A Tight Nonlinear Approximation Theory for Time Dependent Closed Quantum Systems

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Abstract

The approximation of fixed points by numerical fixed points was presented in the elegant monograph of Krasnosel’skii et al. (1972). The theory, both in its formulation and implementation, requires a differential operator calculus, so that its actual application has been selective. The writer and Kerkhoven demonstrated this for the semiconductor drift-diffusion model in 1991. In this article, we show that the theory can be applied to time dependent quantum systems on bounded domains, via evolution operators. In addition to the kinetic operator term, the Hamiltonian includes both an external time dependent potential and the classical nonlinear Hartree potential. Our result can be paraphrased as follows: For a sequence of Galerkin subspaces, and the Hamiltonian just described, a uniquely defined sequence of Faedo-Galerkin solutions exists; it converges in Sobolev space, uniformly in time, at the maximal rate given by the projection operators.
1 Introduction.

The topic of this article is the convergence analysis for the Faedo-Galerkin method, as applied to a model for time dependent density functional theory (TDDFT). We consider closed quantum systems on bounded domains, with potentials described by a time varying external potential and by the Hartree potential. Exchange correlation potentials, for which there is no consensus in the physics community, are not included. A systematic approximation theory is used for the convergence analysis, which is spatially uniform over a specified time interval.

An operator calculus for approximation of the fixed points of nonlinear mappings by numerical fixed points, in general Banach spaces, was developed by Krasnosel’skii and his coworkers [18], and is intended for nonlinear equations and systems. It was applied to the semiconductor model in [13] (see also [9]) by the analysis of implicit fixed point mappings, obtained by Gummel decomposition (iteration). It was shown by the author in [8] that the inf-sup theory [2], used for stability/convergence in finite element applications to linear problems, is logically implied by the Krasnosel’skii theory. In section 2 particularly Theorem 2.1, we shall summarize the theory of [18] as it applies here.

TDDFT was introduced into the physics community in [19]. A readable account of the subject may be found in [21]. It has emerged as a significant tool in application fields [3], especially those which study the physical properties of subatomic particles, since it is formulated to track electronic charge exactly. The TDDFT model is to be distinguished from the nonlinear Schrödinger equation [4, 5], much studied in the mathematical community, by the presence of time dependent potentials in the Hamiltonian. From the perspective of mathematical analysis, this means that evolution operators, not semigroups, are the preferred tool (for a development of these operators, due originally to Kato, see [15][16][7]). In fact, the evolution operators, together with fixed point analysis, were used in [14][10], to establish strong and weak solutions, resp. They were shown to be an effective computational tool in [6]. In this article, we coordinate the explicit fixed point mappings, induced by the evolution operators, with the operators of the Krasnosel’skii calculus. We demonstrate the following (Th. 5.2): For a sequence of Galerkin subspaces of $H^1_0$, with dense union, a uniquely defined sequence of Faedo-Galerkin solutions exists for the system, and converges in $H^1_0$, uniformly in time, to the unique solution $\Psi$ of the quantum system. The order of convergence is the same as that given by the orthogonal projection operators, as applied to both the solution and the initial datum. Also, $\Psi$ is the unique fixed point of an operator $K$ defined by the evolution operator. The principal assumption of the theory may be interpreted as a regularization property of the linear operator $K' (\Psi)$. 

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2 The Krasnosel’skii Calculus

Given a fixed point \( x_0 \) of a smooth mapping \( T \), a numerical approximation map \( T_n \), with numerical fixed point \( x_n \), and a linear projection map \( P_n \), a theory is constructed to estimate \( \| x_n - P_n x_0 \| \). The result is stated as Theorem 2.1 below. We now discuss the basic results of the theory.

2.1 The abstract calculus

Let \( E \) be a Banach space and \( T \) a mapping from an open subset \( \Omega_0 \) of \( E \) into \( E \). We assume the existence of a fixed point \( x_0 \) for \( T \):

\[
Tx_0 = x_0. \tag{1}
\]

If \( \{E_n\} \) denotes a sequence of closed subspaces of \( E \), suppose that \( T_n : \Omega_n \mapsto E_n \), \( \Omega_n := \Omega_0 \cap E_n \), has a fixed point:

\[
T_n x_n = x_n. \tag{2}
\]

Finally, let \( \{P_n\} \) be a family of bounded linear projections from \( E \) onto \( E_n \):

- \( P_n^2 = P_n \),
- \( P_n E = E_n \).

We have the following [13, Th. 19.1].

**Theorem 2.1.** Let the operators \( T \) and \( P_n T \) be Fréchet-differentiable in \( \Omega_0 \), and \( T_n \) Fréchet-differentiable in \( \Omega_n \). Assume that (1) has a solution \( x_0 \in \Omega_0 \) and the linear operator \( I - T'(x_0) \) is continuously invertible in \( E \). Let

\[
\|P_n x_0 - x_0\| \to 0, \tag{3}
\]
\[
\|P_n T P_n x_0 - T x_0\| \to 0, \tag{4}
\]
\[
\|P_n T'(P_n x_0) - T'(x_0)\| \to 0, \tag{5}
\]
\[
\|[T_n - P_n T] P_n x_0\| \to 0, \tag{6}
\]
\[
\|[T_n - (P_n T)'](P_n x_0)\| \to 0, \tag{7}
\]

as \( n \to \infty \). Finally, assume that for any \( \epsilon > 0 \) there exist \( n_\epsilon \) and \( \delta_\epsilon > 0 \) such that

\[
\|T_n'(x) - T_n'(P_n x_0)\| \leq \epsilon \text{ for } (n \geq n_\epsilon; \|x - P_n x_0\| \leq \delta_\epsilon, x \in \Omega_n). \tag{8}
\]

Then there exist \( n_0 \) and \( \delta_0 > 0 \) such that, when \( n \geq n_0 \), equation (2) has a unique solution \( x_n \) in the ball \( \|x - x_0\| \leq \delta_0 \). Moreover,

\[
\|x_n - x_0\| \leq \|[I - P_n] x_0\| + \|x_n - P_n x_0\| \to 0 \text{ as } n \to \infty, \tag{9}
\]

and \( \|x_n - P_n x_0\| \) satisfies the following two-sided estimate \( (c_1, c_2 > 0) \):

\[
c_1 \|P_n T x_0 - T_n P_n x_0\| \leq \|x_n - P_n x_0\| \leq c_2 \|P_n T x_0 - T_n P_n x_0\|. \tag{10}
\]
Remark 2.1. In order to convert the result of the theorem into a useful form, it is convenient to use the triangle inequality as applied to the bounds of (10):
\[ \|P_nT x_0 - T_n P_n x_0\| \leq \|(P_n - I) T x_0\| + \| T x_0 - T P_n x_0\| + \|(T - T_n) P_n x_0\|. \]
The rhs of this inequality dictates the convergence of the overall approximation.

