ERRATA OF "A THEORETICAL INVESTIGATION OF TIME-DEPENDENT KOHN-SHAM EQUATIONS"

M. SPRENGEL*, G. CIARAMELLA†, AND A. BORZÌ‡

Abstract. The paper [3] (SIAM J. Math. Anal., 49 (2017), pp. 1681–1704.) contains wrong estimates concerning the solution to the given time-dependent Kohn-Sham equations. The correct statements, similar to [3], are given in this errata subject to slight partial modification of the assumptions. The proofs of these statements are given in [1].

Key words. Theory of PDEs, time-dependent Kohn-Sham equations, nonlinear Schrödinger equation, quantum optimal control

AMS subject classifications. 35Q93, 81Q99

1. Additional notation and assumptions. In this errata, we refer to [3] for notation and all definitions unless otherwise stated. Further, we consider the following additional Banach spaces and the corresponding norms

$$
\begin{aligned}
Z &:= H_0^1(\Omega;\mathbb{C}) \cap H^2(\Omega;\mathbb{C}), & \|\Phi\|_{H^2}^2 &:= \sum_{0\le|\boldsymbol{\alpha}|\le 2} \|\partial^{\boldsymbol{\alpha}}\Phi\|^2,\\
Y_{\infty,0} &:= L^\infty(0,T;L^2(\Omega;\mathbb{C})), & \|\Phi\|_{Y_{\infty,0}} &:= \operatorname{ess\,sup}_{t\in(0,T)}\|\Phi(t)\|,\\
Y_{\infty,1} &:= L^\infty(0,T;H^1(\Omega;\mathbb{C})), & \|\Phi\|_{Y_{\infty,1}} &:= \operatorname{ess\,sup}_{t\in(0,T)}\|\Phi(t)\|_{H^1},\\
\widehat{Y} &:= L^\infty(0,T;Z), & \|\Phi\|_{\widehat{Y}} &:= \operatorname{ess\,sup}_{t\in(0,T)}\|\Phi(t)\|_{H^2}.
\end{aligned}
$$

Moreover, we introduce the following changes to Assumptions 2 in [3]:

(a') The domain $\Omega \subset \mathbb{R}^3$ is bounded and $\partial\Omega \in C^{2,1}$;

(b') (replacing [3] Assumption 2 b–d) For every $\Phi \in Z$ it holds that $V_{xc}(\Phi)\Phi \in Z$ and there exist positive constants K and $\widetilde{K}$ such that

$$\|V_{xc}(\Phi)\Phi - V_{xc}(\Lambda)\Lambda\| \le K\|\Phi-\Lambda\|, \tag{1}$$

$$\|V_{xc}(\Phi)\Phi - V_{xc}(\Lambda)\Lambda\|_{H^2} \le \widetilde{K}\|\Phi-\Lambda\|_{H^2}, \tag{2}$$

for any $\Phi, \Lambda \in Z$;

(e') V_0, $V_u \in W^{2,\infty}(\Omega;\mathbb{R})$, where $W^{2,\infty}(\Omega;\mathbb{R})$ is a standard Sobolev space; see, e.g., [2];

(f') $u \in L^\infty(0,T;\mathbb{R})$;

(g') $\Psi_0 \in Z$.

Notice that the enumeration of the equations and formulae in this errata is not related to that of the referred papers.

2. Energy estimates. In the proof of the energy estimates [3, Theorem 10], in Equations (37), (38), and (39) we made use of the following

$$i\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\Psi\|_{L^2}^2 = i\left(\partial_t\Psi,\, \Psi\right)_{L^2}. \tag{3}$$

*— (martin-sprengel@web.de).

† Fachbereich Mathematik, Universität Konstanz, Germany (gabriele.ciaramella@uni-konstanz.de).

‡Institut für Mathematik, Universität Würzburg, Emil-Fischer-Strasse 30, 97074 Würzburg, Germany (alfio.borzi@mathematik.uni-wuerzburg.de).

However, this equation only holds for real-valued functions. For complex-valued wave functions, the correct equation is

$$i\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\Psi\|_{L^2}^2 = i\,\mathrm{Re}\,(\partial_t\Psi,\ \Psi)_{L^2}\,. \tag{4}$$

The corrected energy estimates are as follows. Let $G \in \widehat{Y}$ be a given function and define $V = V_0 + V_u\,u$. Consider the auxiliary problem

$$i(\partial_t\Psi,\Phi) = (\nabla\Psi,\nabla\Phi) + (V\Psi,\Phi) + (G,\Phi) \text{ a.e. in } (0,T),\ \forall\Phi\in H_0^1(\Omega;\mathbb{C}). \tag{5}$$

Then the following energy estimates hold for the Galerkin solution Ψ_m^a of (5).

THEOREM 1. *(Energy estimates for the auxiliary problem) Let $G \in \widehat{Y}$. Then for almost all $t \in (0,T)$ there exist positive constants C_∇, $C_{1,\Delta}$, $C_{2,\Delta}$, $C_{3,\Delta}$, K_{-1} and K_{-2} (independent of m) such that*

$$\|\Psi_m^a(t)\|^2 \le \exp(T)\Big[\|\Psi_0\|^2 + T\|G\|_{Y_{\infty,0}}^2\Big], \tag{6}$$

$$\|\nabla\Psi_m^a(t)\|^2 \le \exp(C_\nabla T)\Big[\|\nabla\Psi_0\|^2 + T\|G\|_{Y_{\infty,1}}^2\Big], \tag{7}$$

$$\|\Delta\Psi_m^a(t)\|^2 \le \exp(C_{1,\Delta}T)\Big[\|\Delta\Psi_0\|^2 + T\big[C_{2,\Delta}\|\nabla\Psi_0\|^2 + C_{3,\Delta}\|G\|_{\widehat{Y}}^2\big]\Big], \tag{8}$$

$$\|\partial_t\Psi_m^a(t)\|_{H^{-1}} \le K_{-1}, \tag{9}$$

$$\|\partial_t\Psi_m^a(t)\| \le K_{-2}, \tag{10}$$

where K_{-1} depends on $\|G\|_{Y_{\infty,1}}$ and $\|\Psi_0\|_{H^1}$, and K_{-2} depends on $\|G\|_{\widehat{Y}}$ and $\|\Psi_0\|_{H^2}$.

