FORMULATION AND NUMERICAL SOLUTION OF QUANTUM CONTROL PROBLEMS
– ERRATA & ADDITIONS –

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1. Errata and additions

In this short note, we provide some errata and additions to the book "Formulation and Numerical Solution of Quantum Control Problems".
All the errata and additions are given in the following list.

(1) Page 57, The first paragraph should be extended as follows:
"A reasonable choice is to take ψ_j^0, $j = 1, \dots, N$, equal to the N orthogonal eigenfunctions of the eigenproblem (2.74) with the lowest energy. If the initial wavefunctions are chosen to be orthogonal, this property is preserved by the evolution given in (2.82) and Lemma 2.11 can be used to obtain the density as given in the last line of (2.82)."

(2) Page 130, we add the definition of Z and $Z_\star$:
We define the following spaces of functions of time and space with values in $\mathbb{C}^N$ and their norms:

$$
\begin{aligned}
&Y := L^2(0,T;L^2(\Omega;\mathbb{C}^N)), && \|u\|_Y^2 = \int_0^T \|u(t)\|_{L^2}^2 \mathrm{d}t,\\
&X := L^2(0,T;H_0^1(\Omega;\mathbb{C}^N)), && \|u\|_X^2 = \int_0^T \|u(t)\|_{H^1}^2 \mathrm{d}t,\\
&X^* = L^2(0,T;H^{-1}(\Omega;\mathbb{C}^N)), && \|u\|_{X^*} = \sup_{v\in X\setminus\{0\}} \frac{|u(v)|}{\|v\|_X},\\
&W := \{u \in X \text{ such that } u' \in X^*\}, && \|u\|_W^2 = \|u\|_X^2 + \|u'\|_{X^*}^2,\\
&Z_\star := L^\infty(0,T;H^2(\Omega;\mathbb{C}^N)\cap H_0^1(\Omega;\mathbb{C}^N)), && \|u\|_{Z_\star} = \operatorname*{ess\,sup}_{t\in[0,T]} \|u(t)\|_{H^2(\Omega;\mathbb{C}^N)},\\
&Z := \{u \in Z_\star \text{ such that } u' \in X^*\}, && \|u\|_Z^2 = \|u\|_{Z_\star}^2 + \|u'\|_{X^*}^2.
\end{aligned}
$$

Moreover, Assumption 2 has to be improved as follows.

- Assumption 2 (page 130): "We assume that the correlation potential V_c is continuous from $L^2(\Omega;\mathbb{C}^N)$ to $L^2(\Omega)$, and the map $\Psi \mapsto V_c(\Psi)\Psi$ is continuously real-Fréchet differentiable with bounded derivative from Z to Y."

(3) Page 131, in formula (3.131) the space W has to be replaced with Z. Moreover, the sentence after the formula has to be replaced with
"In what follows, we assume that $\Psi^0 \in H_0^1(\Omega;\mathbb{C}^N)\cap H^2(\Omega;\mathbb{C}^N)$."

(4) Page 132, Lemma 3.47 is wrong, should be removed. It is only used to prove Lemma 3.53; see page 135-136 for an amendment of this proof.

(5) Page 133, Lemma 3.49 has some typos in its statement and proof. It should be as follows.

Lemma 1 (Lemma 3.49)**.** *The exchange potential term $V_x(\Psi)\Psi$ is Lipschitz continuous, in the sense that there exist positive constants L and $\tilde{L}$ such that*

$$\|V_x(\Psi(t))\Psi(t) - V_x(\Upsilon(t))\Upsilon(t)\|_{L^2(\Omega;\mathbb{C}^N)} \leq L\|\Psi(t) - \Upsilon(t)\|_{L^2(\Omega;\mathbb{C}^N)}$$

and

$$\|V_x(\Psi)\Psi - V_x(\Upsilon)\Upsilon\|_{X^*} \leq \tilde{L}\|\Psi - \Upsilon\|_X.$$