Remark 2.2. The authors of [18] permit the projection operators to be unbounded; some further assumptions are required in this case. They observe that, when $P_n$ is bounded, the differentiability of $P_nT$ follows from that of $T$, and $(P_nT)'(x) = P_nT'(x)$. Our application is confined to the case when $P_n$ is bounded.

3 The Model

In its original form, TDDFT includes three components for the potential: an external potential, the Hartree potential, and a general non-local term representing the exchange-correlation potential, which is assumed to include a time history part. The exchange-correlation term is suppressed here for the analysis, since there is not a consensus on its representation. When included, its required analytical properties resemble those of the Hartree potential. If $\hat{H}$ denotes the Hamiltonian operator of the system, then the state $\Psi(t)$ of the system obeys the nonlinear Schrödinger equation,
\[ i\hbar \frac{\partial \Psi(t)}{\partial t} = \hat{H} \Psi(t). \]

Here, $\Psi = \{\psi_1, \ldots, \psi_N\}$ consists of $N$ orbitals, and the charge density $\rho$ is defined by
\[ \rho(x, t) = |\Psi(x, t)|^2 = \sum_{k=1}^{N} |\psi_k(x, t)|^2. \]

An initial condition,
\[ \Psi(0) = \Psi_0, \quad (12) \]
and boundary conditions are included. The particles are confined to a bounded region $\Omega \subset \mathbb{R}^3$ and homogeneous Dirichlet boundary conditions hold within a closed system. $\Psi$ denotes a finite vector function of space and time. The effective potential $V_e$ is a real scalar function of the form,
\[ V_e(x, t, \rho) = V(x, t) + W * \rho. \]

Here, $W(x) = 1/|x|$ and the convolution $W * \rho$ denotes the Hartree potential. If $\rho$ is extended as zero outside $\Omega$, then, for $x \in \Omega$,
\[ W * \rho (x) = \int_{\mathbb{R}^3} W(x - y)\rho(y) \, dy, \]
which depends only upon values $W(\xi)$, $\|\xi\| \leq \text{diam}(\Omega)$. We may redefine $W$ smoothly outside this set, so as to obtain a function of compact support for which Young’s inequality applies. The Hamiltonian operator is given by,

\[ \hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + V(x, t) + W * \rho, \quad (13) \]

and $m$ designates the effective mass and $\hbar$ the normalized Planck’s constant.

### 3.1 Definition of weak solution

The solution $\Psi$ is continuous from the time interval $J$, to be defined shortly, into the finite energy Sobolev space of complex-valued vector functions which vanish in a generalized sense on the boundary, denoted $H^1_0(\Omega)$: $\Psi \in C(J; H^1_0(\Omega))$. The time derivative is continuous from $J$ into the dual $H^{-1}$ of $H_0^1$: $\Psi \in C^1(J; H^{-1})$. The spatially dependent test functions $\zeta$ are arbitrary in $H^1_0$. The duality bracket is denoted $\langle f, \zeta \rangle$. Norms and inner products are discussed in the appendix.

**Definition 3.1.** For $J = [0, T_0]$, the vector-valued function $\Psi = \Psi(x, t)$ is a weak solution of (11, 12, 13) if $\Psi$ satisfies the initial condition (12) for $\Psi_0 \in H^1_0$, and if $\forall 0 < t \leq T$:

\[ i\hbar \langle \frac{\partial \Psi(t)}{\partial t}, \zeta \rangle = \int_\Omega \frac{\hbar^2}{2m} \nabla \Psi(x, t) \cdot \nabla \zeta(x) + V_e(x, t, \rho) \Psi(x, t) \zeta(x) dx. \quad (14) \]

### 3.2 Hypotheses for the Hamiltonian and theorem statement

- The so-called external potential $V$ is assumed to be continuously differentiable on the closure of the space-time domain.

The following theorem was proved in [10], based upon the evolution operator as presented in [7].

**Theorem 3.1.** For any interval $[0, T_0]$, the system (14) in Definition 3.1, with Hamiltonian defined by (13), has a unique weak solution $\Psi$ if the hypothesis stated for $V$ holds.

We briefly summarize the method of [10]. Specifically, we identify the mapping $K : C(J; H^1_0) \rightarrow C(J; H^1_0)$ for which the unique solution $\Psi$ of Theorem 3.1 is the unique fixed point of the restriction of $K$ to an appropriate closed ball on which $K$ is invariant and strictly contractive.

**Definition 3.2.** For each $\Psi^*$ in the domain $C(J; H^1_0)$ of $K$ we obtain the image $K\Psi^* = \Psi$ by the following decoupling.

- $\Psi^* \mapsto \rho = \rho(x, t) = |\Psi^*(x, t)|^2$. 

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• $\rho \mapsto \Psi$ by the solution of the associated linear problem (14) where the potential $V_e$ uses $\rho$ in its final argument.

**Remark 3.1.** One can implement the second stage of the previous definition as follows. Introduce the linear evolution operator $U(t,s)$: for given $\Psi^*$ in $C(J;H^1_0)$, set $U(t,s) = U^\rho(t,s)$ so that

$$\Psi(t) = U^\rho(t,0)\Psi_0.$$  \hspace{1cm} (15)

For each $t$, $\Psi(t)$ is a function of $x$. Moreover, $\Psi = K\Psi^*$. The properties of $K$ can be derived with the assistance of the evolution operators. The following theorem is quoted from the results of [12, sections 3.3–3.5].

