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**Time-Dependent Density-Functional Theory**

**Editorial**

**Time-dependent density-functional theory**

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Time-dependent current density functional theory via time-dependent deformation functional theory: a constrained search formulation in the time domain

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The logical structure and basic theorems of time-dependent current density functional theory (TDCDFT) are analyzed and reconsidered from the point of view of recently proposed time-dependent deformation functional theory (TDDeF). It is shown that the formalism of TDDeF allows to avoid a traditional external potential-to-density/current mapping. Instead the theory is formulated in a form similar to the constrained search procedure in the ground state DFT. Within this formulation of TDCDFT all basic functionals appear from the solution of a constrained universal many-body problem in a comoving reference frame, which is equivalent to finding a conditional extremum of a certain universal action functional. As a result the physical origin of the universal functionals entering the theory, as well as their proper causal structure become obvious. In particular, this leaves no room for any doubt concerning the predictive power of the theory.

I. Introduction

The last decades have witnessed the growing popularity of time-dependent density functional theory (TDDFT) as a practical tool for studying dynamics of various quantum many-body systems (see ref. 2 and references therein). The range of applications of TDDFT (including its current-based version, the time-dependent current density functional theory (TDCDFT)) is impressively broad. The interaction of atoms, molecules and solids with electromagnetic radiation, transport phenomena in nanostructured systems, dynamics of nuclear matter and ultracold trapped atomic gases form a by far incomplete list of modern TDDFT/TDCDFT applications.

A birth of TDDFT can be dated back to the time of the late 70s/early 80s, when the first generalizations of the Hohenberg–Kohn theorem to time-dependent phenomena were established in the linear response regime and for arbitrary strong, but periodic with time, external potentials. This early period of the theory was completed in 1984 with the work by Runge and Gross who proved a time-dependent density functional theory in the time domain

definition of xc potentials in TDDFT. Presently we have many explanations and resolutions of this paradox, but, surprisingly, the most straightforward and elementary resolution of the causality problem has been proposed only in the last year. Another puzzling surprise that appeared in the last year was an observation made by Baer. He found that in a lattice formulation of the theory, in contrast to the ground state DFT on a lattice, there are apparently reasonable time-dependent densities which are not \( v \)-representable. This problem has been discussed and clarified in two very recent papers, but it became quite clear that \( v \)-representability, which is commonly taken for granted in TDDFT and TDCDFT, can be a serious issue. The second fundamental issue of TDDFT, the density-to-potential mapping, was also under debate in the last year. The authors of ref. 20 attempted to analyze a causal structure of the mapping from the density-to-external potential and arrived at a conclusion that TDDFT in the Kohn-Sham (KS) formulation cannot predict the dynamics of the density as the exchange-correlation (xc) potential does depend on a “future” in a form of a second time derivative of the density. In a recent comment Maier, et al., have demonstrated that this conclusion is based on a misunderstanding of the basic mapping theorem and proved that KS-TDDFT has full predictive power. However at the present stage of the theory this can be shown only for the KS-TDDFT while for the other, for example, hydrodynamic formulations of the theory the question raised in ref. 20 is still formally valid. In general, one should honestly say that the causal structure of all basic functionals in TDDFT and TDCDFT is not well studied and understood. Hence in the last year we have seen a great deal of papers debating all of the most fundamental aspects of TDDFT and
related approaches. Therefore it is timely to carefully re-examine the foundations and the logical structure of the theory and to formulate it, from the very beginning, in a way that takes into account our current level of understanding and the most recent developments in the field.

This work is an attempt at such a re-examination. Below I concentrate on the current density version of the theory (TDCDFT), bearing in mind its generality and numerous recent applications of TDDFT-based methods to the transport theory where the exact knowledge of the current is vital.

