The Quantum Faedo-Galerkin Equation: Evolution Operator and Time Discretization

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Abstract

Time dependent quantum systems have become indispensable in science and nanotechnology. Disciplines including chemical physics and electrical engineering have used approximate evolution operators to solve these systems for targeted physical quantities. Here, we discuss the approximation of closed time dependent quantum systems on bounded domains via evolution operators. The work builds upon the use of weak solutions, which includes a framework for the evolution operator based upon dual spaces. We are able to derive the corresponding Faedo-Galerkin equation as well as its time discretization, yielding a fully discrete theory. We obtain corresponding approximation estimates. These estimates make no regularity assumptions on the weak solutions, other than their inherent properties. Of necessity, the estimates are in the dual norm, which is natural for weak solutions. This appears to be a novel aspect of this approach.

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1 Introduction

This article continues the analysis of time dependent closed quantum mechanical systems, begun in [1] and continued in [2] for the system derived for time dependent density functional theory (cf. [3, 4, 5]). The emphasis in [1] was a rigorous study of discretization and well-posedness for strong solutions, based upon the evolution operator; this is consistent with the applications' literature [6, 7, 8, 9, 10]. In [2], we derived a global existence and uniqueness theorem, achieved via the contraction mapping theorem, for weak solutions. What is missing is a rigorous bridge to a space-time approximation theory, forming the basis for the computations employed in [11]. This is the topic of the current study. We derive a rigorous initial value problem for the Faedo-Galerkin approximate method; also, the time discretization of this equation. It will be necessary to discuss the evolution operator for the general system since estimation constants should be independent of the Galerkin subspace selected. We shall not attempt a survey of the Faedo-Galerkin method; the reader can consult [12] for a powerful analytical application of the method to nonlinear partial differential equations.

1.1 Time dependent quantum systems

In this article, we discuss linear systems. There is no loss of generality in this. In both [1, 2], the nonlinear systems were analyzed via fixed point mappings implemented by the linear evolution operator. Moreover, successive approximation, based on linear systems, was justified in [2]. Thus, we study the analog of the linear evolution operator, based upon a Galerkin approximation of the Hamiltonian. We review the Schrödinger system, which obeys the equation,

$$i\hbar \frac{\partial \Psi(t)}{\partial t} = \hat{H}\Psi(t). \tag{1}$$

Here, $\Psi = \{\psi_1, \ldots, \psi_N\}$. For mathematical well-posedness, an initial condition,

$$\Psi(0) = \Psi_0, \tag{2}$$

consisting of N orbitals, and boundary conditions must be adjoined. We will assume in this article that the particles are confined to a bounded region $\Omega \subset \mathbb{R}^d$ and that homogeneous Dirichlet boundary conditions hold for the evolving quantum state within a closed system. In general, Ψ denotes a finite vector function of space and time. In the mathematical arguments below, we will consider the case of arbitrary Euclidean dimension d. The Hamiltonian operator assumes the standard form, where V_{eff} is the effective potential,

$$\hat{H}(t) = -\frac{\hbar^2}{2m}\nabla^2 + V_{\text{eff}}(\cdot\,, t). \tag{3}$$

What separates this study, and the more general studies of [1], [2], from current mathematical studies of the Schrödinger system (see the monograph [13], for

example) is that the potential is time dependent. This necessitates the evolution operator, and is particularly important in the case of time dependent density functional theory.

1.2 The weak solution

We require the solution to be continuous from the time interval into H_0^1. The time derivative is required to be continuous from the time interval into H^{-1}. Finally, the spatially dependent test functions are arbitrary in the space H_0^1. We formalize this.

Definition 1.1. *For $J = [0, T]$, the vector-valued function $\Psi = \Psi(\mathbf{x}, t)$ is a weak solution of (1, 2, 3) if*

$$\Psi \in C(J; H_0^1(\Omega)) \cap C^1(J; H^{-1}(\Omega)),$$

if Ψ satisfies the initial condition (2) for $\Psi_0 \in H_0^1$, and if $\forall\, t \in J$ the following integral relation holds

$$i\hbar\langle \frac{\partial \Psi(\mathbf{x}, t)}{\partial t}, \zeta(\mathbf{x})\rangle = \int_\Omega \left\{ \frac{\hbar^2}{2m} \nabla\Psi(\mathbf{x}, t)\cdot \nabla\zeta(\mathbf{x}) + V_{\text{eff}}(\mathbf{x}, t)\Psi(\mathbf{x}, t)\zeta(\mathbf{x}) \right\} d\mathbf{x}.$$

Here, $\zeta \in H_0^1(\Omega)$ is arbitrary and V_{eff} is a function which is nonnegative and continuously differentiable on its space-time domain.