**Theorem 3.2.** The mapping $K$ is differentiable on $C(J;H^1_0)$, with a locally Lipschitz derivative. Moreover, at its unique fixed point $\Psi$, the linear mapping $I - K'(\Psi)$ is invertible with continuous inverse. For each $\psi \in C(J;H^1_0)$, and $\rho = |\psi|^2$, the derivative is given explicitly by

$$K'[\psi](\omega) = \frac{2i}{h} \int_0^t U^\rho(t,s) \left[ \text{Re}(\bar{\psi}\omega) * W \right] U^\rho(s,0)\Psi_0 ds.$$ \hspace{1cm} (16)

**Remark 3.2.** The identity,

$$U^\rho_1\Psi_0(t) - U^\rho_2\Psi_0(t) = \frac{i}{h} \int_0^t U^\rho_1(t,s)[V_e(s,\rho_1) - V_e(s,\rho_2)]U^\rho_2(s,0)\Psi_0 ds,$$ \hspace{1cm} (17)

and the inequality,

$$\|V_e(\rho_1) - V_e(\rho_2)\|_{C(J;H^1_0)} \leq C\|\Psi_1 - \Psi_2\|_{C(J;H^1_0)}\|\psi\|_{H^1_0},$$ \hspace{1cm} (18)

are used to prove the preceding theorem. Here, $C$ is a locally defined constant. Some adjustments of [14] are also employed. Full details are given in [12, sect. 3]. The identity (17) is derived by differentiating $U^\rho_1(t,s)U^\rho_2(s,0)\Psi_0$ with respect to $s$, and integrating from $0$ to $t$ after using differentiation properties of the evolution operators. As derived, the operator $U^\rho(t,s)$, within the integral on the rhs of the identity, is interpreted as acting on the dual space. However, because of (18), the operator $U^\rho(t,s)$ may be interpreted as acting invariantly on $H^1_0$ for each fixed $s$. Finally, the identity (17), in conjunction with (18) and the invariance properties of the evolution operator, gives the local Lipschitz property of $K$.

### 4 The Projection Mappings

The program carried out here is intended to provide the appropriate mathematical structure to accommodate the classical Faedo-Galerkin method in conjunction with the Krasnosel’skii calculus introduced earlier.

From Theorem 3.2, we see that $\Omega_0 = E = C(J;H^1_0)$ in the notation of section two. We now discuss the projections $P_n$. 


4.1 The approximation spaces

**Definition 4.1.** Let \( \{F_n\}_{n \geq 1} \) be a sequence of finite-dimensional subspaces of the Hilbert space \( H_0^1 \), and let \( Q_n \) denote the orthogonal projection onto \( F_n \) for each \( n \). We suppose that \( \|Q_n f - f\|_{H_0^1} \to 0 \), \( n \to \infty \), for all \( f \in H_0^1 \). Suppose a basis \( \{f_j, j = 1, \ldots, k(n)\} \) is given for \( F_n \). If \( J = [0, T_0] \), then \( E_n \subset C(J; H_0^1) \) is defined by

\[
E_n = \left\{ \sum_{j=1}^{k(n)} \alpha_j(t) f_j(x), \alpha_j \in C(J), j = 1, \ldots, k(n) \right\}.
\]

Finally, if \( \psi \in C(J; H_0^1) \), define \( P_n \psi(\cdot, t) := Q_n \psi(\cdot, t) \), for each \( t \).

**Remark 4.1.** In the following proposition, we will verify the consistency of this definition and the compatibility with the Krasnosel’skii calculus. The subspaces \( E_n \) are not vector subspaces, since the basis coefficients are functions and not scalars. In the mathematical literature, \( E_n \) is a free module over a ring (of continuous functions). It seems to be the appropriate concept for the analysis of the Faedo-Galerkin method.

**Proposition 4.1.** In Definition 4.1

1. \( \{E_n\} \) are closed subspaces of \( C(J; H_0^1) \).

2. \( P_n \) maps \( C(J; H_0^1) \) onto \( E_n \) and \( P_n^2 = P_n \).

**Proof.** We begin with statement (1), which involves two steps. The first is to show that \( E_n \subset C(J; H_0^1) \). We observe that, by use of the classical Gram-Schmidt procedure, we may assume that the basis \( \{f_j\} \) of \( F_n \) is orthonormal in \( H_0^1 \). Continuity of the coefficients is preserved. With this property, if \( t_0 \in J \) and \( t \in J \), then, for \( g \in E_n \):

\[
\|g(t) - g(t_0)\|^2_{H_0^1} = \sum_{j=1}^{k(n)} |\alpha_j(t) - \alpha_j(t_0)|^2,
\]

which has zero limit as \( t \to t_0 \). It follows that \( E_n \subset C(J; H_0^1) \). We now prove that \( E_n \) is closed. Suppose that \( \{g_\ell\} \subset E_n \) converges in the norm of \( C(J; H_0^1) \) to a limit \( g \). In particular, \( \{g_\ell\} \) is a Cauchy sequence. Again, under the assumption that the basis in \( F_n \) is orthonormal, we write

\[
\|g_\ell(t) - g_m(t)\|^2_{H_0^1} = \sum_{j=1}^{k(n)} |\alpha_j^\ell(t) - \alpha_j^m(t)|^2,
\]

so that the individual coefficient sequences are Cauchy sequences in the Banach space \( C(J) \). It follows that the limits \( \alpha_j(t) \) are continuous on \( J \) and that \( g = \sum \alpha_j f_j \). We conclude that \( E_n \) is a closed subspace of \( C(J; H_0^1) \).
In order to prove statement (2), we must show that the coefficients induced by the orthogonal projection $Q_n$ are continuous functions of $t$. In fact, the difference of these coefficients is given explicitly by the inner product,

$$ \alpha_j(t) - \alpha_j(t_0) = (\psi(\cdot, t) - \psi(\cdot, t_0), f_j)_{H^1_0}, $$

which is estimated in norm by $\|\psi(\cdot, t) - \psi(\cdot, t_0)\|_{H^1_0}$. By the definition of the Banach space $C(J; H^1_0)$, this has a zero limit as $t \to t_0$. The remaining statements of (2) are evident.

4.2 The hypotheses of the Krasnosel’skii calculus: I

The propositions of this section deal with hypotheses pertaining to the fixed point mapping and its relation to the projections.

**Proposition 4.2.** The hypotheses (3) and (4) hold for the case $T = K$, $x_0 = \Psi$, and $P_n$ as defined in Definition 4.1. Specifically,

$$ \|P_n\Psi - \Psi\|_{C(J; H^1_0)} \to 0, \quad (19) $$

$$ \|P_nKP_n\Psi - K\Psi\|_{C(J; H^1_0)} \to 0, \quad (20) $$

as $n \to \infty$.

**Proof.** The hypothesis (19) has been built into the definition of the projection family. We rewrite (20) as follows, using the triangle inequality, the fixed point property, and the property $\|P_n\| = 1$.

$$ \|P_nKP_n\Psi - K\Psi\|_{C(J; H^1_0)} \leq \|P_nKP_n\Psi - P_nK\Psi\|_{C(J; H^1_0)} + \|P_nK\Psi - K\Psi\|_{C(J; H^1_0)} \leq $$

$$ \|K P_n\Psi - K\Psi\|_{C(J; H^1_0)} + \|P_n\Psi - \Psi\|_{C(J; H^1_0)}. $$

The (local Lipschitz) continuity of $K$ and (19) imply the convergence expressed in (20).