From conceptual point of view TDCDFT is a reduced theory which allows one to describe the behavior of the current \( j \) and the density \( n \) formally ignoring the rest of complicated microscopic dynamics of a quantum many-body system. In other words, TDCDFT is a formally closed theory of convective motion. It is most natural to formulate such a theory in a form of a closed system of equations of motion for the basic variables, the density and the current. This is the hydrodynamic formulation of TDCDFT, which is analyzed in detail in section II of the present paper. I show how hydrodynamic equations of motion are related to the microscopic many-body dynamics, and how one can make them closed by employing the traditional formulations of the TDCDFT mapping theorem.\(^{3,4} \) The main concern of section II is to prove an equivalence of different sets of basic variables which can be used in TDCDFT to describe the convective degrees of freedom. These are: (i) the current and the density \( (j,n) \); or (ii) the velocity field and the density \( (v,n) \) in the Eulerian description of convective dynamics; and (iii) a continuous set of trajectories \( x(\xi,t) \) of infinitesimal fluid element in the Lagrangian description. The hydrodynamic equations of TDCDFT for all three possible choices of basic variables are derived and compared. I also derive a KS formulation of TDCDFT and show how the basic universal functionals entering the hydrodynamic-TDCDFT and the KS-TDCDFT are related to each other. The most important part of the paper is section III where the foundations of TDCDFT are reconsidered from the point of view of recently proposed time-dependent deformation functional theory (TDDefFT).\(^{23} \) I prove the equivalence of these two theories and present a new logical structure of TDCDFT which is based on TDDefFT. The main idea of the new formulation is simple and physically transparent. From the very beginning we choose the Lagrangian trajectories to be a set of basic variables describing the convective motion, and separate the convective degrees of freedom by transforming the many-body Schrödinger equation to a reference frame moving with fluid elements. After this transformation an appearance of a closed theory of the convective dynamics becomes obvious. In fact, TDDefFT and thus TDCDFT take a form which very similar to the constrained search formulation of the ground state DFT.\(^{24–26} \) In the Conclusion section I briefly discuss the main results of this work and some perspectives for the further development of the theory.

Throughout this paper I am trying to avoid long algebraic manipulations and simply state the results when they are physically plausible (some detailed calculations, especially those related formalities of nonlinear transformations of coordinates can be found in ref. 22, 23 and 27). Instead, I am concentrating on the logical structure of the theory and on discussions of some delicate mathematical questions, such as the equivalence of different descriptions, uniqueness and existence of solutions, etc. I believe that this way of presentation is more suitable for the purpose of this work.

II. Hydrodynamic formulation of TDCDFT

A Starting point: general formulation of the quantum many-body problem

Let us consider a system of \( N \) identical particles in the presence of time dependent external scalar \( U(x,t) \) and vector \( A(x,t) \) potentials. The corresponding many-body wave function \( \Psi(x_1,\ldots,x_N,t) \) is a solution to the time-dependent Schrödinger equation

\[
\frac{i}{\hbar} \frac{\partial \Psi(x_1,\ldots,x_N,t)}{\partial t} = H \Psi(x_1,\ldots,x_N,t)
\]

with the following Hamiltonian

\[
H = \sum_{j=1}^{N} \left[ \left( \frac{\partial^2}{\partial x_j^2} + \frac{A(x_j,t)}{2m} \right)^2 + U(x_j,t) \right] + \frac{1}{2} \sum_{j \neq k} \left| V(x_j - x_k) \right|
\]

where \( V(x - x') \) is the interaction potential. For a given initial condition,

\[
\Psi(x_1, \ldots, x_N, 0) = \Psi_0(x_1, \ldots, x_N),
\]

the dynamics of the system is completely specified by eqn (2.1).