Proof. The function $f : \mathbb{C}^N \to \mathbb{C}^N$, $f(z) = V_x(z)z$ is continuously differentiable with bounded derivative, hence Lipschitz continuous with Lipschitz constant $\tilde{L}$ from $\mathbb{C}^N$ to $\mathbb{C}^N$. Moreover, since $V_x(\Psi) \in L^\infty(0,T;L^\infty(\Omega;\mathbb{R}))$, we have that $V_x(\Psi)\Psi \in Y$. With this preparation, the Lipschitz continuity from L^2 to L^2 is obtained as follows

$$\int_\Omega |V_x(\Psi(x,t))\Psi(x,t) - V_x(\Upsilon(x,t))\Upsilon(x,t)|^2 \mathrm{d}x \le \int_\Omega L^2 |\Psi(x,t) - \Upsilon(x,t)|^2 \mathrm{d}x.$$

Similarly, the Lipschitz continuity from X to X^* is deduced as follows

$$\begin{aligned}
&\|V_x(\Psi)\Psi - V_x(\Upsilon)\Upsilon\|_{X^*}^2 \le C\|V_x(\Psi)\Psi - V_x(\Upsilon)\Upsilon\|_Y^2 \\
&= C\int_0^T \|V_x(\Psi(x,t))\Psi(x,t) - V_x(\Upsilon(x,t))\Upsilon(x,t)\|_{L^2(\Omega;\mathbb{C}^N)}^2 \mathrm{d}t \\
&\le C\int_0^T L^2\|\Psi(x,t) - \Upsilon(x,t)\|_{L^2(\Omega;\mathbb{C}^N)}^2 \mathrm{d}t = \tilde{L}^2\|\Psi - \Upsilon\|_Y^2 \le \tilde{L}^2\|\Psi - \Upsilon\|_X^2,
\end{aligned}$$

where we use the Gelfand triple $X \hookrightarrow Y \hookrightarrow X^*$. □

(6) Page 133, Definition 3.50, the sentence after the formulas should be:
"The space of real-linear maps from X to Y is a Banach space and is denoted by $\mathcal{L}(X,Y)$ in this section."

(7) Page 135, the statement of Lemma 3.53 slightly changes:

Lemma 2 (Lemma 3.53)**.** *The map $Z \ni \Psi \mapsto V_x(\Psi)\Psi \in Y$ is continuously real-Fréchet differentiable with derivative $\mathrm{D}(V_x(\Psi)\Psi) = A(\Psi)$, where $A(\Psi) \in \mathcal{L}(Z,Y)$ is given in Lemma 3.52.*

(8) Page 135–136. in the proof of Lemma 3.53:
- the first sentence has to be:
"We prove that the real-Gâteaux derivative $A(\Psi)$ of $V_x(\Psi)\Psi$ at Ψ is continuous from Z to $\mathcal{L}(Z,Y)$. Then the real-Fréchet differentiability follows immediately from [11,Proposition A.3]."
- the statement
"for all $\epsilon > 0$ $\exists\delta > 0$ such that $\|A(\Psi) - A(\Phi)\|_{\mathcal{L}(W,Y)} < \epsilon$ $\forall\|\Psi - \Phi\|_W < \delta$."
has to be replaced with
"$\forall\epsilon > 0$ $\exists\delta > 0$ s.t. $\|A(\Psi) - A(\Phi)\|_{\mathcal{L}(Z,Y)} < \epsilon$, $\forall\Psi,\Phi \in Z$ s.t. $\|\Psi - \Phi\|_Z < \delta$."
- On page 136, the first line should be "Together, we have Hölder continuity for all $\Psi \in Z$,"
- On page 136, some changes are required such that Lemma 3.47 is not used. In particular, the second part of the proof has to be updated as follows:

