N = 64$



(c) $\|v_{K,N}^* - v_N^*\|_{C^0((-1,1))}$ with respect to computation time for a Crank-Nicolson scheme, an order 4 Runge-Kutta scheme, and the global in time Chebyshev approach, for $N = 64$

Fig. 2

DEFINITION B.1. Let $u, f \in L^2(J, \mathcal{H})$. We say that $(i\partial_t - H - B(t))u = f$ holds weakly if and only if

$$(B.1) \quad \forall \varphi \in \mathcal{C}_c^0(J, D(H)) \cap \mathcal{C}_c^1(J, \mathcal{H}), \quad (u | (i\partial_t - H)\varphi)_{L^2(J, \mathcal{H})} = (f | \varphi)_{L^2(J, \mathcal{H})},$$

where $D(H)$ is equipped with the graph norm of H .

We first deal with the case $B(t) = 0$.

PROPOSITION B.2. Let $u \in L^2(J, \mathcal{H})$, and $v = e^{itH} u$. The following are equivalent :

1. $(i\partial_t - H)u \in L^2(J, \mathcal{H})$.
2. $i\partial_t v \in L^2(J, \mathcal{H})$.

In particular, if 1. and 2. hold, u and v both belong to $\mathcal{C}^0(J, \mathcal{H})$. Moreover, in this case, $i\partial_t v = e^{itH}(i\partial_t - H)u$, and

$$(B.2) \quad \forall t \in J, \quad u(t) = e^{-itH} u(0) - i \int_0^t ds e^{-i(t-s)H} (i\partial_t - H)u(s).$$

Proof. Assume $(i\partial_t - H)u = f \in L^2(J, \mathcal{H})$, then, for any $\varphi \in \mathcal{C}_c^\infty(J, D(H^2))$,

$$(v | i\partial_t \varphi)_{L^2(J, \mathcal{H})} = (u | e^{-itH} i\partial_t \varphi)_{L^2(J, \mathcal{H})} = (u | (i\partial_t - H) e^{-itH} i\partial_t \varphi)_{L^2(J, \mathcal{H})} = (f | e^{-itH} \varphi)_{L^2(J, \mathcal{H})}.$$

By density, this identity extends to all $\varphi \in \mathcal{C}_c^1(J, \mathcal{H})$, and we conclude that $v \in H^1(J, \mathcal{H})$ with $i\partial_t v = e^{itH} f$. Conversely, assume $i\partial_t v = g \in L^2(J, \mathcal{H})$. Then for any $\varphi \in \mathcal{C}_c^\infty(J, D(H^2))$,

$$(u | (i\partial_t - H)\varphi)_{L^2(J, \mathcal{H})} = (v | e^{itH} (i\partial_t - H)\varphi)_{L^2(J, \mathcal{H})} = (v | i\partial_t e^{itH} \varphi)_{L^2(J, \mathcal{H})} = (g | e^{itH} \varphi)_{L^2(J, \mathcal{H})}.$$

By density, the identity extends to all $\varphi \in \mathcal{C}_c^0(J, D(H)) \cap \mathcal{C}_c^1(J, \mathcal{H})$, so $(i\partial_t - H)u = e^{-itH} g \in L^2(J, \mathcal{H})$. Moreover, we then have for all $t \in J$

$$\begin{aligned} u(t) &= e^{-itH} v(t) = e^{-itH} (v(0) - i \int_0^t ds g(s)) \\ &= e^{-itH} u(0) - i \int_0^t ds e^{-i(t-s)H} (i\partial_t - H)u(s). \end{aligned} \quad \square$$

COROLLARY B.3. *For any $f \in L^2(J, \mathcal{H})$ and $u_0 \in \mathcal{H}$, there exists exactly one $u^* \in L^2(J, \mathcal{H})$ such that $(i\partial_t - H)u^* = f$ and $u^*(0) = u_0$.*

Proof. Existence: Let $f \in L^2(J, \mathcal{H})$. Define

$$v^*(t) = u_0 - i \int_0^t ds e^{isH} f(s),$$

and $u^* = e^{-itH} v^*$. Then, by Proposition B.2, $(i\partial_t - H)u^* = e^{-itH} e^{itH} i\partial_t v^* = f$, and $u^*(0) = u_0$.