In order to address hypothesis (5), we require a regularization hypothesis for $K'(\Psi)$.

**Definition 4.2.** Denote by $B$ the closed unit ball of $H^1_0$, and by $C$ the set $C(J; B)$. Finally, set $K = K'(\Psi)C$. If the maximal dispersion of the set $K$ from $E_n$ is defined by

$$ \mathcal{E}(K; E_n) := \sup_{\phi \in K} \|\phi - P_n\phi\|_{C(J; H^1_0)}, $$

then the regularization hypothesis asserts that

$$ \lim_{n \to \infty} \mathcal{E}(K; E_n) = 0. $$

Naturally, one wishes to find subspaces $F_n \subset H^1_0$ such that the dispersion $\mathcal{E}$ is minimized. This represents a mild extension of an important topic in approximation theory, termed the $n$-width, which characterizes minimal dispersion.
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from $n$-dimensional subspaces. Here, we have the additional structure of time dependence. The $n$-width was introduced by A. N. Kolmogorov in [17], and has been intensively studied by many authors.

According to classical approximation theory, one expects the regularization hypothesis to hold if members of $\mathcal{K}$ have spatial regularity exceeding that for $H^1_0$. The exact formula for $\mathcal{K}'(\Psi)$, given by (16), allows some observations. For example, the middle (convolution) term is in $C(J;H^2)$, as can be shown by distributing the second order derivative, and then applying the general Young’s inequality. There is a bound dependent only on that of $\omega$. Moreover, it was shown in [14] that $U^{\rho}(s,0)\Psi_0$ is in $C(J;H^2 \cap H^1_0)$ if $\Psi_0 \in H^2 \cap H^1_0$. One expects a product of such $H^2$ functions to be in a fractional order Sobolev space with index greater than one. This means that the hypothesis is not unrealistic.

**Proposition 4.3.** Suppose the regularization hypothesis of Definition 4.2 holds. Then (5) holds for the case $T = K$, $x_0 = \Psi$, and $P_n$ as defined in Definition 4.1. We have:

$$\|P_nK'(P_n\Psi) - K'(\Psi)\| \to 0, \quad n \to \infty. \quad (21)$$

**Proof.** The norms used here are those of the uniform operator topology. Explicitly:

$$\|P_nK'(P_n\Psi) - K'(\Psi)\| \leq \|P_nK'(P_n\Psi) - P_nK'(\Psi)\| + \|P_nK'(\Psi) - K'(\Psi)\|.$$  

The continuity of $K'$, the definition of $P_n$, and the definition of the uniform operator topology imply the estimate for the first term. The second term requires the regularization hypothesis of Definition 4.2. Thus, we obtain (21).

5 The Numerical Fixed Point Map

We identify the mapping $K_n : E_n \mapsto E_n$ which serves as the numerical fixed point map. It is the analog of the mapping $K$ of Definition 3.2.

**Definition 5.1.** For each $u^*$ in the domain $E_n$ of $K_n$ we obtain the image $K_nu^* = u \in E_n$ by the following decoupling.

- $u^* \mapsto \rho = \rho(x,t) = |u^*(x,t)|^2$.
- $\rho \mapsto u$ by the solution of the linear system (23) to follow, where the potential $V_e$ uses $\rho$ in its final argument.

5.1 The Galerkin operator

**Definition 5.2.** Let $F_n \subset H^1_0(\Omega)$ be a given finite dimensional linear subspace, with positive dimension $k(n)$. Define, for each fixed $t \in [0,T_0]$, and $u(\cdot,t) \in F_n$, the relation,

$$G(t,u)[v] = \int_\Omega \left\{ \frac{\hbar^2}{2m} \nabla u(x,t) \cdot \nabla v(x) + V_e(x,t,\rho)u(x,t)v(x) \right\} dx, \quad \forall v \in F_n,$$  

(22)
where \( \rho = |u^*|^2 \), for a given \( u^* \in E_n \). Finally, \( u \in E_n \) is a solution of the linear Faedo-Galerkin equation if
\[
i \hbar \frac{\partial u}{\partial t} = \mathcal{G}(t, u), \quad u(\cdot, 0) = Q_n \Psi_0,
\]
(23)
for \( \partial u/\partial t \) a continuous linear functional on \( E_n \). Here, \( Q_n \) retains its meaning as the orthogonal projection onto \( F_n \). In the event that \( \rho = |u|^2 \), we say that \( u \) is a solution of the nonlinear Faedo-Galerkin equation.

**Remark 5.1.** There are three separate points of analysis remaining for the numerical fixed point map \( K_n \). We state them here.

- **Definition 5.1** is consistent. In particular, this entails a liner theory for equation (23).
- \( K_n \) is continuously differentiable.
- Convergence properties (6), (7), and (8) hold in the present context.

We take these up in the following subsections. Note that the existence of numerical fixed points is a consequence of the theory; it is not necessary to establish this independently.

### 5.2 The linear problem: Faedo-Galerkin evolution operators

The Galerkin operator \( \mathcal{G} \) and the Galerkin Cauchy problem (23) are solved by the evolution operators associated with the subspace \( E_n \), where \( E_n \) has the meaning of Definition 4.1. A less general potential, consisting only of an external potential, was considered in [11] with simpler estimates.

**Theorem 5.1.** The linear approximate Cauchy problem (23) is solvable for \( u = \Psi_\mathcal{G} \) by the formula,
\[
\Psi_\mathcal{G}(\cdot, t) = U_\mathcal{G}(t, 0)Q_n \Psi_0.
\]
Here, \( U_\mathcal{G}(t, s) \) denotes the time-ordered evolution operator, which acts invariantly on \( F_n \) and is strongly differentiable in both arguments. As a function of \( x \) and \( t \), \( \Psi_\mathcal{G} \) is in \( E_n \) and is interpreted as the linear Faedo-Galerkin approximation.

