3.4.3 Time Propagation of the Semi-Discrete Problem: Variational Splitting

Consider one time step $u_0 \mapsto S_{\Delta t}(u_0) =: u_1$ which is split into the three following substeps:

1) Compute $u_-^{1/2} \in \mathcal{M}$ as the solution at time $\frac{\Delta t}{2}$ of the variational principle
   Compute $\dot{u} \in T_u \mathcal{M}$ s.t.
   $$\langle v \,|\, \dot{u} - \tfrac{1}{i} T u \rangle = 0 \quad \forall v \in T_u \mathcal{M} \qquad (1)$$
   with initial value $u(0) = u_0$
2) Compute $u_+^{1/2} \in \mathcal{M}$ as the solution at time Δt of the variational principle
   Compute $\dot{u} \in T_u \mathcal{M}$ s.t.
   $$\langle v \,|\, \dot{u} - \tfrac{1}{i} V u \rangle = 0 \quad \forall v \in T_u \mathcal{M}$$
   with initial value $u(0) = u_-^{1/2}$.
3) Compute $u_1 \in \mathcal{M}$ as the solution at time Δt of the variational principle (1) with initial value $u(\frac{\Delta t}{2}) = u_+^{1/2}$.

Remarks:

1) The procedure was first proposed in [34].
The analysis given in [34] applies to bounded potentials and will be outlined below.

2) If $u_0 \in \mathcal{M}$, then (1) decouples into linear free Schrödinger equations
$$i\dot{\phi}_{j_k}^{(k)} = T\phi_{j_k}^{(k)}, \quad j_k = 1,\dots,N_k, \; k=1,\dots,f.$$
Numerical methods for these problems will be discussed later in this course.

3) Thus, with the gauging from p. 48, the subproblems correspond with those resulting from the classical Strang splitting into the vector fields (we write $\hat{H} := \hat{T} + \hat{V}$)
$$\hat{T} := -i(0, T)^T, \quad \hat{V} := -i(\mathcal{A}_V, B_V)^T$$

4) The advantage of the splitting is the following: The kinetic part $\hat{T}$ is associated with fast-varying solutions requiring small time steps, while $\hat{V}$ comprises the computationally expensive meanfield integrals.

3.4.4 The Calculus of Lie Derivatives

This is a convenient formalism with suggestive notation, to write the flow of a PDE in formal analogy to the fundamental matrix for linear ODEs!

F ... vector field on $\mathcal{M}$

$$\mathcal{M} \ni u \mapsto F(u) \in T_u\mathcal{M}$$

(e.g., $F = \hat{T}, \hat{V}, \hat{H} \in T_u\mathcal{M}$, since $\dot{u} = \mathcal{J}(u) H u$)

φ_F^t ... flow of the differential equation $\dot{u} = F(u)$ on $\mathcal{M}$

$\varphi_F^t(v)$ ... solution of $\dot{u} = F(u), u(0) = v$ at t.

G ... another vector field on $\mathcal{M}$

$D_F G$ ... Lie derivative,

$$(D_F G)(v) = \frac{d}{dt}\Big|_{t=0} G(\varphi_F^t(v)) = G'(v)F(v).$$

Write

$$[\exp(tD_F)G](v) = G(\varphi_F^t(v)).$$

For example, $G = \mathrm{Id}$ reproduces the exact flow as

$$\exp(tD_F)\,\mathrm{Id}(v) = \varphi_F^t(v).$$

Properties: •) $\frac{d}{dt}\exp(tD_F)G(v) = (\exp(tD_F)D_F G)(v) =$

$$= (D_F \exp(tD_F) G)(v)$$

•) Commutator $[D_F, D_G] := D_F D_G - D_G D_F$: $[D_F, D_G] = D_{[G,F]}$

3.4.5 Error Analysis for Variational Splitting

We make the following assumptions:

1) $e^{-itT} u \in \mathcal{M}$ for $u \in \mathcal{M}$, $t \in \mathbb{R}$

$\iff Tu \in \mathcal{T}_u \mathcal{M}$ for $u \in \mathcal{M} \cap D(T)$.

2) $\|V\varphi\| \leq \beta \|\varphi\| \quad \forall \varphi \in \mathcal{H}$.

3) The manifold $\mathcal{M}$ satisfies curvature bounds, (similar to those proven in the finite-dimensional case for the dynamical low rank approximation of time dependent matrices)

$$\|(\mathcal{P}(u) - \mathcal{P}(v))\varphi\| \leq \varkappa \|u-v\| \|\varphi\| \qquad (1)$$

$$\|\mathcal{P}^{\perp}(v)(u-v)\| \leq \varkappa \|u-v\|^2, \qquad (2)$$

where $\mathcal{P}(u)$ is the orthogonal projection onto $\mathcal{T}_u \mathcal{M}$, $\mathcal{P}^{\perp} := I - \mathcal{P}$, for $u, v \in \mathcal{M}$, $\varphi \in \mathcal{H}$.