Uniqueness: Assume $(i\partial_t - H)u_1^* = (i\partial_t - H)u_2^* = f \in L^2(J, \mathcal{H})$ and $u_1^*(0) = u_2^*(0) = u_0$. Define $v_j^* = e^{itH} u_j^*$ ($j = 1, 2$), we then have $\partial_t v_1^* = \partial_t v_2^*$. Since $v_1^*(0) = v_2^*(0) = u_0$, uniqueness follows. \square

We now add a time-dependent part $B(t)$, assumed to be a strongly continuous family of uniformly bounded self-adjoint operators (that is, for any $t \in J$, $B(t)$ is a bounded self-adjoint operator, and $\sup_{t \in J} \|B(t)\| < \infty$).

PROPOSITION B.4. *Assume J is **bounded**. For any $f \in L^2(J, \mathcal{H})$ and $u_0 \in \mathcal{H}$ there exist a unique $u^* \in L^2(J, \mathcal{H})$ such that $(i\partial_t - H - B(t))u^* = f$ and $u(0) = u_0$. Furthermore, the following continuity estimate holds:*

$$(B.3) \quad \|u^*\|_{\mathcal{C}^0(J, \mathcal{H})} \leq \sqrt{2} \left(|u_0|^2 + T \|f\|_{L^2(J, \mathcal{H})}^2 \right)^{\frac{1}{2}}$$

Proof. The result is proved by a standard fixed-point argument for ODEs. For simplicity, we assume here $J = (0, T)$ for some $T > 0$. The extension to negative times is straightforward. Set

$$M = \sup_{t \in J} \|B(s)\|.$$

We also define, for $\mu > 0$,

$$\forall u \in L^2(J, \mathcal{H}), \quad \|u\|'_{L^2(J, \mathcal{H})} = \left(\int_0^T dt e^{-\mu t} |u(t)|^2 \right)^{\frac{1}{2}},$$

which is a norm on $L^2(J, \mathcal{H})$ equivalent to $\|\cdot\|_{L^2(J, \mathcal{H})}$.

For any $u \in L^2(J, \mathcal{H})$ and $t \in J$, set

$$\Phi(u)(t) = e^{-itH} u_0 - i \int_0^t ds e^{-i(t-s)H} (f(s) - B(s)u(s)).$$

Clearly $\Phi(u) \in L^2(J, \mathcal{H})$, and for any $u, v \in L^2(J, \mathcal{H})$,

$$\begin{aligned} \|\Phi(u) - \Phi(v)\|'_{L^2(J, \mathcal{H})}^2 &= \int_0^T dt e^{-\mu t} \left| \int_0^t ds e^{-i(t-s)H} B(s)(v(s) - u(s)) \right|^2 \\ &\leq M^2 T \int_0^T dt e^{-\mu t} \int_0^T ds |u(s) - v(s)|^2 \\ &\leq M^2 T \int_0^T ds |u(s) - v(s)|^2 \int_s^\infty dt e^{-\mu t} \\ &\leq \frac{M^2 T}{\mu} \int_0^T ds e^{-\mu s} |u(s) - v(s)|^2. \end{aligned}$$

Choosing μ such that $\frac{M^2 T}{\mu} < 1$, this proves that Φ is contractive for $\|\cdot\|'_{L^2(J, \mathcal{H})}$, hence admits a unique fixed point u^* which satisfies for all $t \in \mathcal{H}$

$$(B.4) \quad u^*(t) = e^{-itH} u_0 - i \int_0^t ds e^{-i(t-s)H} (f(s) - B(s)u^*(s)),$$

which, by Proposition B.2, is equivalent to $(i\partial_t - H - B(t))u = f$ and $u(0) = u_0$.