**Proof.** The generation of the evolution operators from a family of stable, strongly continuous semigroups on a frame space \( X \) is discussed in [7, Ch. 6], based on Kato’s original results in [15, 16]. For the model considered here, and, indeed, a somewhat more general one, the details are presented in [10] for the family \( \{-i/\hbar\{H(t)\} \) of generators of contractive semigroups \( \{W(t, s)\} \) on \( H^{-1} \). These semigroups are shown to act stably on \( H_0^1 \) via a similarity relation which is a cornerstone of Kato’s theory. Equivalently, this is expressed as a commutator relation. The proof here amounts to the verification that the generators
\((-i/\hbar)\{G(t)\}\) enjoy similar properties on \(F_n\) and its dual, resp. We may obtain these semigroups, denoted \(\{W_G(t,s)\}\), from the family \(\{W(t,s)\}\) as follows. If \(\ell\) is a (continuous) linear functional on \(F_n\), extend \(\ell\) to \(\hat{\ell} \in H^{-1}\) by defining \(\hat{\ell}\) to be zero on the orthogonal complement of \(F_n\) in \(H^1_0\). We can define

\[ W_G(t,s)[\ell] := W(t,s)[\hat{\ell}] |_{F_n}. \]

The remainder of the proof deals with the invariance of \(\{W_G(t,s)\}\) on \(F_n\). We recall that for the full Hamiltonian, this means that

\[ S\hat{H}(t)S^{-1} = \hat{H}(t) + B(t), \tag{24} \]

where \(S\) is an isomorphism from \(H^1_0\) to \(H^{-1}\), and where \(B(t)\) represents a bounded operator on (all of) \(H^{-1}\), with norm uniformly estimated in \(t\). It was shown in [10] that, if \(S\) is the canonical isomorphism from \(H^1_0\) to \(H^{-1}\), then \(B(t)\) is given explicitly on \(H^{-1}\) by:

\[ \langle B(t)\ell, \zeta \rangle = \int_{\Omega} \left[ \frac{\hbar^2}{2m} \psi \nabla V_e \cdot \nabla \zeta \right] \, dx, \; \forall \zeta \in H^1_0, \tag{25} \]

where \(\psi = S^{-1}\ell\). For the Faedo-Galerkin case, one replaces (24) by

\[ S_G\hat{G}(t)S_G^{-1} = \hat{G}(t) + B_G(t), \tag{26} \]

where \(S_G\) is an induced isomorphism from \(F_n\) to its dual, and (25) is replaced by

\[ \langle B_G(t)\ell, \zeta \rangle = \int_{\Omega} \left[ \frac{\hbar^2}{2m} \psi \nabla V_e \cdot \nabla \zeta \right] \, dx, \; \forall \zeta \in F_n, \tag{27} \]

where \(\psi = S_G^{-1}\ell\). The estimate is obtained by the generalized Hölder inequality, with \(\psi \in L^6, \nabla V_e \in L^3, \nabla \zeta \in L^2\). In particular, we obtain the evolution operator \(U_G(t,s)\) and the corresponding theory for the Cauchy problem.

\begin{remark}
The \(L^3\) property of \(\nabla V_e\) is established in [12] in Lemma 3.1 and its proof. It is possible to extend \(U_G\) to all of \(C(J;H^1_0)\) as follows: For fixed \(t\), for \(s < t\), and \(\psi \in C(J;H^1_0)\), set

\[ U_G(t,s)\psi(\cdot, s) := U_G(t,s)Q_n\psi(\cdot, s). \]

In words, we consider the action only on the orthogonal projection of a given function at time \(s\).

For later use, we observe that the same reasoning can be applied to a construction of the evolution operators associated with \(I - Q_n\).
\end{remark}

### 5.3 Differentiability of \(K_n\)

There are two steps in the analysis of the differentiability of \(K_n\):

- The verification of the existence of the Gâteaux derivative at each member of \(C(J;E_n)\) with its accompanying formula;
• The verification of the continuity of the Gâteaux derivative, hence the existence of the continuous Fréchet derivative with the same formula.

We begin with a preliminary lemma.

**Lemma 5.1.** Suppose that \( \psi_\epsilon \) converges to \( \psi \) in \( E_n \) as \( \epsilon \to 0 \). Then \( U^\rho G^\epsilon \) converges to \( U^\rho G \) in the operator topology, uniformly in \( t, s \). In fact, the convergence is of order \( O(\|\psi_\epsilon - \psi\|_{C(J, H^0)}) \).

**Proof.** The proof adapts the proof of [12, Lemma 3.2]. The version of (17) appropriate here is the operator equation,

\[
U^\rho_1 G(t, s) - U^\rho_2 G(t, s) = \frac{i}{\hbar} \int_s^t U^\rho_1 G(t, r) [V_e(r, \rho_1) - V_e(r, \rho_2)] U^\rho_2 G(r, s) dr. \tag{28}
\]

If we identify \( \rho_1 \) with \( \rho_\epsilon \) in the formula, and \( \rho_2 \) with \( \rho \), then the convergence follows from (18); note that \( U^\rho \epsilon \psi G(t, s) \) is uniformly bounded in \( \epsilon \), as explained in the following remark.

**Remark 5.3.** The uniform boundedness of \( U^\rho \epsilon \psi G(t, s) \) can be derived from the construction of the evolution operators (see [7]). Specifically, a bound can be obtained by appropriately exponentiating a bound for (27) over the global time interval.

**Proposition 5.1.** The numerical fixed point mapping \( K_n \) is Gâteaux differentiable on \( E_n \) with derivative,

\[
K'_n[\psi](\omega) = \frac{2i}{\hbar} \int_0^t U^\rho G(t, s) \left[ \text{Re}(\overline{\psi}\omega) * W \right] U^\rho G(s, 0) Q_n \Psi_0 \, ds. \tag{29}
\]

Here, \( \psi \) and \( \omega \) are arbitrary in \( E_n \) and \( \rho = |\psi|^2 \). In fact, the derivative is continuous, hence \( K_n \) is continuously Fréchet differentiable.

**Proof.** Let \( \psi \) be a given element of \( E_n \) and set \( \rho = |\psi|^2 \). Set

\[
\rho_\epsilon = |\psi + \epsilon \omega|^2, \text{ for } \omega \in E_n, \, \epsilon \in \mathbb{R}, \, \epsilon \neq 0.
\]

We will use (28) as applied to \( Q_n \Psi_0 \):

\[
U^\rho G Q_n \Psi_0(t) - U^\rho G Q_n \Psi_0(t) = \frac{i}{\hbar} \int_0^t U^\rho G(t, s) [V_e(s, \rho_\epsilon) - V_e(s, \rho)] U^\rho G(s, 0) Q_n \Psi_0 \, ds. \tag{30}
\]

This identity and the inequality (18) are used as in [12, sections 3.3-3.4]. By direct calculation, we obtain

\[
\frac{U^\rho G Q_n \Psi_0(t) - U^\rho G Q_n \Psi_0(t)}{\epsilon} = \frac{2i}{\epsilon} \int_0^t U^\rho G(t, s) \left[ \text{Re}(\overline{\psi}\omega) * W \right] U^\rho G(s, 0) Q_n \Psi_0 \, ds + \frac{i}{\hbar} \int_0^t U^\rho G(t, s) [\omega^2 * W] U^\rho G(s, 0) Q_n \Psi_0 \, ds.
\]
In [12], this limit was computed in the $C(J; H^1_0)$ topology. Here, we may use the same topology. Specifically, the first term converges to the derivative (cf. Lemma 5.1), and the second term converges to zero. Note that the multiplier of $\epsilon$ remains bounded.