It follows as a special case of [2] that there is a unique weak solution of (1, 2, 3). The assumption on V_{eff} can be weakened (cf. section 4).

1.3 Hilbert space framework

In [2], the L^2 pivot space paradigm was employed, whereby the Sobolev spaces may be characterized as dense and nested. H^{-1} was realized as a reflexive Banach space. For the present study, it is more convenient to follow the idea used in [14, p. 32], where H^{-1} is represented as a real Hilbert space. We summarize the basic properties. Consider the dual space $H^{-1}(\Omega, \mathbb{C}^N)$ of continuous linear functionals on $H_0^1(\Omega, \mathbb{C}^N)$ and, for $u \in H^{-1}$, consider the uniquely determined element $\phi_u \in H_0^1$ satisfying

$$-\frac{\hbar^2}{2m}\Delta\phi_u + \phi_u = u \ (S\phi_u = u). \tag{4}$$

Here, we have noted the isomorphism $S : H_0^1 \mapsto H^{-1}$. The vector space H^{-1} is equipped with the scalar product,

$$(u, v)_{H^{-1}} = (\phi_u, \phi_v)_{H_0^1} = \text{Re}\ \left[\frac{\hbar^2}{2m} \int_\Omega \nabla\phi_u \cdot \overline{\nabla\phi_v}\ dx + \int_\Omega \phi_u \bar{\phi}_v\ dx \right].$$

Remark 1.1. *In [2], the Lumer-Phillips theorem in reflexive Banach spaces [15, 16] was employed to obtain contractive semigroups on H^{-1} generated by $\frac{-i}{\hbar}\hat{H}(t)$. The required properties for the generators are the dissipative property and the surjectivity of the generator, perturbed by a multiple of the identity. The authors of [14] obtain an equivalent theory expressed in terms of m-dissipative operators on real Hilbert spaces. This is the point of view we adopt here.*

Proposition 1.1. *The family $\frac{-i}{\hbar}\hat{H}(t)$ generates a contractive, in fact, isometric semigroup on the real Hilbert space H^{-1}. We write $T(t,s) = e^{-\frac{i}{\hbar}\hat{H}(s)t}$ for the semigroup.*

Proof. We summarize the details. By adapting the straightforward proof of [14, Prop. 2.6.14], we conclude that the negative Hamiltonian,

$$-\hat{H}(t) = \Delta - V(\cdot\,, t),\ \mathrm{Dom}_{\hat{H}} = H_0^1 \subset H^{-1},$$

is self-adjoint and nonpositive on H^{-1}. By [14, Cor. 2.4.8], this operator is m-dissipative; it follows that $\frac{-i}{\hbar}\hat{H}(t)$ generates a contractive, in fact, isometric semigroup on the real Hilbert space H^{-1} [14, Th. 3.2.3], written $T(t,s) = e^{-\frac{i}{\hbar}\hat{H}(s)t}$. □

1.4 The evolution operator and the Cauchy problem

We briefly summarize the theory here since it is relevant to the Galerkin evolution operator. The solvability of the Cauchy problem is a direct consequence of the existence of the time ordered evolution operator (see [17, 18, 19]; also, [20, Ch. 6]). There are similar results in [21]. For the interested reader, the exact statements are reproduced in the appendix of [1]. We state a summary version here, applicable to the contractive semigroups associated with the Schrödinger system.

Theorem 1.1. *Let X and Y be Banach spaces such that Y is densely and continuously embedded in X. Let $\{-A(t), 0 \le t \le T\}$ generate contractive semigroups on X, and assume the following.*

1. *If S is an isomorphism of Y onto X, then the family*

$$A_1(t) = SA(t)S^{-1}$$

   defines a collection of negative generators of strongly continuous semigroups on X.