  "Define $Z_1 := L^\infty(0,T;H^2(\Omega;\mathbb{C}))$. Now, we turn our attention to $A_2(\Psi)$ and use the Hölder continuity of $\tilde{A}_2(\Psi)\psi_j\psi_m$ to obtain the following estimate. We have

$$\begin{aligned}
&\|A_2(\Psi)(\delta\Psi) - A_2(\Phi)(\delta\Psi)\|_Y^2 \\
&= \sum_{m=1}^N \int_0^T \int_\Omega \left| \tilde{A}_2(\Psi)\psi_m \sum_{j=1}^N (\psi_j\overline{\delta\psi_j} + \overline{\psi_j}\delta\psi_j) - \tilde{A}_2(\Phi)\phi_m \sum_{j=1}^N (\phi_j\overline{\delta\psi_j} + \overline{\phi_j}\delta\psi_j) \right|^2 \mathrm{d}x\mathrm{d}t \\
&\le \sum_{m=1}^N \int_0^T \int_\Omega \sum_{j=1}^N \left| \overline{\delta\psi_j}(\tilde{A}_2(\Psi)\psi_j\psi_m - \tilde{A}_2(\Phi)\phi_j\phi_m) \right|^2 \mathrm{d}x\mathrm{d}t \\
&\quad + \sum_{m=1}^N \int_0^T \int_\Omega \sum_{j=1}^N \left| \delta\psi_j(\tilde{A}_2(\Psi)\overline{\psi_j}\psi_m - \tilde{A}_2(\Phi)\overline{\phi_j}\phi_m) \right|^2 \mathrm{d}x\mathrm{d}t \\
&\le c\sum_{j=1}^N \|\delta\psi_j\|_{Z_1}^2 \sum_{m=1}^N \Big(\|\tilde{A}_2(\Psi)\psi_j\psi_m - \tilde{A}_2(\Phi)\phi_j\phi_m)\|_{Y_1}^2 + \|\tilde{A}_2(\Psi)\overline{\psi_j}\psi_m - \tilde{A}_2(\Phi)\overline{\phi_j}\phi_m\|_{Y_1}^2 \Big) \\
&\le c_1 \sum_{j=1}^N \|\delta\psi_j\|_{Z_1}^2 \sum_{m=1}^N \|\Psi - \Phi\|_Y^{2\alpha} \\
&= c'\|\delta\Psi\|_{Z_\star}^2 N\|\Psi - \Phi\|_Y^{2\alpha} < c'\|\delta\Psi\|_{Z_\star}^2 N\delta^{2\alpha}.
\end{aligned}$$

Furthermore, by the Hölder continuity of V_x and the embedding $Z \hookrightarrow Y$, we have

$$\begin{aligned}\|A_1(\Psi)(\delta\Psi) - A_1(\Phi)(\delta\Psi)\|_Y &\leq c_2\|A_1(\Psi) - A_1(\Phi)\|_{Y_1}\|\delta\Psi\|_{Z_\star}\\ &\leq c_3\|\Psi - \Phi\|_Y^{2/n}\|\delta\Psi\|_{Z_\star} \leq c''\delta^\alpha\|\delta\Psi\|_{Z_\star}.\end{aligned}$$

Now, we have the following:

$$\begin{aligned}\|A(\Psi) - A(\Phi)\|_{\mathcal{L}(Z,Y)} &= \sup_{\delta\Psi\in Z\setminus\{0\}} \frac{\|A(\Psi)(\delta\Psi) - A(\Phi)(\delta\Psi)\|_Y}{\|\delta\Psi\|_Z}\\ &\leq (\sqrt{c'N} + c'')\delta^\alpha \sup_{\delta\Psi\in Z\setminus\{0\}} \frac{\|\delta\Psi\|_{Z_\star}}{\|\delta\Psi\|_Z} \leq (\sqrt{c'N} + c'')\delta^\alpha =: \epsilon.\end{aligned}$$

This completes the proof of the continuous real-Fréchet differentiability of $V_x(\Psi)\Psi$."