The continuity of $K'_n$ can be inferred directly from the formula (29) by using Lemma 5.1 together with Lemma 3.1 of [12].

5.4 The hypotheses of the Krasnosel’skii calculus: II

We will prove convergence properties (6), (7), and (8) in turn. However, we begin with a fundamental proposition on the approximation of $K$ by $K_n$. The following proposition is required for the proofs of Lemma 5.2 and Theorem 5.2 to follow.

Proposition 5.2. If $\Psi$ is the unique fixed point of $K$, given by $\Psi = U^\rho(t, 0)\Psi_0$, then

$$\|K_n P_n \Psi - K P_n \Psi\|_{C(J; H^1_0)} \to 0, \text{ as } n \to \infty.$$ 

In fact, the convergence is of the order,

$$O(\|P_n \Psi - \Psi\|_{C(J; H^1_0)}) + O(\|Q_n \Psi_0 - \Psi_0\|_{H^1_0}),$$

as $n \to \infty$.

Proof. Set $P_n = |P_n \Psi|^2$. By the definitions of $K$ and $K_n$, we have

$$K P_n \Psi - K_n P_n \Psi = U^\rho_n \Psi_0 - U^G_n Q_n \Psi_0.$$

We write this difference as the sum,

$$K P_n \Psi - K_n P_n \Psi = U^\rho_n [\Psi_0 - Q_n \Psi_0] + [U^\rho_n - U^G_n] Q_n \Psi_0.$$

By the boundedness of the evolution operators, the first term converges to zero with order,

$$O(\|\Psi_0 - Q_n \Psi_0\|_{H^1_0}).$$

We analyze the second difference, by writing it as the sum,

$$[U^\rho_n - U^G_n] Q_n \Psi_0 = [P_n U^\rho_n - U^G_n] Q_n \Psi_0 + (I - P_n) U^\rho_n Q_n \Psi_0. \quad (31)$$

The first rhs term is zero, as we now show. We will require the following representation to show this:

$$P_n U^\rho_n (t, 0) Q_n \Psi_0 - U^G_n (t, 0) Q_n \Psi_0 = P_n [U^\rho_n (t, 0) Q_n \Psi_0 - U^G_n (t, 0) Q_n \Psi_0]$$

$$= \left( \frac{1}{\hbar} \right) P_n \int_0^t U^\rho_n (t, r) [\hat{H}(\rho_n) - \mathcal{G}(\rho_n)] U^G_n (r, 0) Q_n \Psi_0 \, dr. \quad (32)$$

Now the difference, $\hat{H}(\rho_n) - \mathcal{G}(\rho_n)$, for each fixed $t$, is a continuous linear functional which vanishes on $F_n$. We may therefore regard $U^\rho_n (t, s)$ as acting invariantly on the orthogonal complement of $F_n$ in $H^1_0$. Time integration preserves...
the invariance, and the result is annihilated by $P_n$. We write the second term on the rhs of (34) as,

\[ (I - P_n)U^{\rho_n}(t,0)Q_n\Psi_0 = (I - P_n)[U^{\rho_n}(t,0) - U^{\rho}(t,0)]Q_n\Psi_0 + (I - P_n)U^{\rho}(t,0)Q_n\Psi_0. \] (33)

According to [12, Lemma 3.2], the convergence of $\|U^{\rho_n}(t,0) - U^{\rho}(t,0)\|$ in the operator norm is of order, $O(\|\Psi - P_n\Psi\|_{C(J;H^1)})$. The remaining term of (33) is written as,

\[ (I - P_n)U^{\rho}(t,0)Q_n\Psi_0 = (I - P_n)U^{\rho}(t,0)\Psi_0 + (I - P_n)U^{\rho}(t,0)(Q_n - I)\Psi_0. \] (34)

The first term on the rhs of (34) is rewritten as $(I - P_n)\Psi$; its estimation is obvious. The second term is of order, $O(\|Q_n\Psi_0 - \Psi_0\|_{H^1})$. This completes the proof.

\[ \square \]

**Lemma 5.2.** The limit relation (7) holds in the case

\[ T_n \mapsto K_n, T \mapsto K, x_0 \mapsto \Psi. \]

More precisely,

\[ \|P_nK P_n\Psi - K_nP_n\Psi\|_{C(J;H^1)} \to 0, \ n \to \infty. \] (35)

Here, $\Psi$ designates the unique fixed point of $K$ in $C(J;H^1)$, and the projection $P_n$ is defined in Definition 4.1.

**Proof.** We begin with the triangle inequality, and estimate the resulting terms.

\[ \|P_nK P_n\Psi - K_nP_n\Psi\|_{C(J;H^1)} \leq \|P_nK P_n\Psi - K\Psi\|_{C(J;H^1)} + \|K\Psi - K P_n\Psi\|_{C(J;H^1)} + \|K P_n\Psi - K_nP_n\Psi\|_{C(J;H^1)}. \]

The first term has already been estimated. It is relation (20), as proved in Proposition 4.2. The third term is estimated by Proposition 5.2. The second term is estimated by the local Lipschitz continuity of $K$. This concludes the proof.

\[ \square \]

**Lemma 5.3.** The limit relation (7) holds, with the same identifications as the previous lemma. Specifically,

\[ \|[K_n' - P_nK'](P_n\Psi)\| \to 0, \ as \ n \to \infty. \] (36)

**Proof.** To clarify the notation, set $\psi_n = P_n\Psi, \rho_n = |\psi_n|^2$. For arbitrary $\omega \in E_n, \|\omega\|_{C(J;H^1)} \leq 1$, we write the difference of $P_nK'[\psi_n](\omega)$ and $K'_n[\psi_n](\omega)$ as:

\[ P_nK'[\psi_n](\omega) - K'_n[\psi_n](\omega) = \]

\[ \frac{2i}{\hbar} \int_0^t P_nU^{\rho_n}(t,s) [\text{Re}(\bar{\psi}_n\omega) * W] \ U^{\rho_n}(s,0)(I - Q_n)\Psi_0 \ ds + \]

...
\[ \frac{2i}{\hbar} \int_0^t P_n U^\rho_n(t, s) \left[ \text{Re}(\bar{\psi}_n \omega) * W \right] U^\rho_n(s, 0) Q_n \Psi_0 \, ds - \]

\[ \frac{2i}{\hbar} \int_0^t U^\rho_G(t, s) \left[ \text{Re}(\bar{\psi}_n \omega) * W \right] U^\rho_G(s, 0) Q_n \Psi_0 \, ds. \]

