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The computational foundations of time dependent density functional theory JAMES WHITFIELD, University of Vienna — The mathematical foundations of TDDFT are established through the formal existence of a fictitious non-interacting system (known as the Kohn-Sham system), which can reproduce the one-electron reduced probability density of the actual system. We build upon these works and show that on the interior of the domain of existence, the Kohn-Sham system can be efficiently obtained given the time-dependent density. Since a quantum computer can efficiently produce such time-dependent densities, we present a polynomial time quantum algorithm to generate the time-dependent Kohn-Sham potential with controllable error bounds. Further, we find that systems do not immediately become non-representable but rather become ill-representable as one approaches this boundary. A representability parameter is defined in our work which quantifies the distance to the boundary of representability and the computational difficulty of finding the Kohn-Sham system.

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