(9) Page 137, proof of Lemma 3.54, in the last estimates a constant is missing. It should be

$$\begin{aligned}&\frac{\|V_H(\Psi+\delta\Psi)(\Psi+\delta\Psi) - V_H(\Psi)\Psi - \mathrm{D}(V_H(\Psi)\Psi)(\delta\Psi)\|_{X^*}^2}{\|\delta\Psi\|_W^2}\\ &\leq C\frac{\|V_H(\Psi+\delta\Psi)(\Psi+\delta\Psi) - V_H(\Psi)\Psi - \mathrm{D}(V_H(\Psi)\Psi)(\delta\Psi)\|_Y^2}{\|\delta\Psi\|_W^2}\\ &\leq \frac{C'}{\|\delta\Psi\|_W^2}\left(\int_0^T \|\delta\Psi\|_{L^2(\Omega;\mathbb{C}^N)}^2\|\Psi\|_{H^1(\Omega;\mathbb{C}^N)}^2\|\delta\Psi\|_{L^2(\Omega;\mathbb{C}^N)}^2\right.\\ &\left.+\|\delta\Psi\|_{L^2(\Omega;\mathbb{C}^N)}^2\|\delta\Psi\|_{H^1(\Omega;\mathbb{C}^N)}^2\|\Psi\|_{L^2(\Omega;\mathbb{C}^N)}^2 + \|\delta\Psi\|_{H^1(\Omega;\mathbb{C}^N)}^2\|\delta\Psi\|_{L^2(\Omega;\mathbb{C}^N)}^4\mathrm{d}t\right)\\ &\leq \frac{C'}{\|\delta\Psi\|_W^2}\left(\max_{0\leq t\leq T}\|\delta\Psi\|_{L^2(\Omega;\mathbb{C}^N)}^4\left(\|\Psi\|_X^2 + \|\delta\Psi\|_X^2\right)\right.\\ &\left.+\max_{0\leq t\leq T}\|\delta\Psi\|_{L^2(\Omega;\mathbb{C}^N)}^2\max_{0\leq t\leq T}\|\Psi\|_{L^2(\Omega;\mathbb{C}^N)}^2\|\delta\Psi\|_X^2\right)\\ &\leq C''\frac{\|\delta\Psi\|_W^4\left(\|\Psi\|_X^2 + \|\delta\Psi\|_X^2\right) + \|\delta\Psi\|_W^2\|\Psi\|_W^2\|\delta\Psi\|_X^2}{\|\delta\Psi\|_W^2}\\ &\leq C''\|\delta\Psi\|_W^2\left(\|\Psi\|_X^2 + \|\delta\Psi\|_X^2\right) + C''\|\delta\Psi\|_W^2\|\Psi\|_W^2 \to 0 \text{ for } \|\delta\Psi\|_W \to 0,\end{aligned}$$

for some positive constants C, C', and C''.

(10) Page 138, the following paragraph should be added to the remark at the beginning of the page

"Further, notice that using the embedding $Z \hookrightarrow W$, it follows that a function f that is real-Fréchet differentiability from W to Y at $a \in Z$ is also real-Fréchet differentiable from Z to Y at a as follows:"

$$\lim_{\|h\|_Z\to 0}\frac{\|f(a+h) - f(a) - Df(a)(h)\|_Y}{\|h\|_Z} \leq \lim_{\|h\|_Z\to 0}\frac{\|f(a+h) - f(a) - Df(a)(h)\|_Y}{\|h\|_W} = 0.$$

(11) Page 138, Theorem 3.55 has to be changed as follows:

Theorem 1 (Theorem 3.55)**.** *The map $c : Z \times H_0^1(0,T;\mathbb{R}) \to X^*$, defined in (3.135) is continuously real-Fréchet differentiable.*

Proof. In the first part of the proof we have shown that $\tilde{c} : W \times U \to X^*$ is Fréchet differentiable, and its derivative $\mathrm{D}\,\tilde{c}$ given by

$$\mathrm{D}\,\tilde{c}(\Psi,u)(\delta\Psi,\delta u) = \tilde{c}(\delta\Psi,u) - V_u\delta u\Psi = i\frac{\partial\delta\Psi}{\partial t} - \left(-\nabla^2 + V_0 + V_u u\right)\delta\Psi - V_u\delta u\Psi.$$

This derivative is continuous from $W \times U$ to X^*. By the remark on page 138 (see point 10) this means $\tilde{c}$ is continuously differentiable from $Z \times U$ to X^*.