Note that we commuted \( Q_n \) and \( \int_0^t \), and then replaced \( Q_n \) by \( P_n \). Because of the boundedness of the evolution operator on \( H_0^1 \), the first term is estimated by a constant \( \| \Psi_0 - Q_n \Psi_0 \|_{H_0^1} \). Here, we directly use [12, Lemma 3.1]. The indicated difference between the second and third terms can be written as the sum of the two differences, \( d_1, d_2 \), where \( d_1 = \]

\[ \frac{2i}{\hbar} \int_0^t P_n U^\rho_n(t, s) \left[ \text{Re}(\bar{\psi}_n \omega) * W \right] (U^\rho_n(s, 0) - U^\rho_G(s, 0)) Q_n \Psi_0 \, ds, \]

and where \( d_2 = \]

\[ \frac{2i}{\hbar} \int_0^t [P_n U^\rho_n(t, s) - U^\rho_G(t, s)] \left[ \text{Re}(\bar{\psi}_n \omega) * W \right] U^\rho_G(s, 0) Q_n \Psi_0 \, ds. \]

Now \( d_1 \) can be estimated by using the proof of Proposition 5.2 beginning with (4), where it was shown that

\[ \| (U^\rho_n - U^\rho_G) Q_n \Psi_0 \|_{C(J; H^1_0)} \to 0, \quad n \to \infty, \]

with order of convergence, \( O(\| \Psi - P_n \Psi \|_{C(J; H^1_0)}) + O(\| \Psi_0 - Q_n \Psi_0 \|_{H^1_0}) \). This is maintained for \( d_1 \) via [12, Lemma 3.1]. Also, \( d_2 = 0 \). We show this by writing

the term as the sum,

\[ \frac{2i}{\hbar} \int_0^t [P_n U^\rho_n(t, s) - U^\rho_G(t, s)] \left[ \text{Re}(\bar{\psi}_n \omega) * W \right] U^\rho_G(s, 0) Q_n \Psi_0 \, ds = \]

\[ \frac{2i}{\hbar} \int_0^t [P_n U^\rho_n(t, s) - U^\rho_G(t, s)] P_n \left[ \text{Re}(\bar{\psi}_n \omega) * W \right] U^\rho_G(s, 0) Q_n \Psi_0 \, ds + \]

\[ \frac{2i}{\hbar} \int_0^t [P_n U^\rho_n(t, s) - U^\rho_G(t, s)] (I - P_n) \left[ \text{Re}(\bar{\psi}_n \omega) * W \right] U^\rho_G(s, 0) Q_n \Psi_0 \, ds. \]

Since the operator,

\[ P_n U^\rho_n(t, s) - U^\rho_G(t, s), \]

vanishes on \( E_n \) and on the subspace, which, for each fixed time, is the orthogonal complement of \( F_n \), we draw the conclusion that \( d_2 = 0 \).

This concludes the proof. \( \square \)

The proof of this result allows a generalization to the case where \( \psi_n \) is in a closed \( E_n \) neighborhood of \( P_n \Psi \). This will be required for the verification of the hypothesis (38) to follow.
Corollary 5.1. Let \( \epsilon > 0 \) be specified. Then there is a real number \( \delta_\epsilon > 0 \) and an integer \( n_\epsilon \) such that, for

\[
\| \psi_n - P_n \Psi \|_{C(J; H^1_\delta)} \leq \delta_\epsilon, \quad \psi_n \in E_n, \quad n \geq n_\epsilon,
\]

then

\[
\|[K'_n - P_nK](\psi_n)\| \leq \epsilon. \tag{37}
\]

Proof. We telescope the representations of the previous proof as follows. Note that \( \psi_n \) and \( \rho_n \) have the new interpretation as specified in the corollary.

\[
P_nK'(\psi_n)(\omega) - K'_n[\psi_n](\omega) =
\]

\[
\frac{2i}{\hbar} \int_0^t P_n U^{\rho_n}(t, s) \left[ \text{Re}(\bar{\psi}_n\omega) \ast W \right] U^{\rho_n}(s, 0)(I - Q_n)\Psi_0 \, ds +
\]

\[
\frac{2i}{\hbar} \int_0^t P_n U^{\rho_n}(t, s) \left[ \text{Re}(\bar{\psi}_n\omega) \ast W \right] (U^{\rho_n}(s, 0) - U^{\rho_n}_G(s, 0))Q_n\Psi_0 \, ds +
\]

\[
\frac{2i}{\hbar} \int_0^t [P_n U^{\rho_n}(t, s) - U^{\rho_n}_G(t, s)] \left[ \text{Re}(\bar{\psi}_n\omega) \ast W \right] U^{\rho_n}_G(s, 0)Q_n\Psi_0 \, ds.
\]

As before, the first term is estimated by a constant times \( \| \Psi_0 - Q_n\Psi_0 \|_{H^1_\delta} \), and the third term is zero. The only difference is the second term, which reduces to a study of the term,

\[
\|(U^{\rho_n} - U^{\rho_n}_G)Q_n\Psi_0\|_{C(J; H^1_\delta)},
\]

with the new interpretation of \( \rho_n \). This requires a new analysis of the second term on the rhs of (34) which we rewrite as follows.

\[
(I - P_n)U^{\rho_n}Q_n\Psi_0 = [(I - P_n)U^{\rho_n}Q_n\Psi_0 - (I - P_n)U^{[P_n\Psi]^2}Q_n\Psi_0] +
\]

\[
(I - P_n)U^{[P_n\Psi]^2}Q_n\Psi_0.
\]

When the triangle inequality is applied, (34) leads to an estimate, previously derived, for the final term. The difference expression is a term of order \( O(\|\psi_n - P_n\Psi\|_{C(J; H^1_\delta)}) \), which will satisfy a bound of \( \epsilon/2 \) by choice of \( \delta_\epsilon \). Now \( n_\epsilon \) can be chosen according to the remaining terms, so that an additional \( \epsilon/2 \) is added to the estimate. This concludes the proof. \( \square \)

Lemma 5.4. The limit relation (5) holds, with the same identifications as the previous lemmas. Specifically, for any \( \epsilon > 0 \), there exist \( n_\epsilon \) and \( \delta_\epsilon > 0 \) such that

\[
\|K'_n(\psi) - K'_n(P_n\Psi)\| \leq \epsilon \quad \text{for} \quad (n \geq n_\epsilon; \|\psi - P_n\Psi\| \leq \delta_\epsilon, \psi \in E_n). \tag{38}
\]