4) $\|[\hat{T}, \hat{V}](u)\| \leq c_1 \|u\|_{H^1}$

$\|[\hat{T}, [\hat{T}, \hat{V}]](u)\| \leq c_2 \|u\|_{H^2}$.

Remark: We will not prove the commutator bounds 4) on p. 58. However, note the formal computation

$$[\hat{T}, \hat{V}](u) = \hat{T}\,\hat{V}(u) - \hat{V}'(u)\hat{T}u \,, \quad \text{with}$$
$$\hat{V}'(u)\hat{T}u = \frac{d}{d\tau}\Big|_{\tau=0} \hat{V}(e^{\tau\hat{T}}u).$$

The commutator bounds become plausible when we look at the case where $\hat{V}$ is linear, e.g. a multiplication operator $\hat{V}: u \mapsto Vu$:

$$\left[\frac{d}{dx}, V(x)\right] u(x) = \frac{d}{dx}\big(V(x)u(x)\big) - V(x)\frac{d}{dx}u(x) =$$
$$= V'u + Vu' - Vu' = V'u$$
$$\left[\frac{d^2}{dx^2}, V(x)\right] u(x) = \frac{d^2}{dx^2}(Vu) - Vu'' = V''u + 2V'u' +$$
$$+ Vu'' - Vu'' = V''u + 2V'u'.$$

i.e., for $V \in C^2$ the commutators 4) do not depend on the highest derivatives of u!

We will prove the following convergence result:

<u>Theorem</u>: Under the conditions 1)–4) from p. 58, the error of the variational splitting method is bounded by

$$\| u_n - u(t_n) \| \le C(t_n) (\Delta t)^2 \max_{0 \le \tau \le t_n} \| u(\tau) \|_{H^2},$$

where $C(t_n)$ depends on β, c_1, c_2.

The proof proceeds by the classical recipe "consistency + stability $\Rightarrow$ convergence". Thus the following lemmas are proven:

<u>Lemma 1</u>: With the assumptions of the last theorem, the local error is bounded by $(C = C(\beta, c_1, c_2))$

$$\| u_1 - u(\Delta t) \| \le C (\Delta t)^3 \max_{0 \le \tau \le \Delta t} \| u(\tau) \|_{H^2}.$$

<u>Lemma 2</u>: Let $u_1 = S_{\Delta t}(u_0)$, $v_1 = S_{\Delta t}(v_0)$, $\|u_0\| = \|v_0\| = 1$, $\|u_0 - v_0\| \le c \Delta t$. Then

$$\| u_1 - v_1 \| \le e^{\gamma \Delta t} \| u_0 - v_0 \|,$$

$\gamma = \varkappa \delta + O(\Delta t)$, $\delta = \operatorname{dist}(V v_0, T_{v_0} \mathcal{M})$.

Noting

$$u_n - u(t_n) = \sum_{j=0}^{n-1} \left[S_{\Delta t}^{n-1-j} \left(S_{\Delta t}(u(t_j)) - S_{\Delta t}^{n-j-1} (u(t_{j+1})) \right) \right]$$

yields the proposition of the Theorem with $C(t) = \frac{e^{\gamma t} - 1}{\gamma} C$.

Proof of Lemma 1: For notational simplicity, we omit 'hats' in subscripts of Lie derivatives, i.e. $D_H \leftarrow D_{\hat{H}}$, $D_V \leftarrow D_{\hat{V}}$, $D_T \leftarrow D_{\hat{T}}$.

The nonlinear variation of constant formula ("Gröbner-Alexeev Lemma", [38]) yields

$$u(\Delta t) = \exp(\Delta t D_H) Id(u_0) =$$

$$= \exp(\Delta t D_T) Id(u_0) + \int_0^{\Delta t} \exp((\Delta t - s) D_H) D_V \exp(s D_T) Id(u_0)\, ds =$$

$$= \exp(\Delta t D_T) Id(u_0) + \int_0^{\Delta t} \exp((\Delta t - s) D_T) D_V \exp(s D_T) Id(u_0)\, ds + r_1,$$

$$r_1 = \int_0^{\Delta t}\int_0^{\Delta t - s} \exp((\Delta t - s - \sigma) D_H) D_V \exp(\sigma D_T) D_V \exp(s D_T) Id(u_0)\, d\sigma\, ds$$

It can be shown that $\|r_1\| \le C(\Delta t)^2$, $C = C(\beta)$.

On the other hand,

$$u_1 = \exp(\tfrac{1}{2}\Delta t D_T) \exp(\Delta t D_V) \exp(\tfrac{1}{2}\Delta t D_T) Id(u_0) =$$

$$= \exp(\Delta t D_T) Id(u_0) + \Delta t \exp(\tfrac{1}{2}\Delta t D_T) D_V \exp(\tfrac{1}{2}\Delta t D_T) Id(u_0) + r_2,$$

$$r_2 = (\Delta t)^2 \int_0^1 (1-\theta) \exp(\tfrac{1}{2}\Delta t D_T) \exp(\theta \Delta t D_V) D_V^2 \cdot \exp(\tfrac{1}{2}\Delta t D_T) Id(u_0)\, d\theta.$$

Also, $\|r_2\| \le C(\Delta t)^2$, $C = C(\beta)$.