Proof. The proof is given in [1], Theorem 3.1. ∎

These energy estimates can be used to prove results similar to those in [3] concerning existence and uniqueness of solutions to the TDKS equation.

3. Existence of a unique solution. In Eq. (75) in the proof of Theorem 13 in [3] there is the real part missing as in (3).

Therefore, we modify Theorems 12 and 13 of [3] in the following way. We prove existence and regularity results for the problem

$$i(\partial_t\Psi,\Phi) = (\nabla\Psi,\nabla\Phi) + (V\Psi,\Phi) + (V_{H_{xc}}(\Psi)\Psi,\Phi) \quad \text{a.e. in } (0,T), \tag{11}$$

and for all $\Phi \in H_0^1(\Omega;\mathbb{C})$, where $V_{H_{xc}} = V_H + V_{xc}$ is added to the right-hand side of our equation.

For this purpose, we consider the following new assumptions.

(b'2) For any $\Phi \in H_0^1(\Omega;\mathbb{C})$ it holds that $V_{xc}(\Phi)\Phi \in H_0^1(\Omega;\mathbb{C})$ and there exist positive constants K_1 and K_2 such that

$$\|V_{xc}(\Phi)\Phi - V_{xc}(\Lambda)\Lambda\| \le K_1\|\Phi-\Lambda\|, \tag{12}$$

$$\|V_{xc}(\Phi)\Phi - V_{xc}(\Lambda)\Lambda\|_{H^1} \le K_2\|\Phi-\Lambda\|_{H^1}, \tag{13}$$

for any $\Phi,\Lambda \in H_0^1(\Omega;\mathbb{C})$;

(e'2) $V_0,\ V_u \in W^{1,\infty}(\Omega;\mathbb{R})$;

(f'2) $u \in L^\infty(0,T;\mathbb{R})$;

(g'2) $\Psi_0 \in H_0^1(\Omega;\mathbb{C})$.

With these assumptions, we can prove the following

THEOREM 2 (Existence and uniqueness of solution to the TDKS problem). *Under the assumptions* (a'), (e'), (f'), (b'2), (e'2), (f'2) *and* (g'2), *there exists a unique weak solution* $\Psi \in W(0,T)$ *to* (11) *with* $\Psi(0) = \Psi_0$.

Proof. The proof is given in [1], Theorem 5.6. ∎

This theorem is similar to Theorems 12 and 13 of [3]. The differences are in the assumption on the boundary regularity ($C^{2,1}$ instead of C^2), on the regularity of the initial condition function Ψ_0 ($H_0^1(\Omega)$ instead of $L^2(\Omega)$), and the potentials V_0, V_u, V_{xc} that are required to be weakly differentiable.

Notice that in [3] an additional right-hand side in the TDKS equation is considered. This function is denoted with F, and assuming $F \in \hat{Y}$, Theorem 2 above can be proved to cover also this non-homogeneous case.

On the other hand, notice that in [1], we have the notation $F(\Psi) = V_{H_{xc}}(\Psi)\Psi$.

4. Higher regularity. In [3], in the proof of Theorem 16 there is an i missing at the left hand side of Eq. (82). Further, below Eq. (85) as well as in Eq. (91) in the proof of Theorem 17, the wrong equality (3) is used instead of the correct (4).

By amending these mistakes and using Assumptions (a')–(g') we obtain the following correct result

THEOREM 3. *There exists a unique solution* $\Psi \in W(0,T)$ *to* (11) *with* $\Psi(0) = \Psi_0$. *In particular, it holds that*

$$\Psi \in L^\infty(0,T;Z), \quad \partial_t\Psi \in L^\infty(0,T;L^2(\Omega;\mathbb{C})) \quad \textit{and} \quad \Psi \in C([0,T];H_0^1(\Omega;\mathbb{C})).$$

Proof. The proof is given in [1], Theorem 4.3. ∎

Notice that this result is the same as in [3], only the assumptions have been slightly changed. In particular, we require additional regularity of the initial condition $\Psi_0 \in Z$. Further, also in this case we have a slightly stronger assumption on the boundary regularity ($C^{2,1}$ instead of C^2), and the potentials V_0, V_u, V_{xc} are required to be twice weakly differentiable.

REFERENCES

[1] G. Ciaramella, M. Sprengel, and A. Borzì, *A theoretical investigation of time-dependent Kohn–Sham equations: new proofs*, Applicable Analysis, (2019), pp. 1–20, https://doi.org/10.1080/00036811.2019.1679792.

[2] P. G. Ciarlet, *Linear and Nonlinear Functional Analysis with Applications*, Society for Industrial and Applied Mathematics, Philadelphia, PA, 2013.

[3] M. Sprengel, G. Ciaramella, and A. Borzì, *A theoretical investigation of time-dependent Kohn-Sham equations*, SIAM J. Math. Anal., 49 (2017), pp. 1681–1704.