New global space-time variational formulation for the time-dependent Schrödinger equation

Mi-Song Dupuy[3], Virginie Ehrlacher[1,2], Clément Guillot[1,2]

[1]Ecole des Ponts ParisTech

[2]INRIA Paris

[3]Sorbonne Université

École des Ponts ParisTech

MATHerials

Inria INVENTEURS DU MONDE NUMÉRIQUE

European Research Council
Established by the European Commission

Exploiting Algebraic and Geometric Structure in Time Integration methods, 3rd April 2024

Outline of the talk

1. Aim and motivation
2. Variational formulation of the time-dependent Schrödinger equation
3. Application to the many-body electronic Schrödinger problem
4. Global space-time discretization methods
5. Dynamical low-rank approximations
6. Summary

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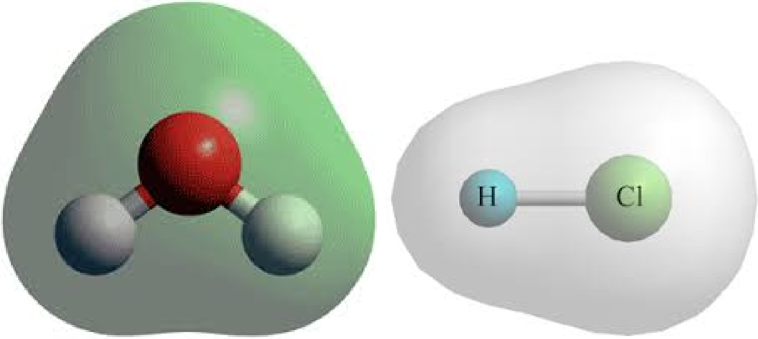
Motivation: electronic structure calculation for molecules



Computation of the **evolution in time of the state of the set of electrons** in a molecule: electrical, magnetical, optical properties...

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Let us consider a physical system composed of

- M nuclei, that are assumed to be (fixed) classical point charges, whose positions and electric charges are denoted by $R_1, \ldots, R_M \in \mathbb{R}^3$ and $Z_1, \ldots, Z_M \in \mathbb{N}^*$ respectively;

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- N electrons, considered as quantum particles: at time $t \in \mathbb{R}$, the state of the electrons is represented by a complex-valued function $\psi(t) : \mathbb{R}^{3N} \to \mathbb{C}$. The function $\psi(t)$ is called the **wavefunction** of the system of electrons at time $t \in \mathbb{R}$.

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Physical interpretation of the wavefunction:

For $x_1, \ldots, x_N \in \mathbb{R}^3$, the quantity $|\psi(t, x_1, \ldots, x_N)|^2$ represents the probability density at time t of the positions $x_1, \ldots, x_N$ of the N electrons.

For $B \subset \mathbb{R}^{3N}$,

$$\int_B |\psi(t, \cdot)|^2 : \text{ probability that the electrons are located in the set } B \text{ at time } t.$$

Time-dependent Schrödinger equation

$$\begin{cases} i\partial_t \psi(t) - H\psi(t) = 0, & t \in (0,T) \\ \psi(0) = \psi_0 \end{cases} \tag{1}$$

where the operator $H = H_0 + A$ is a self-adjoint operator on $\mathcal{H} = L^2(\mathbb{R}^{3N})$ with domain $D(H) = H^2(\mathbb{R}^{3N})$ called the **Hamiltonian** of the system of electrons and is given by

$$H_0 = -\Delta_{x_1,\dots,x_N} \quad \text{(kinetic energy)}$$

and

$$A = V(x_1,\dots,x_N) = \sum_{k=1}^{M}\sum_{i=1}^{N} \frac{-Z_k}{|x_i - R_k|} + \sum_{1\leqslant i<j\leqslant N} \frac{1}{|x_i - x_j|} \quad \text{(coulombic energy)}$$

Goal: quadratic variational formulation of the TD Schrödinger equation

Our aim here is to express equivalently the solution ψ of (7) as the solution of a variational problem of the form

$$\forall \varphi \in \mathcal{X}_H, \quad a(\psi, \varphi) = b(\varphi)$$

with

- $\mathcal{X}_H$ a Hilbert space of functions depending both on the time and space variable;
- $a : \mathcal{X}_H \times \mathcal{X}_H$ a continuous hermitian coercive sesquilinear form
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so that

$$\psi = \operatorname*{argmin}_{\varphi \in \mathcal{X}_H} \mathcal{E}(\varphi)$$

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There are several ways to do so!