To prove the continuity estimate, we first assume $f \in C^0(J, \mathcal{H})$, and write for any $t \in J$

$$|u^*(t)|^2 = \left| u_0 - i \int_0^t ds e^{isH} (f(s) - B(s)u^*(s)) \right|^2,$$

from which we deduce

$$\begin{aligned} \frac{d}{dt} |u^*(t)|^2 &= 2\Re \langle u_0 - i \int_0^t ds e^{isH} (f(s) - B(s)u^*(s)), -i e^{itH} (f(t) - B(t)u^*(t)) \rangle \\ &= 2\Im \langle u^*(t), f(t) - B(t)u^*(t) \rangle = 2\Im \langle u^*(t), f(t) \rangle. \end{aligned}$$

This yields

$$\forall t \in J, \quad \left| \frac{d}{dt} |u^*(t)|^2 \right| \leq 2 |u^*(t)| |f(t)|.$$

Let $\varepsilon > 0$ and $w_\varepsilon(t) = \varepsilon + |u_0| + \int_0^t ds |f(s)|$. Let $K_\varepsilon = \{w_\varepsilon \geq |u^*|\} \subset \bar{J}$, which is closed (by continuity of w and u^*) and contains 0. Now assume $t_0 := \inf \bar{J} \setminus K_\varepsilon < T$. By continuity, it holds $|u^*(t_0)| = w(t_0) \geq \varepsilon > 0$, and there exists a $\delta > 0$ such that $[t_0, t_0 + \delta] \subset J$ and $|u^*(t)|$ for every $t \in [t_0, t_0 + \delta]$. Therefore,

$$\forall t \in [t_0 - \delta, t_0 + \delta], \quad 2 |u^*(t)| \frac{d}{dt} |u^*(t)| = \frac{d}{dt} |u^*(t)|^2 \leq 2 |f(t)| |u^*(t)|,$$

which yields

$$\forall t \in [t_0, t_0 + \delta], \quad \frac{d}{dt} |u^*(t)| \leq |f(t)|.$$

It follows by integration that

$$\forall t \in [t_0, t_0 + \delta], \quad |u^*(t)| \leq |u^*(t_0)| + \int_{t_0}^t ds |f(s)| = w(t),$$

which contradicts the definition of t_0 . Therefore,

$$\forall t \in \bar{J}, \quad |u^*(t)| \leq w_\varepsilon(t) \leq \varepsilon + |u_0| + \sqrt{T} \|f\|_{L^2(J, \mathcal{H})} \leq \varepsilon + \sqrt{2} \left(|u_0|^2 + T \|f\|_{L^2(J, \mathcal{H})}^2 \right)^{\frac{1}{2}}.$$

Since this holds for any $\varepsilon > 0$, we obtain the desired inequality.

For general $f \in L^2(J, \mathcal{H})$, we take a sequence $(f_n)_{n \geq 0}$ such that $\|f_n - f\|_{L^2(J, \mathcal{H})} \rightarrow 0$, and define u_n^* the unique element of $L^2(J, \mathcal{H})$ such that

$$(B.5) \quad u_n^*(t) = e^{-itH} u_0 - i \int_0^t ds e^{-i(t-s)H} (f_n(s) - B(s)u_n^*(s)).$$

As earlier, we compare u_n^* and u^* in term of $\|\cdot\|'_{L^2(J, \mathcal{H})}$, and obtain with (B.4) and (B.5)

$$\|u_n^* - u^*\|'_{L^2(J, \mathcal{H})}^2 \leq C \|f_n - f\|_{L^2(J, \mathcal{H})}^2 + \frac{M^2 T}{\mu} \|u_n^* - u^*\|'_{L^2(J, \mathcal{H})}^2,$$

yielding

$$\|u_n^* - u^*\|'_{L^2(J, \mathcal{H})} \leq C \|f_n - f\|_{L^2(J, \mathcal{H})},$$

for some constant $C > 0$. This proves that $u_n^* \rightarrow u^*$ in $L^2(J, \mathcal{H})$, and using (B.4) and (B.5) again we deduce that $u_n^* \rightarrow u^*$ in $C^0(J, \mathcal{H})$. The result appears by taking $n \rightarrow \infty$ in

$$\forall n \geq 0, \quad \|u_n^*\|_{C^0(J, \mathcal{H})} \leq \sqrt{2} \left(|u_0|^2 + T \|f_n\|_{L^2(J, \mathcal{H})}^2 \right)^{\frac{1}{2}}. \quad \square$$

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