EXISTENCE OF PROPAGATORS FOR COULOMB-LIKE POTENTIALS IN DENSITY FUNCTIONAL THEORY

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Density Functional Theory (DFT) is one of the most widely used methods for electronic structure calculations in materials science. It was realized that for $N \geq 10^3$ electrons, it is impractical to find the N particle wave function for this system. One of the gems of DFT is the Hohenberg-Kohn Theorem, which says that the ground state electron density alone provides all properties of a given static system. When the system is allowed to evolve in time, the corresponding time dependent theory (TDDFT) was initiated by E. Runge and E. K. U Gross in the early 1980's, and is one of the most popular theories for computing electronic excitation spectra. Runge and Gross proved a time dependent analog of the Hohenberg-Kohn Theorem, which is the starting point for our work. While attempting to develop a new proof of the Runge-Gross Theorem, there came a need to solve a Schrödinger equation with time dependent Hamiltonian in $\mathbb{R}^{3N}$. By smoothing out the classical Coulomb potential, we show existence of unitary propagators for a general time dependent Schrödinger equation where we allow the atomic nuclei to move along classical trajectories. By appealing to a classical 1973 result of Barry Simon, we can also understand the spectrum of the underlying time dependent Hamiltonian. This is joint work with Maxim Gilula (MSU) and is inspired by work of John Perdew (Temple).

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