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Two main interests/motivations:

- **global space-time Galerkin discretization** methods: given $\mathcal{X}_d \subset \mathcal{X}_H$ a finite-dimensional subspace of $\mathcal{X}_H$, compute $\psi_d \in \mathcal{X}_d$ solution to

$$\forall \varphi_d \in \mathcal{X}_d, \quad a(\psi_d, \varphi_d) = b(\varphi_d)$$

Cea's lemma: $\|\psi - \psi_d\|_{\mathcal{X}_H} \leqslant C \inf_{\varphi_d \in \mathcal{X}_d} \|\psi - \varphi_d\|_{\mathcal{X}_H}$

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- **dynamical low-rank approximations** well-defined on the whole time interval $(0, T)$ whatever the value of the final time T

References on global space-time discretization methods for TD Schrödinger equations

Petrov-Galerkin discretizations:

[Demkowicz et al., 2017], [Gomez, Moiola, 2022], [Gomez, Moiola, 2024], [Hain, Urban, 2022]

At least up to our knowledge, all restricted to

- bounded spatial domains;
- bounded/smooth interaction potentials.

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Notation and definition of weak solutions

- Let $\mathcal{H}$ be a Hilbert space equipped with a scalar product $\langle \cdot, \cdot \rangle$ and associated norm $|\cdot|$
- Let H be a self-adjoint operator on $\mathcal{H}$ with domain $D(H)$
- Let $I := (0, T)$ and consider the Bochner space $L^2(I; \mathcal{H})$

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For all $u_0 \in \mathcal{H}$ and $f \in L^2(I; \mathcal{H})$, consider $u^\star$ the unique weak solution to

$$\begin{cases} i\partial_t u^\star(t) - Hu^\star(t) = f(t), & t \in I, \\ u^\star(0) = u_0 \end{cases} \tag{2}$$

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Definition (Notion of weak solutions)

A function $u^\star \in L^2(I; \mathcal{H})$ is said to be a weak solution to (2) if and only if

(C1) $\forall v \in \mathcal{C}_c^0(I, D(H)) \cap \mathcal{C}_c^1(I, \mathcal{H})$,

$$(u^\star | (i\partial_t - H)v)_{L^2(I;\mathcal{H})} = (f|v)_{L^2(I;\mathcal{H})}$$

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Remark: Actually, (C1) implies that $u^\star \in \mathcal{C}^0(\bar{I}; \mathcal{H})$, which enables to give a meaning to (C2)

A first variational formulation (not useful)

Define

$$\mathcal{X}_H = \left\{ u^\star \in L^2(I;\mathcal{H}) : \ \exists (u_0, f) \in \mathcal{H} \times L^2(I;\mathcal{H}) \text{ such that } u^\star \text{ solves (2)} \right\}$$

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This space is a Hilbert space when equipped with the inner product

$$\forall u, v \in \mathcal{X}_H, \ (u,v)_{\mathcal{X}_H} = \langle u(0), v(0)\rangle + T((i\partial_t - H)u|(i\partial_t - H)v)_{L^2(I;\mathcal{H})} \tag{3}$$

The associated norm is then denoted by

$$\forall u \in \mathcal{X}_H, \ \|u\|_{\mathcal{X}_H} = \left(|u(0)|^2 + T\|(i\partial_t - H)u\|^2_{L^2(I,\mathcal{H})}\right)^{\frac{1}{2}} \tag{4}$$

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Equivalent formulation:

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Problem: what is the space $\mathcal{X}_H$?

First characterization of $\mathcal{X}_H$

Theorem

The application

$$\left\{ \begin{array}{ccc} L^2(I;\mathcal{H}) & \to & L^2(I;\mathcal{H}) \\ u & \mapsto & e^{itH} u \end{array} \right. \quad (5)$$

defines an isomorphism between $\mathcal{X}_H$ *and* $H^1(I;\mathcal{H})$.

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Problem again: the evolution group e^{-itH} is not easy to compute/characterize in general

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The proofs of the following results rely on **Kato's smoothing theory** *[Reed, Simon, 1978]*

Assumptions on H_0 and A

Assumptions (A):

(A1) The operator H_0 is a self-adjoint operator on $\mathcal{H}$ with domain $D(H_0)$

(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

$$\sup_{\lambda \in \mathbb{R}} \left\| A(H_0 - \lambda \pm i\varepsilon)^{-1} \right\| < 1 \quad (6)$$

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- *It holds that $\mathcal{X}_H = \mathcal{X}_{H_0}$*
- *There exist constant $\alpha, C > 0$ independent of T such that*