2. *The space $Y \subset D_{A(t)}$ and the mapping $t \mapsto A(t)$ is continuous from $[0,T]$ to the normed space $B[Y,X]$ of bounded linear operators from Y to X.*

Under these conditions the evolution operators $U(t,s)$ exist uniquely as bounded linear operators on X, $0 \le s \le t \le T$ with the following properties.

I The family $\{U(t,s)\}$ *is strongly continuous on* X*, jointly in* (t,s)*, with:*

$$U(s,s) = I,\ \|U(t,s)\|_X \leq 1.$$

II The time ordering is expressed by:

$$U(t,r) = U(t,s)U(s,r).$$

III If D_t^+ *denotes the right derivative in the strong sense, then*

$$[D_t^+ U(t,s)g]_{t=s} = -A(s)g,\ g \in Y,\ 0 \leq s < T.$$

IV If d/ds *denotes the two-sided derivative in the strong sense, then*

$$(d/ds)U(t,s)g = U(t,s)A(s)g,\ g \in Y,\ 0 \leq s \leq t \leq T.$$

This is understood as one-sided if $s = t$ *or* $s = 0$*.*

Remark 1.2. *The identifications* $X = H^{-1}, Y = H_0^1$*, together with the isomorphism defined above in (4), allows one to obtain the evolution operator* $U(t,s)$ *for the Schrödinger system. Details were provided in [2] for the more complicated version considered. For the reader's convenience, we summarize the discussion regarding the operators* A_1 *at the conclusion of the introduction.*

This leads to the solution of the Cauchy problem, our principal goal [20, Prop. 6.4.1].

Theorem 1.2 (Cauchy problem)**.** *The Cauchy problem, for* $A(t) = \frac{i}{\hbar}\hat{H}(t)$*,*

$$\frac{d\Psi}{dt} + A(t)\Psi(t) = 0,\ \Psi(0) = \Psi_0, \tag{5}$$

is solvable for $\Psi_0 \in H_0^1$ *by the formula,*

$$\Psi(\cdot\,, t) = U(t,0)\Psi_0.$$

The verification of the second assumption of Theorem 1.1 is routine. The verification of the first assumption is a consequence of the following.

Proposition 1.2. *For* S *defined earlier in (4), we have:*

$$\hat{H}(t) = (S - I + V_{\text{eff}}). \tag{6}$$

In particular, we have the similarity relation,

$$SA(t)S^{-1} = A(t) + B(t),$$

for a family $B(t)$*, which can be extended as bounded linear operators on* H^{-1}*. In particular, the assumption on* $A_1(t)$ *holds. A uniform bound for* $\|U(t,s)\|$ *in* H_0^1 *is provided by* $Ce^{(t-s)\beta}$*, where* C *is a constant depending on* S*, and* β *serves as a uniform bound for* $\|B(t)\|_{H^{-1}}$*.*

Proof. All of the statements except the final one are verified in [2]. The final statement is proved in the monograph [20, Prop. 6.3.1; Eq. (6.3.20)]. □

Remark 1.3. *See [2, Eq. (7)] for an estimate on* β *in terms of the gradient of* V_{eff}*.*

2 The Galerkin Operator

Let $\mathcal{A} \subset H_0^1(\Omega)$ be given, with positive dimension m. $\mathcal{A}$ is a finite dimensional Hilbert subspace of H_0^1. Define, for each fixed $t \in [0,T]$, and $u(\cdot\,,t) \in \mathcal{A}$, the relation,

$$\mathcal{G}(t,u)[v] = \int_\Omega \left\{ \frac{\hbar^2}{2m} \nabla u(\mathbf{x},t) \cdot \nabla v(\mathbf{x}) + V_{\text{eff}}(\mathbf{x},t) u(\mathbf{x},t) v(\mathbf{x}) \right\} d\mathbf{x}, \ \forall v \in \mathcal{A}. \quad (7)$$

Definition 2.1. *Let $W(t,s) = T(t,s)|_{\mathcal{A}^*}$, where $T(t,s)$ has been introduced in Proposition 1.1 We identify W with the semigroup generated by $-\frac{i}{\hbar}\mathcal{G}(t)$.*

The interpretation of W is that it acts only on those linear functionals which are continuous on the dual of $\mathcal{A}$. These linear functionals Λ are represented as follows:

$$\Lambda(P\phi) = \ell(P\phi), \ \ell \in H^{-1},$$

where P is the orthogonal projection in H_0^1 onto $\mathcal{A}$.

