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Convergent iteration in Sobolev space for time dependent closed quantum systems

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ABSTRACT

Time dependent quantum systems have become indispensable in science and its applications, particularly at the atomic and molecular levels. Here, we discuss the approximation of closed time dependent quantum systems on bounded domains, via iterative methods in Sobolev space based upon evolution operators. Recently, existence and uniqueness of weak solutions were demonstrated by a contractive fixed point mapping defined by the evolution operators. Convergent successive approximation is then guaranteed. This article uses the same mapping to define quadratically convergent Newton and approximate Newton methods. Estimates for the constants used in the convergence estimates are provided. The evolution operators are ideally suited to serve as the framework for this operator approximation theory, since the Hamiltonian is time-dependent. In addition, the hypotheses required to guarantee quadratic convergence of the Newton iteration build naturally upon the hypotheses used for the existence/uniqueness theory.

1. Introduction

Time dependent density functional theory (TDDFT) dates from the seminal article [1]. A current account of the subject and a development of the mathematical model may be found in [2]. For the earlier density functional theory (DFT), we refer the reader to [3,4]. Our focus in this article is TDDFT only. Closed quantum systems on bounded domains of $\mathbb{R}^3$ were analyzed in [5,6], via time-ordered evolution operators. The article [5] includes simulations based on approximations of the evolution operator, employing a spectral algorithm. The article [6] extended the existence results of [5] to include weak solutions via a strict contraction argument for an operator K; [6] also includes the exchange–correlation component of the Hamiltonian potential not included in [5]. TDDFT is a significant field for applications (see [7–11]), including the expanding field of chemical physics, which studies the response of atoms and molecules to external stimuli.

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By permitting time dependent potentials, TDDFT extends the nonlinear Schrödinger equation, which has been studied extensively [12,13].

In this article, we build upon [6] by introducing a Newton iteration argument for $I-K$. This is examined at several levels, including classical Newton iteration and also that of approximate Newton iteration, defined by residual estimation. It is advantageous that the existence/uniqueness theory of [6] employs strict contraction on a domain with an 'a priori' norm bound. One consequence is that the local requirements of Newton's method can, in principle, be satisfied by preliminary Picard iteration (successive approximation). The results of this article should be viewed as advancing understanding beyond that of an existence/uniqueness theory; they are directed toward ultimately identifying a successful constructive approach to obtaining solutions. In the following subsections of the introduction, we familiarize the reader with the model, and summarize the basic results of [6], which serve as the starting point for the present article. In this presentation, we provide explicit estimates for the domain and contraction constant used for the application of the Banach contraction theorem. Section two cites and derives essential operator results regarding Newton iteration in Banach spaces. Section three is devoted to an exact Newton iteration, with quadratic convergence, for the quantum TDDFT model, whereas section four considers an approximate quadratically convergent Newton iteration for the TDDFT model. Section five is a brief 'Conclusion' section. Appendices are included, which state the hypotheses used in [6] (Appendix A), basic definitions of the norms and function spaces adopted for this article (Appendix B), and a general Banach space lemma characterizing quadratic convergence for approximate Newton iteration (Appendix C).

The constants which appear in the analysis are directly related to the components of the potential. The external potential and the Hartree potential present no problem. However, as observed in [2], there is no explicit universally accepted representation of the exchange–correlation potential, which is required to be non-local in our approach. It follows that the explicit convergence estimates we present are strongest in the absence of this potential, or in the case when concrete approximations are employed. This is developed later in the article.

1.1. The model

TDDFT includes an external potential, the Hartree potential, and the exchange–correlation potential. If $\hat{H}$ denotes the Hamiltonian operator of the system, then the state $\Psi(t)$ of the system obeys the nonlinear Schrödinger equation,

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

Here, $\Psi = \{\psi_1, \ldots, \psi_N\}$ and the charge density ρ is defined by

$$\rho(\mathbf{x}, t) = |\,\Psi(\mathbf{x}, t)|^2 = \sum_{k=1}^{N} |\psi_k(\mathbf{x}, t)|^2.$$

For well-posedness, an initial condition,

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

consisting of N orbitals, and boundary conditions must be adjoined. We will assume that the particles are confined to a bounded region $\Omega \subset \mathbb{R}^3$ 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.