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

Consequence: second variational formulation

$$u^\star = \operatorname*{argmin}_{u \in \mathcal{X}_{H_0}} |u(0) - u_0|^2 + \|(i\partial_t - H_0 - A)u - f\|^2_{L^2(I;\mathcal{H})}$$

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$$v^\star = \operatorname*{argmin}_{v \in H^1(I;\mathcal{H})} |(e^{-itH_0} v)(0) - u_0|^2 + \left\|(i\partial_t - H_0 - A)(e^{-itH_0} v) - f\right\|^2_{L^2(I;\mathcal{H})}$$

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- $(e^{-itH_0} v)(0) = v(0)$
- since the evolution group e^{itH_0} is a unitary group, it holds that

$$\left\|(i\partial_t - H_0 - A)(e^{-itH_0} v) - f\right\|^2_{L^2(I;\mathcal{H})} = \left\|e^{itH_0}(i\partial_t - H_0 - A)(e^{-itH_0} v) - e^{itH_0} f\right\|^2_{L^2(I;\mathcal{H})}$$

Consequence: second variational formulation

$$u^\star = \underset{u \in \mathcal{X}_{H_0}}{\operatorname{argmin}} |u(0) - u_0|^2 + \|(i\partial_t - H_0 - A)u - f\|^2_{L^2(I;\mathcal{H})}$$

$$\mathcal{X}_{H_0} = \left\{ e^{-itH_0} v : \; v \in H^1(I;\mathcal{H}) \right\}$$

Let $v^\star \in H^1(I;\mathcal{H})$ such that $u^\star = e^{-itH_0} v^\star$. We then have

$$v^\star = \underset{v \in H^1(I;\mathcal{H})}{\operatorname{argmin}} |(e^{-itH_0} v)(0) - u_0|^2 + \left\|(i\partial_t - H_0 - A)(e^{-itH_0} v) - f\right\|^2_{L^2(I;\mathcal{H})}$$

- $(e^{-itH_0} v)(0) = v(0)$
- since the evolution group e^{itH_0} is a unitary group, it holds that

$$\left\|(i\partial_t - H_0 - A)(e^{-itH_0} v) - f\right\|^2_{L^2(I;\mathcal{H})} = \left\|e^{itH_0}(i\partial_t - H_0 - A)(e^{-itH_0} v) - e^{itH_0} f\right\|^2_{L^2(I;\mathcal{H})}$$

- for all $v \in H^1(I;\mathcal{H})$, $e^{itH_0}(i\partial_t)e^{-itH_0} v = e^{itH_0} e^{-itH_0}(H_0 + i\partial_t)v = (H_0 + i\partial_t)v$

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Consequence: second variational formulation

Theorem

Let H_0 and A be operators on $\mathcal{H}$ satisfying (A). Let $u_0 \in \mathcal{H}$ and $f \in L^2(I; \mathcal{H})$.

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Theorem

Let H_0 and A be operators on $\mathcal{H}$ satisfying (A). Let $u_0 \in \mathcal{H}$ and $f \in L^2(I;\mathcal{H})$. Then, the solution $u^\star$ to (2) *is given by $u^\star = e^{-itH_0} v^\star$ where $v^\star \in H^1(I;\mathcal{H})$ is the unique solution to*

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$$F(v) = |v(0) - u_0|^2 + T \left\| (i\partial_t - e^{itH_0} A e^{-itH_0}) v - e^{itH_0} f \right\|_{L^2(I;\mathcal{H})}$$

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Moreover, there exists $\alpha, C > 0$ independent on T such that

$$\forall v \in H^1(I;\mathcal{H}), \quad \frac{\alpha}{1+T} \|v - v^\star\|_{H^1(I;\mathcal{H})} \leqslant \sqrt{F(v)} \leqslant C(1+T)\|v - v^\star\|_{H^1(I;\mathcal{H})}$$

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Remark: We obtain a similar result in the case when $u^\star$ is the solution of a time-dependent Schrödinger equation of the form

$$\begin{cases} i\partial_t u^\star(t) - (H_0 + A + B(t))u^\star(t) = f(t), \quad t \in I, \\ u^\star(0) = u_0 \end{cases}$$

where $B : \overline{I} \ni t \mapsto B(t)$ is a strongly continuous family of **bounded** self-adjoint operators on $\mathcal{H}$.

