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Time-Dependent Density-Functional Theory in Massively

...

This theorem has since
been extended to the
time-dependent
domain to develop
time-dependent
density functional

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theory (TDDFT), which can be used to describe excited states. The second H-K theorem defines an energy functional for the system and proves that the correct ground-state electron density minimizes this energy functional.

**7th Time-Dependent
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Simulating One-Photon
Absorption and

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Density
Resonance Raman
Scattering Spectra
Using Analytical
Excited State Energy
Gradients within Time-
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Functional Theory. DOI:
10.1021/ct4007772.
Daniel W. Silverstein,
Chris B. Milojevich, Jon
P. Camden, and Lasse
Jensen.

**Time-dependent
density functional
theory -**

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Time-dependent density-functional theory (TDDFT) describes the quantum dynamics of interacting electronic many-body systems formally exactly and in a practical and efficient manner.

Progress in Time-Dependent Density-Functional Theory ...

Density-Functional Theory for Time-Dependent Systems. A

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Density-functional formalism comparable to the Hohenberg-Kohn-Sham theory of the ground state is developed for arbitrary time-dependent systems. It is proven that the single-particle potential $v(\mathbf{r} \rightarrow t)$ leading to a given v -representable density $n(\mathbf{r} \rightarrow t)$ is uniquely determined so that the corresponding map $v \rightarrow n$ is invertible.

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Density (PDF) Time- Dependent Density Functional Response Theory ...

Time-dependent density-functional theory (TDDFT) is a formally exact approach to the time-dependent electronic many-body problem which is widely used for calculating excitation energies. We present a survey of the fundamental framework, practical

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Density
aspects, and
applications of TDDFT.

Concepts And Applications **Density functional theory - Wikipedia**

Time-dependent
density-functional
theory (TDDFT)
describes the quantum
dynamics of interacting
electronic many-body
systems formally
exactly and in a
practical and efficient
manner. TDDFT has
become the leading
method for calculating

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excitation energies and optical properties of large molecules, with accuracies that rival traditional wave-function based methods, but at a fraction of the computational cost.

Amazon.com: Time-Dependent Density-Functional Theory ...

In view of the success of density functional methods in the treatment of stationary

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many-body systems and in view of their numerical simplicity, a time-dependent version of density functional theory appears highly desirable, both within and beyond the regime of linear response.

TIME-DEPENDENT DENSITY FUNCTIONAL THEORY | Annual Review ...

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density-functional theory (TDDFT) extends the basic ideas of ground-state density-functional theory (DFT) to the treatment of excitations or more general time-dependent phenomena.

Time-Dependent Density-Functional Theory: Concepts and ...

- Abstract Time-dependent density

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functional theory (TDDFT) can be viewed as an exact reformulation of time-dependent quantum mechanics, where the fundamental variable is no longer the many-body wave function but the density.

Density-Functional Theory for Time-Dependent Systems

...

In this article, we show how time-dependent

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density-functional theory (TDDFT) in real time can be a very competitive approach to study the excited states of electronic systems in massively parallel architectures, especially when combined with a spatial grid representation.

**A brief compendium
of time-dependent
density-functional
theory**

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The classic density-functional theory (DFT) formalism introduced by Hohenberg, Kohn, and Sham in the mid-1960s is based on the idea that the complicated N -electron wave function can be replaced with the mathematically simpler 1-electron charge density in electronic structure calculations of the ground stationary state. As such, ordinary DFT

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Density
cannot treat time-
dependent (TD) Theory
problems nor describe
excited electronic
states.
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Time Dependent Density Functional Theory

Time-dependent
density-functional
theory (TDDFT) is a
quantum mechanical
theory used in physics
and chemistry to
investigate the

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properties and dynamics of many-body systems in the presence of time-dependent potentials, such as electric or magnetic fields. The effect of such fields on molecules and solids can be studied with TDDFT to extract features like excitation energies, frequency-dependent response properties, and photoabsorption spectra.

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Time-Dependent Density-Functional Theory: Concepts and ...

A density-functional formalism comparable to the theory of Hohenberg, Kohn and Sham is developed for electronic systems subject to time-dependent external fields.

Density functional theory of time-

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dependent

phenomena ...

Time-dependent density-functional theory (TDDFT) is an extension of density functional theory (DFT)

to time-dependent problems, and can be viewed as an alternative formulation of time-dependent quantum mechanics.

As in DFT, the wave-function no longer has the leading role: the basic variable of TDDFT

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is the one-body
electron density, $n(\mathbf{r},t)$.

Time-dependent Density Functional Theory

Time-dependent
density-functional
response theory (TD-
DFRT) is presented
from the point of view
of quantum chemistry.
The extension of
density-functional
theory (DFT) into the
time-domain is
reviewed from the

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Density
point of view of Runge,
Gross, and Kohn.
Functional Theory

Concepts And Applications **Time-Dependent Density Functional Response Theory for**

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response theory (TD-
DFRT) is presented
from the point of view
of quantum chemistry.
The extension of
density-functional
theory (DFT) into the
time-domain is...

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Density Functional Theory of Time- Dependent Systems Applications

The time-dependent density determines uniquely the time-dependent external potential and hence all physical observables for fixed initial state.

$\rho(r, t) \rightarrow \rho(r, t) \rightarrow \rho(r, t) \rightarrow \rho(r, t)$

TDKS theorem: The time-dependent density of the interacting system of

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interest can be
calculated as density of
an auxiliary non-
interacting (KS) system
with the local potential.

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Time-dependent density functional theory - Wikipedia

Time-dependent
density-functional
theory (TDDFT) is a
quantum mechanical
framework which
describes the dynamics
of interacting
electronic many-body

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systems formally
exactly and in a
computationally
efficient manner. This
book presents the
concepts of TDDFT at
the graduate level.