Proof. We write, for \( \psi \) in a neighborhood of \( P_n\Psi \) in \( E_n \) as yet to be determined,

\[
K'_n(\psi) - K'_n(P_n\Psi) = [K'_n(\psi) - P_nK'(\psi)] +
\]

\[
[P_nK'(\psi) - P_nK'(P_n\Psi)] + [P_nK'(P_n\Psi) - K'_n(P_n\Psi)].
\]
To estimate the second term, choose a Lipschitz constant $C$ such that $K'$ is Lipschitz continuous, with this constant, in the closed ball of radius one centered at $\Psi$ in $C(J; H^{1}_{0})$. Choose $N$ sufficiently large so that, for $n \geq N$, $P_{n}\Psi$ is in the concentric ball of radius $1/2$. Then select $\delta'$ as follows:

$$\delta' = \min \left(1/2, \frac{\epsilon}{3C}\right).$$

We can choose $n$ and $\delta''$ so that $n \geq N$ and the first and third terms do not exceed $\epsilon/3$ for $n \geq n_{*}$. This is possible by an application of Lemma 5.3 to the third expression, and Corollary 5.1 to the first expression. We conclude that if

$$\delta := \min(\delta', \delta''),$$

then condition (38) is satisfied, and the proof is concluded.

### 5.5 The main result

**Theorem 5.2.** Suppose that $\Psi$ is the unique solution satisfying Definition 4.7 and guaranteed by Theorem 4.7. Suppose that the subspaces $E_{n} \subset C(J; H^{1}_{0})$ are defined as in Definition 4.1, with associated projections $P_{n}$. Suppose that the regularization hypothesis of Definition 4.2 holds. There is a pair $\delta_{0}, n_{0}$, such that, in the closed ball $B(\Psi, \delta_{0}) \subset C(J; H^{1}_{0})$, and for $n \geq n_{0}$, there is a unique solution of the (nonlinear) Faedo-Galerkin equation (23), with $\rho = |u|^{2}$. If we designate the solutions by $u = \Psi_{n}$, then these approximations converge to the unique solution $\Psi$ with order $O(\|\Psi - P_{n}\Psi\|_{C(J; H^{1}_{0})}) + O(\|\Psi_{0} - Q_{n}\Psi_{0}\|_{H^{1}_{0}})$. This is the maximal expected order of convergence.

**Proof.** We have verified the hypotheses of Theorem 2.1 in sections 4.2 and 5.4. This yields the unique local existence of the nonlinear Faedo-Galerkin approximations $\Psi_{n}$ for sufficiently large $n$. According to Remark 2.1, we have

$$\|P_{n}K\Psi - K_{n}P_{n}\Psi\| \leq \|(P_{n} - I)K\Psi\| + \|K\Psi - KP_{n}\Psi\| + \|(K - K_{n})P_{n}\Psi\|.$$

The first two of these expressions are of the order $O(\|I - P_{n}\|)$ in $C(J; H^{1}_{0})$. In fact, since $\Psi$ is a fixed point of $K$, the convergence of the first term on the rhs is a consequence of (19). The convergence of the second term follows from the local Lipschitz property of $K$, combined with (19). The convergence of the third term follows from Proposition 5.2 and is of order $O(\|\Psi - P_{n}\Psi\|_{C(J; H^{1}_{0})}) + O(\|\Psi_{0} - Q_{n}\Psi_{0}\|_{H^{1}_{0}})$. This completes the proof.

### 6 Summary

We have employed a powerful and precise operator calculus to obtain a sharp convergence theory for Faedo-Galerkin approximations for solutions of time dependent closed quantum systems with Kohn-Sham potentials. Computation has not been discussed in the article. This topic was discussed in [14], where
it was shown that a spectral method, embodied in the algorithm FEAST, can accommodate the evolution operator approach, extending to time and spatial discretization. The evolution operator is especially appropriate for a fixed point approximation theory, as used here, because it permits explicit analytical calculation.

Natural extensions of the present study include the incorporation of time discretization, and additional potentials to account for exchange-correlation. The latter is particularly important to track charge exactly, and thus the physical properties which use exact charge.

Since the evolution operator accommodates convergent iteration, it would be especially valuable if the iteration analyzed in [12] could be extended to standard finite dimensional approximation theory.

We are not aware of any other systematic approach to Faedo-Galerkin approximation for this model. For a special choice of $F_n$, based on a smooth orthonormal system, the authors of [20] demonstrate convergence, as part of an existence analysis for a quantum control model.

Finally, we make the following observation, which paraphrases that of [18]. Although six separate convergence estimates are required for the application of the theory, it is only those cited in Remark 2.1 which govern the rate of convergence, established in Theorem 5.2. If $\Psi$ and $\Psi_0$ have additional regularity, one expects these estimates to confirm increased order of convergence from standard approximation theory, when applicable.

### A Notation and Norms

We employ complex Hilbert spaces in this article.

$$L^2(\Omega) = \{ f = (f_1, \ldots, f_N)^T : |f_j|^2 \text{ is integrable on } \Omega \}.$$

$$(f, g)_{L^2} = \sum_{j=1}^{N} \int_{\Omega} f_j(x) \overline{g_j(x)} \, dx.$$

However, $\int_{\Omega} f g$ is interpreted as

$$\sum_{j=1}^{N} \int_{\Omega} f_j g_j \, dx.$$

For $f \in L^2$, as just defined, if each component $f_j$ satisfies $f_j \in H_0^1(\Omega; \mathbb{C})$, we write $f \in H_0^1(\Omega; \mathbb{C}^N)$, or simply, $f \in H_0^1(\Omega)$. The inner product in $H_0^1$ is

$$(f, g)_{H_0^1} = (f, g)_{L^2} + \sum_{j=1}^{N} \int_{\Omega} \nabla f_j(x) \cdot \overline{\nabla g_j(x)} \, dx.$$

$\int_{\Omega} \nabla f \cdot \nabla g$ is interpreted as

$$\sum_{j=1}^{N} \int_{\Omega} \nabla f_j(x) \cdot \nabla g_j(x) \, dx.$$
Finally, $H^{-1}$ is defined as the dual of $H^1_0$, and its properties are discussed at length in [1]. The Banach space $C(J; H^1_0)$ is defined in the traditional manner:

$$C(J; H^1_0) = \{ u : J \mapsto H^1_0 : u(\cdot) \text{ is continuous} \},$$

$$\|u\|_{C(J; H^1_0)} = \sup_{t \in J} \|u(t)\|_{H^1_0}.$$ 

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