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Many-body electronic Schrödinger problem

$$\begin{cases} i\partial_t \psi(t) - H\psi(t) = 0, & t \in (0, T) \\ \psi(0) = \psi_0 \end{cases} \tag{7}$$

where the operator $H = H_0 + A$ is a self-adjoint operator on $\mathcal{H} = L^2(\mathbb{R}^{3N})$ with domain $D(H) = H^2(\mathbb{R}^{3N})$ is given by

$$H_0 = -\Delta_{x_1,\dots,x_N} \quad \text{(kinetic energy)}$$

and

$$A = V(x_1, \dots, x_N) = \sum_{k=1}^{M} \sum_{i=1}^{N} \frac{-Z_k}{|x_i - R_k|} + \sum_{1 \leqslant i < j \leqslant N} \frac{1}{|x_i - x_j|} \quad \text{(coulombic energy)}$$

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Theorem

Let H_0 and A be operators on $\mathcal{H}$ satisfying (A1)-(A2).

Kato smoothing theory

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Let H_0 and A be operators on $\mathcal{H}$ satisfying (A1)-(A2).
Then, if

$$\sup_{\varphi\in\mathcal{H},\ |\varphi|=1} \int_{\mathbb{R}} dt |Ae^{-itH_0}\varphi|^2 < \infty,$$

then H_0 and A satisfy (A3).

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$$\sup_{\varphi \in L^2(\mathbb{R}^{3N}),\ \|\varphi\|_{L^2(\mathbb{R}^{3N})}=1} \int_{\mathbb{R}} dt \left\| Ve^{it\Delta}\varphi \right\|^2_{L^2(\mathbb{R}^{3N})} \leqslant 2\sqrt{\frac{2}{\pi}} \left(N \sum_{k=1}^{M} Z_k + \frac{N(N-1)}{2\sqrt{2}} \right) \tag{8}$$

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stems from **Kato-Yajima inequality**: *[Kato,Yajima,1989], [Burq, 2004]*

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Let $u_0 \in L^2(\mathbb{R}^{3N})$*. Let* ψ *be the solution to* (7)*, and* $v^\star := e^{-it\Delta}\psi$*.*

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Let $u_0 \in L^2(\mathbb{R}^{3N})$. Let ψ be the solution to (7), and $v^\star := e^{-it\Delta}\psi$.
Define for any $v \in H^1(I; L^2(\mathbb{R}^{3N}))$ the functional

$$F(v) = \|v(0) - u_0\|^2_{L^2(\mathbb{R}^{3N})} + T\left\|(i\partial_t - e^{-it\Delta}Ve^{it\Delta})v\right\|^2_{L^2(I,L^2(\mathbb{R}^{3N}))}. \quad (9)$$

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

$$\frac{\alpha}{1+T}\|v - v^\star\|_{H^1(I, L^2(\mathbb{R}^{3N}))} \leqslant \sqrt{F(v)} \leqslant C\sqrt{1+T}\,\|v - v^\star\|_{H^1(I, L^2(\mathbb{R}^{3N}))} \tag{10}$$

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4 Global space-time discretization methods

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Electronic many-body Schrödinger case

$$v^\star = \operatorname*{argmin}_{v \in H^1(I; L^2(\mathbb{R}^{3N}))} F(v)$$

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$$\|v^\star - v_d^\star\|_{H^1(I; L^2(\mathbb{R}^{3N}))} \leqslant C \inf_{v_d \in V_d} \|v^\star - v_d\|_{H^1(I; L^2(\mathbb{R}^{3N}))}$$

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Ongoing work:

- Hagedorn functions *[Lasser, Lubich, 2020]*
- Space-time wavelets (on-going work with Markus Bachmayr)

Preliminary results on a simpler test case

Periodic boundary conditions on $[0,1]^2$:

$$\begin{cases} i\partial_t u^\star = (-\Delta_{x,y} + V(t,x,y))u^\star, \\ u(0) = u_0, \end{cases} \tag{11}$$

with $V(t,x,y) = \cos(2\pi(x - c_1 t)) + \cos(2\pi(y - c_2 t)) + \cos(2\pi(x-y))$ for some constants $c_1, c_2 > 0$.