Next, the exchange potential is continuously real-Fréchet differentiable from Z to Y by Lemma 3.53 (see point 7), the correlation potential from Z to Y by Assumption 2 in page 130 (modified as in point 2), and the Hartree potential from Z to Y by Lemma 3.54 and the remark on page 138 (see point 10). To summarize, we have the real-Fréchet derivative (3.137) in page 139.

□

(12) Page 139, Theorem 3.56 has to be changed as follows:

Theorem 2 (Theorem 3.56)**.** *The control to state map* $u \in H_0^1(0,T;\mathbb{R}) \mapsto \Psi(u) \in Z$ *is real-Fréchet differentiable.*

(13) Page 139, Theorem 3.57 has to be changed as follows:

Theorem 3 (Theorem 3.57)**.** *The cost functional* $J : Z \times U \to \mathbb{R}$ *defined in (3.130) is continuously real-Fréchet differentiable.*

In the proof, we notice that $J_\beta : Z \to \mathbb{R}$ is a well-defined quadratic functional and hence real-Fréchet differentiable. Moreover, it is proved that J_η is continuously real-Fréchet differentiable from W to $\mathbb{R}$. Therefore, by the remark on page 138 (see point 10), it is also continuously real-Fréchet differentiable from Z to $\mathbb{R}$.

(14) Page 142, proof of Theorem 3.60, the first estimate has to be replaced with

"Using $\|\Psi_n\|_{L^2} = 1$, the Lipschitz continuity of V_{xc}, and the estimates in [352, Lemma 2, Theorem 3], we obtain that

$$\|V_{ext}\Psi_n\|_Y \leq (\|u_n\|_{C[0,T]}\|V_u\|_{L^\infty(\Omega;\mathbb{C}^N)} + \|V_0\|_{L^\infty(\Omega;\mathbb{C}^N)})\|\Psi_n\|_Y,$$

$$\|V_{Hxc}(\Psi_n)\Psi_n\|_Y \leq (\max(L,\tilde{L}) + c\|\Psi_n\|_X^2)\|\Psi_n\|_Y,$$

which leads to the estimate

$$\left\|\Psi^0 - i\int_0^t g(s)\mathrm{d}s\right\|_{L^2(\Omega;\mathbb{C}^N)} \leq \|\Psi^0\|_{L^2(\Omega;\mathbb{C}^N)} + c\|g\|_Y \leq \|\Psi^0\|_{L^2(\Omega;\mathbb{C}^N)} + c\big(\|V_{ext}\Psi_n\|_Y + \|V_{Hxc}(\Psi_n)\Psi_n\|_Y\big) \leq C,$$

where c and C are positive constants."

(15) Page 144, the beginning of the proof of Lemma 3.61 has to be slightly changed as follows

"To show that the term $D_u\Psi(u)$ is well defined, we use the implicit function theorem, which ensures real-differentiability of the map $u \mapsto \Psi(u)$, $H^1(0,T;\mathbb{R}) \to Z$. To this end, we show that the real-Fréchet derivative $D_\Psi c(\Psi,u) : Z \to X^*$ is a bijection at any $(\Psi,u) \in Z \times H^1(0,T;\mathbb{R})$."

(16) Pages 146–147, in the statement of Theorem 3.63, the space of the local solution (Ψ,u) is $Z \times H^1(0,T;\mathbb{R})$.

(17) Page 147, formula (3.152a) has to be modified as follows

$$D_\Psi L(\Psi^\star, u^\star, \Lambda^\star) = 0 \text{ for all } \delta\Psi \in \{\Phi \in Z \,:\, \Phi(0) = 0\}.$$

(18) Page 147, in the proof of Theorem 3.64 the derivative of c has to be defined from $Z \times H^1(0,T;\mathbb{R})$ to X^*, that is $Dc(\Psi,u) : Z \times H^1(0,T;\mathbb{R}) \to X^*$.

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