2.1 Cauchy problem for the Galerkin operator: Faedo-Galerkin equation

This section deals with the Cauchy problem for the Galerkin operator. We have the following theorem.

Theorem 2.1 (Approximate Cauchy problem)**.** *The approximate Cauchy problem, for $A(t) = \frac{i}{\hbar}\mathcal{G}(t)$,*

$$\frac{d\Psi_{\mathcal{G}}}{dt} + A(t)\Psi_{\mathcal{G}}(t) = 0, \ \Psi_{\mathcal{G}}(0) = P\Psi_0, \quad (8)$$

is solvable for by the formula,

$$\Psi_{\mathcal{G}}(\cdot\,,t) = U_{\mathcal{G}}(t,0)P\Psi_0.$$

Here, $U_{\mathcal{G}}(t,s)$ denotes the time-ordered evolution operator, which acts contractively on $\mathcal{A}^*$, invariantly on $\mathcal{A}$, and is strongly differentiable in both arguments. We may interpret $\Psi_{\mathcal{G}}(t)$ as the Faedo-Galerkin approximation and (8) as the Faedo-Galerkin equation.

Proof. By use of P, the projection in H_0^1 onto $\mathcal{A}$, then we may obtain the analog of (4) as follows. Set

$$S_{\mathcal{G}} = SP,$$

so that the restriction of $S_{\mathcal{G}}$ is an isomorphism from $\mathcal{A}$ to $\mathcal{A}^*$. The arguments for the Hamiltonian are thus also valid for $\mathcal{G}$. This yields the evolution operator $U_{\mathcal{G}}(t,s)$ and the corresponding theory for the Cauchy problem. □

2.2 A calculus for Galerkin approximation

We begin with an operator result which allows the estimation involved in the approximation.

Theorem 2.2 (Fundamental estimation theorem)**.** *We retain our earlier notation for the evolution operators. Then, for $g \in H_0^1$, we have*

$$U_{\mathcal{G}}(t,r)g - U(t,r)g = -\frac{i}{\hbar}\int_r^t U_{\mathcal{G}}(t,s)[\mathcal{G}(s) - \hat{H}(s)]U(s,r)g\, ds, \tag{9}$$

where $U_{\mathcal{G}}$ is understood to act on elements in H_0^1 by first applying the orthogonal projection P.

Proof. One differentiates the expression,

$$U_{\mathcal{G}}(t,s)U(s,r)g,$$

with respect to s, and then integrates from r to t. The result follows from the differentiation formulas of Theorem 1.1. □

We obtain then the norm estimate for Faedo-Galerkin approximation. Although the estimate is in the dual norm, no regularity assumption is made, other than the inherent property satisfied by the weak solution.

Corollary 2.1.

$$\|U_{\mathcal{G}}(t,r)\Psi_0 - U(t,r)\Psi_0\|_{H^{-1}} \leq C(t-r)\tau(\mathcal{A})\|U\|_{\infty,H_0^1},$$

where C is a constant depending only on physical parameters, and on the potential, and $\tau(\mathcal{A})$ represents an order of best approximation in the H_0^1 norm by elements from $\mathcal{A}$.

Proof. We begin by estimating $\hbar$ times the rhs of (9) (with $g \mapsto \Psi_0$) in the H^{-1} norm:

$$\left\|\int_r^t U_{\mathcal{G}}(t,s)[\mathcal{G}(s) - \hat{H}(s)]U(s,r)\Psi_0\, ds\right\|_{H^{-1}} \leq$$
$$(t-r)\|[\mathcal{G}(s) - \hat{H}(s)]U(s,r)\Psi_0\|_{H^{-1}},$$

where we used the contractive property of $U_{\mathcal{G}}(t,s)$ on the dual space. We rewrite the expression within norms as

$$[\mathcal{G}(s) - \hat{H}(s)]U(s,r)\Psi_0 = [(S_{\mathcal{G}} - S) + (V_{\text{eff}} - I)(P - I)]U(s,r)\Psi_0,$$

and apply the triangle inequality to estimate the H^{-1} norm. The first term is estimated from above as

$$\|[S_{\mathcal{G}} - S]U(s,r)\Psi_0\|_{H^{-1}} = \|(I-P)U(s,r)\Psi_0\|_{H_0^1} \leq \tau(\mathcal{A})\|U\|_{\infty,H_0^1}\|\Psi_0\|_{H_0^1}.$$