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- maximal degree of Tchebychev polynomials in the global space-time scheme
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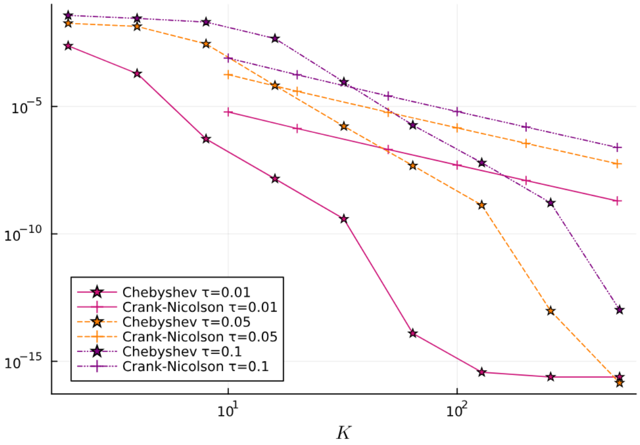
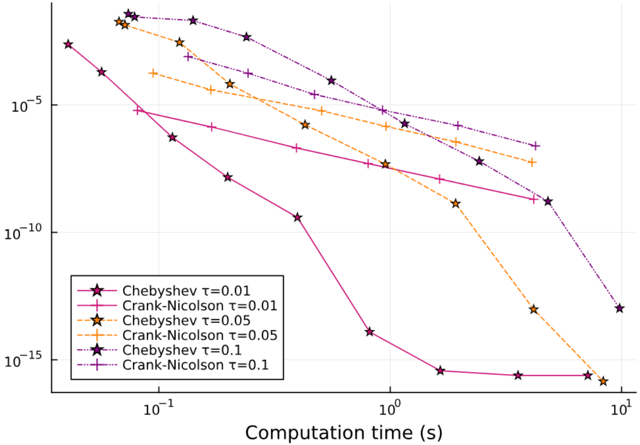
Time interval: $[-\tau, \tau]$

Error in $\| \cdot \|_{\mathcal{C}^0(I;L^2((0,1)^2))}$



Computational time



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1. Aim and motivation
2. Variational formulation of the time-dependent Schrödinger equation
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Low-rank tensor formats

Question: What can we do when N, the number of electrons is large?

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Let $\Sigma \subset \mathcal{H} = L^2(\mathbb{R}^{3N})$ be a susbet of functions of $x_1, \dots, x_N$ which can be represented in some low-rank tensor format (or more generally with low complexity).

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Examples:

- **Pure tensor products:** $\Sigma = \left\{ r_1(x_1) \dots r_N(x_N), \quad r_1, \dots, r_N \in L^2(\mathbb{R}^3) \right\}$ (with antisymmetry: set of Slater determinants)
- **Tucker format** (with antisymmetry: Multi Configuration Self Consistent Field)
- **Tensor Train format**, **Hierarchical Tree format**

Ceruti, Dolgov, Dupuy, Grigori, Hackbusch, Kressner, Khoromskij, Lasser, Lombardi, Lubich, Oseledets, Schneider, Uschmajew,...

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Dynamical low-rank approximation: The aim is to compute an approximation $\widetilde{u}$ of $u^\star$ (or ψ) such that $\widetilde{u}(t) \in \Sigma$ for all t.

Dirac-Frenkel variational principle

Find $\widetilde{u}$ such that for almost all t,

$$\langle (i\partial_t - H)\widetilde{u}(t), \delta\widetilde{u}\rangle = \langle f(t), \delta\widetilde{u}\rangle, \quad \forall \delta\widetilde{u} \in T_{\widetilde{u}(t)}\Sigma, \tag{12}$$

where $T_{\widetilde{u}(t)}\Sigma$ is the tangent space to Σ at point $\widetilde{u}(t)$.

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where $T_{\widetilde{u}(t)}\Sigma$ is the tangent space to Σ at point $\widetilde{u}(t)$.

In general, except in some particular situations, one can only obtain **the local existence in time** of a solution $\widetilde{u}$ to (12).

Alternative variational principle?

Very nice property: $e^{it\Delta}$ is a pure tensor product of operators:

$$e^{it\Delta_{x_1,\dots,x_N}} = e^{it\Delta_{x_1}} \otimes \dots \otimes e^{it\Delta_{x_N}}$$

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Rather look for $\widetilde{u} = e^{it\Delta}\widetilde{v}$ solution to

$$\widetilde{v} \in \underset{\widetilde{w}\in H^1(I;\Sigma)}{\operatorname{argmin}} F(\widetilde{w}) \tag{13}$$

Theorem

Let Σ be a weakly closed subset of $\mathcal{H}$. Then, $H^1(I;\Sigma)$ is a weakly closed subset of $H^1(I;\mathcal{H})$. Hence, there always exists at least one solution to (13).

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In principle, **global in time existence** of dynamical low-rank approximations.

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1. Aim and motivation
2. Variational formulation of the time-dependent Schrödinger equation
3. Application to the many-body electronic Schrödinger problem
4. Global space-time discretization methods
5. Dynamical low-rank approximations
6. Summary

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- **Open question**: how to impose norm conservation in this global space-time formulation?
  Not completely obvious...

Thank you for your attention!