Forming the difference of the former expressions,

$$u_1 - u(\Delta t) = \Delta t \left[\exp\left(\tfrac{1}{2}\Delta t D_T\right) D_V \exp\left(\tfrac{1}{2}\Delta t D_T\right) \mathrm{Id}(u_0) - \ldots\right.$$

$$- \int_0^{\Delta t} \exp((\Delta t - s) D_T) D_V \exp(s D_T) \mathrm{Id}(u_0)\, ds + r_2 - r_1 .$$

Thus, the principal error term corresponds with the quadrature error of the midpoint rule applied to the integral over $[0, \Delta t]$ of the function

$$f(s) := \exp((\Delta t - s) D_T) D_V \exp(s D_T) \mathrm{Id}(u_0) .$$

In "second order Peano form",

$$\Delta t\, f(\Delta t/2) - \int_0^{\Delta t} f(s)\, ds = (\Delta t)^3 \int_0^1 \varkappa_2(\sigma)\, f''(\sigma \Delta t)\, d\sigma ,$$

with the scalar, bounded "Peano kernel" $\varkappa_2$ of the midpoint rule. Rearranging, it follows

$$f''(s) = - \exp((\Delta t - s) D_T) [D_T, [D_T, D_V]] \exp(s D_T) \mathrm{Id}(u_0) =$$

$$= \exp((\Delta t - s) D_T) D_{[\hat{T}, [\hat{T}, \hat{V}]]} \exp(s D_T) \mathrm{Id}(u_0) =$$

$$= \exp(s \hat{T}) [\hat{T}, [\hat{T}, \hat{V}]] \left(\exp((\Delta t - s)\hat{T})\, u_0\right)$$

The commutator bound from Assumption 4) on p. 58 now implies $\|f''\| \leq \text{const} \|u\|_{H^2}$.

Moreover, it can be shown that $\|r_1 - r_2\| \leq C(\Delta t)^3$.

This completes the proof of Lemma 1.

Proof of Lemma 2 :

Noting that the substeps with T, given by the flow of the free Schrödinger equation $e^{-i\Delta t T}$, are propagated by a unitary group of operators (due to the Theorem of Stone), we need to show

$$\| \varphi_V^t(u_0) - \varphi_V^t(v_0) \| \leq e^{\gamma t} \| u_0 - v_0 \|.$$

Writing $u(t) = \varphi_V^t(u_0)$, $v(t) = \varphi_V^t(v_0)$ and recalling $u = P(u)u$ and $v = P(v)v$, we have

$$\dot{u} - \dot{v} = -i P(u) V P(u)(u-v) -$$
$$- i [P(u) V P(u) - P(v) V P(v)] v. \quad | \cdot (u-v)$$

$$\|u-v\| \frac{d}{dt} \|u-v\| = \mathrm{Re} \langle u-v | \dot{u} - \dot{v} \rangle =$$
$$= \mathrm{Re} \langle u-v | -i [P(u) V P(u) - P(v) V P(v)] v \rangle =$$
$$= \mathrm{Im} \langle u-v | P(u) V (P(u) - P(v)) v \rangle +$$
$$+ \mathrm{Im} \langle u-v | [P(u) - P(v)] P(v) V v \rangle +$$
$$+ \mathrm{Im} \langle u-v | [P(u) - P(v)] P^\perp(v) V v \rangle = I + II + III$$

To bound I, we write

$$[P(u) - P(v)] v = -[P^\perp(u) - P^\perp(v)] v = -P^\perp(u) v =$$
$$= P^\perp(u)(u-v).$$

(2) from p. 58 thus gives $|I| \leq \beta \varkappa \|u-v\|^3$

For estimating II, we write

$$\langle u-v \,|\, [P(u)-P(v)]\, P(v)V_v\rangle =$$

$$= -\langle u-v \,|\, [P^\perp(u)-P^\perp(v)]\, P(v)V_v\rangle =$$

$$= -\langle u-v \,|\, P^\perp(u) P(v)V_v\rangle =$$

$$= -\langle P^\perp(u)(u-v) \,|\, P^\perp(u) P(v)V_v\rangle =$$

$$= \langle P^\perp(u)(u-v) \,|\, [P(u)-P(v)]\, P(v)V_v\rangle .$$

With (1)-(2) on p. 58 it follows

$$|II| \le \beta\varkappa^2 \|u-v\|^3 .$$

Finally, from

$$\|P^\perp(v)V_v\| = \mathrm{dist}(V_v, T_v M) = \delta + O(\Delta t)$$

and (1) on p. 58 we have

$$|\underline{III}| \le \varkappa(\delta + O(\Delta t))\|u-v\|^2 .$$

Thus, as long as $\|u-v\| = O(\Delta t)$, we obtain

$$\frac{d}{dt}\|u-v\| \le (\varkappa\delta + O(\Delta t))\|u-v\| . \quad //$$