The second term is estimated by a constant, depending on V_{eff}, times the previous estimate. This completes the proof. □

3 Time Discretization

In this section, we discuss the time discretization induced by the rectangular rule, which permits the approximation of the evolution operator by piecewise semigroups locally in time. It will be advantageous to do this jointly for both the Schrödinger and Faedo-Galerkin operators. The beginning of this section has some overlap with material in [1]; however, it is presented (differently) from the perspective of the current article.

3.1 Numerical evolution operator: Rectangular rule

We present a general result, not restricted to the quantum application. However, for the quantum application, we take $A(t) = \frac{i}{\hbar}\hat{H}(t)$ or $A(t) = \frac{i}{\hbar}\mathcal{G}(t)$.

Definition 3.1 (Rectangular Rule)**.** *Given $\{A(t)\}$ satisfying the hypotheses of Theorem 1.1, define the approximation operators*

$$A_n(t) = A(T[nt/T]/n),\ 0 \le t \le T.$$

Here, $[s]$ denotes the greatest integer less than or equal to s. If $s \le t$, and $s, t \in [t_{j-1}, t_j]$, and $A_n \equiv A$ on this interval, then

$$U_n(t,s) = e^{-(t-s)A}.$$

For other values of s, t, $U_n(t,s)$ is uniquely determined by the condition

$$U_n(t,r) = U_n(t,s)U_n(s,r).$$

These operators may be characterized as numerical evolution operators.

Remark 3.1. *The operators $\{U_n(t,s)\}$ satisfy the following properties.*

1. *Convergence of generator approximations as $n \to \infty$:*

$$\|A(t) - A_n(t)\|_{Y,X} \to 0,\ \textit{uniformly}, t \in [0,T].$$

2. *Invariance and uniform boundedness of evolution operators on Y:*

$$U_n(t,s)Y \subset Y,\ \|U_n(t,s)\|_Y \le Ce^{(t-s)\beta},\ \forall t,s,n.$$

   Here, C, β are defined in Proposition 1.2.

3. *Differentiation:*

$$(d/dt)U_n(t,s)g = -A_n(t)U_n(t,s)g,\ g \in Y,\ \textit{for}\ t \ne \frac{jT}{n}.$$

Theorem 3.1 (General result)**.** *Suppose a partition of the interval $[0,T]$ is given:*

$$0 = t_0 < t_1 < \cdots < t_n.$$

If $\Delta t := \max_{j=1,2,\ldots,n}(t_j - t_{j-1})$*, the rectangular rule is globally convergent: for* $t, r \in [0,T]$*,* $r < t$*,*

$$\|U(t,r)g - U_n(t,r)g\|_X \leq C\|g\|_Y \ (t-r) \sup_{s\in[0,T]} \|A(s) - A_n(s)\|_{Y,X}.$$

Here, If $t, r \in [t_{j-1}, t_j]$*, this global estimate implies the rate of convergence of order* $o(\Delta t)$*. The lengths of the subintervals can be chosen adaptively. Finally,* C *is a uniform bound for* $\|U_n(t,s)\|_{\infty,Y}$*.*

Proof. Consider the identity:

$$U(t,r)g - U_n(t,r)g = -\int_r^t U(t,s)[A(s) - A_n(s)]U_n(s,r)g \, ds, \qquad (10)$$

which follows from the differentiation of $-U(t,s)U_n(s,r)g$ with respect to s, followed by its integration. The estimate is now immediate from the uniform convergence of the generator sequence and the norm estimates satisfied by the evolution operators. □

3.2 Time discretization of the Faedo-Galerkin equation

The result of the preceding section can be applied to both of the evolution operators considered here. It is most natural, however, to apply the approximation to $U_{\mathcal{G}}(t,s)$ since this yields a space-time approximation operator.

