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Time dependent closed quantum systems: Nonlinear Kohn–Sham potential operators and weak solutions

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ABSTRACT

We discuss time dependent quantum systems on bounded domains from the perspective of nonlinear, time-dependent potentials. The time dependence of the Kohn–Sham potentials distinguishes this study from that of the so-called nonlinear Schrödinger equation, much studied in the mathematical community. We are interested in establishing a framework for potentials including the external potential, the Hartree potential and the exchange correlation potential that occur in time dependent density functional theory (TDDFT). As in the previous work, we make use of the time-ordered evolution operator. A departure from the previous work is the use of weak solutions for the nonlinear model; this necessitates a new framework for the evolution operator based upon dual spaces. We are able to obtain unique global solutions. The author thanks Eric Polizzi for discussions leading to the incorporation of a version of the exchange correlation potential in the model.

1. Introduction

This article continues the analysis of a general version of time dependent closed quantum mechanical systems, begun in [12]. The emphasis in this work was on a rigorous study of discretization and well-posedness based upon the evolution operator; this is consistent with the applications' literature [20,4,3,24,17,23]. Here, we extend the analysis to a broader class of nonlinear potentials and a broader class of solutions than considered in our previous work. In particular, we incorporate the exchange correlation potential, in addition to the Hartree potential considered in [12]. The systems which we study are confined to bounded domains with homogeneous Dirichlet boundary values. We now summarize the plan of the article. In the remainder of the introduction, we define the admissible nonlinear quantum systems, via the specification of the Hamiltonian operator. In the second section, we establish the framework for the evolution operator defined with respect to appropriate dual spaces. In section three, we give the details of the global existence and uniqueness theorem, achieved via the contraction mapping theorem.

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1.1. Time dependent quantum systems

Classical density functional theory (DFT) transfers inter-electron effects to the exchange-correlation potential, expressed as a functional of the electron density ρ [15,16]. This theory, and its time-dependent counterpart, TDDFT, proposed in [22], are capable of representing a many-electron system in terms of non-interacting effective particles. We allow for a realization Φ of this term below. The aggregate potential is the effective potential V_{eff}. This leads to the Hamiltonian $\hat{H}$ and its associated Kohn–Sham orbitals. For any usefulness in the applied community, the effective potential must be permitted to include a term (perhaps interpreted as an excitation term) with explicit dependence on time; in addition, the exchange correlation has a time history. This excludes the use of convolution semigroups, except as an approximation tool. The evolution operator is required.

1.2. Initial value problem for Schrödinger systems

We follow the notation and format of [7]. If we denote by $\hat{H}$ 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 [23, Eq. (2.37)]

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

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 $\Omega \subset \mathbb{R}^3$ 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. In the mathematical arguments below, we will consider the classical case of Euclidean dimension $d = 3$. In the final section, we will comment on the cases $d = 1, 2$.

1.3. Specification of the Hamiltonian operator

If, as discussed earlier, the electron charge density is defined by $\rho = |\Psi|^2$, we study potentials which are of the form,

$$V_{\text{eff}}(\mathbf{x}, t, \rho) = V(\mathbf{x}, t) + W * \rho + \Phi(\mathbf{x}, t, \rho),$$

where, for $W(\mathbf{x}) = 1/|\mathbf{x}|$, the convolution $W * \rho$ denotes the Hartree potential, and where Φ represents a time history of ρ:

$$\Phi(\mathbf{x}, t, \rho) = \Phi_0(\mathbf{x}, 0, \rho) + \int_0^t \phi(\mathbf{x}, s, \rho)\, ds.$$