Definition 3.2. *Consider the operators* $\mathcal{G}(t)$*, defined in (7). We denote by* $U_{\mathcal{G},n}$ *the operators described in Definition 3.1 and Remark 3.1.* Y *is interpreted as* $\mathcal{A} \subset H_0^1$ *and* X *as the corresponding dual space. Moreover, on each of the subintervals,* $t_{j-1} \leq t < t_j$*, we define* $\Psi_{\mathcal{G},n}(\cdot\,,t) = U_{\mathcal{G},n}(t,t_{j-1})\Psi_{\mathcal{G},n}(\cdot\,,t_{j-1})$*.*

It is now possible to obtain the corresponding result formulated in Theorem 3.1.

Theorem 3.2 (Estimates for the rectangular rule)**.** *Suppose a partition of the interval* $[0,T]$ *is given:*

$$0 = t_0 < t_1 < \cdots < t_n.$$

If $\Delta t := \max_{j=1,2,\ldots,n}(t_j - t_{j-1})$*, then the approximation order of*

$$\|\Psi_{\mathcal{G}}(\cdot\,,t) - \Psi_{\mathcal{G},n}(\cdot\,,t)\|_{H^{-1}}$$

is $o(\Delta t)$*. The constants depend only on the Schrödinger system as formulated, and not the Galerkin subspace selected for approximation.*

Proof. Theorem 3.1 is applied on each subinterval of the partition. The result follows since the generator convergence is uniform on $[0,T]$. □

3.3 Space-time discretization

It is possible now to obtain error estimates for space-time discretization based on an arbitrary Galerkin method combined with the rectangular rule for time discretization. We have the following.

Theorem 3.3 (Space-time approximation)**.** *Let $\Psi(\cdot\,,t)$ denote the unique weak solution of the Schrödinger system as defined in Definition 1.1. Let $\mathcal{A} \subset H_0^1(\Omega)$ be given, with dimension m, as in Section 2, and suppose Δt is given as in Theorem 3.2. If $\Psi_{\mathcal{G},n}$ denotes the approximation of Theorem 3.2, then the approximation order of*

$$\|\Psi(\cdot\,,t) - \Psi_{\mathcal{G},n}(\cdot\,,t)\|_{H^{-1}}$$

is

$$O(\tau(\mathcal{A})) + o(\Delta t).$$

The constants depend only on the Schrödinger system as formulated, and not the Galerkin subspace selected for approximation.

Proof. The result follows directly from an application of the triangle inequality to the estimates of Corollary 2.1 and Theorem 3.2. □

4 Conclusions and Remarks

In this section, we summarize the results of the article, and indicate that these results are more general than supposed.

4.1 Conclusions

In this article, we have utilized the unifying properties of the evolution operators, specifically those associated with the Hamiltonian, and the Galerkin and time discretized approximate operators. These operators permit a Cauchy formulation in all three cases. The properties of the evolution operators allow the derivation of an approximation theory based on constants independent of the Galerkin subspace and time discretization. Moreover, the estimates, obtained in the dual norm, are independent of additional regularity assumptions, beyond those inherent in the weak solution. The motivation for this special structure lies in the application and computational literature. In terms of the latter, the use of the FEAST algorithm for time prolongation of the (numerical) evolution operator advances the basis coefficients of the Galerkin approximation by a spectral method [11, 1]. The theory developed here supports this.

4.2 Remarks

It is possible, as remarked in the introduction, to weaken the hypothesis on the effective potential; this will depend on the particular application. One requires a bounded potential (the Hamiltonian should be associated with a self-adjoint operator) and one with the regularity to generate a member of the dual

space, appropriately continuous in time. This extension is useful when successive approximation is employed in the more general case of Kohn-Sham potentials. It is possible to employ more sophisticated time discretization, as was demonstrated in [1]. One would expect an analogous theory, with superior estimates. The details are not appropriate here. Similar remarks apply to the spatial estimates, if greater regularity is present.
One of the advantages of the use of the evolution operator, associated with the Hamiltonian, is the theoretical use of the fixed point argument as applied in [2]. Ultimately, the approximation theory is valid, since the solution of the nonlinear problem is characterized via a linear problem, defined by the fixed point equation.

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