In most physically important situations it is not necessarily to know the full many-body wave function. Normally the experimentally measurable response of the system to external probes can be described in terms of reduced “collective” variables—the density of particles \( n(x,t) \), and the density of current \( j(x,t) \)

\[
n(x,t) = \rho(x,x,t),
\]

\[
j(x,t) = \frac{i}{2m} \lim_{\hbar \to 0} \left( \frac{\partial \rho}{\partial x} - \frac{\partial \rho}{\partial x'} \right) \rho(x,x',t) = -\frac{n}{m} A(x,t),
\]

where \( \rho(x,x',t) \) is the one particle reduced density matrix

\[
\rho(x,x',t) = N \int \prod_{j=2}^{N} dx_j \Psi^*(x,x_2,\ldots,x_N,t) \Psi(x',x_2,\ldots,x_N,t)
\]

The main idea of TDCDFT is to reduce, at the formally exact level, the problem of calculation of the density and the current to solving a closed system of equations which involve only \( n(x,t) \) and \( j(x,t) \). In the next two subsections we describe a few equivalent ways to formulate such a closed theory.

B Local conservation laws and TDCDFT hydrodynamics in Eulerian formulation

Using the microscopic definitions of eqn (2.4) and (2.5), and the Schrödinger eqn (2.1) one can derive the following hydrodynamic equations of motion for the density and the current

\[
\partial_t n + \nabla \cdot j = 0,
\]

\[
\rho \partial_t \mu + \nabla \cdot j = -n E + \nabla \cdot \Pi
\]
where \( \mathbf{E}(\mathbf{x},t) \) and \( \mathbf{B}(\mathbf{x},t) \) are electric and magnetic fields generated by the external time-dependent scalar and vector potentials

\[
\mathbf{E}(\mathbf{x},t) = -\partial_t\mathbf{A}(\mathbf{x},t) - \partial_x U(\mathbf{x},t), \tag{2.9}
\]

\[
\mathbf{B}(\mathbf{x},t) = \partial_x \times \mathbf{A}(\mathbf{x},t). \tag{2.10}
\]

Eqn (2.7) is the usual continuity equation, i.e., a local conservation law of the number of particles. The equation of motion for the current, eqn (2.8), physically corresponds to a local momentum conservation law (or a local force balance equation): the time derivative of the current equals to a sum of the external and internal forces. Importantly, the local internal force (the last term in eqn (2.8)) has a form of a divergence of a second rank tensor. Therefore the internal force vanishes after a volume integration in agreement with the Newton’s third law. The momentum flow tensor \( \Pi_{\mu\nu} \) entering eqn (2.8) contains a kinetic and an interaction contributions,\(^{27,28} \)

\[
\Pi_{\mu\nu} = \Pi_{\mu\nu}^{\text{int}} + \Pi_{\mu\nu}^{\text{kin}},
\]

which are expressed in terms of the many-body wave function as follows

\[
\Pi_{\mu\nu}^{\text{int}}(\mathbf{x},t) = \frac{1}{2m} \left\{ \lim_{\mathbf{x} \to \mathbf{x}} \left[ \left( \hat{P}_\mu \hat{P}_\nu + \hat{P}_\nu \hat{P}_\mu \right) \rho(\mathbf{x},\mathbf{x}',t) - \frac{\delta \mu \nu}{2} \hat{\nabla}^2 \rho(\mathbf{x},t) \right] \right\}, \tag{2.11}
\]

\[
\Pi_{\mu\nu}^{\text{kin}}(\mathbf{x},t) = -\frac{1}{2} \int \frac{d\mathbf{x}' \rho(\mathbf{x}',\mathbf{x},t)}{|\mathbf{x}' - \mathbf{x}|} \frac{\partial \hat{V}(\mathbf{x}')}{\partial \mathbf{x}'} \left. \right|_0^t, \tag{2.12}
\]

where \( \hat{P}_\mu = -\partial_\mu + A_\mu(\mathbf{x},t) \) is the kinematic momentum operator, and \( \hat{\Gamma}(\mathbf{x},\mathbf{x}',t) \) is a two particle reduced density matrix

\[
\hat{\Gamma}(\mathbf{x},\mathbf{x}',t) = \langle \mathbf{x} | \mathbf{x}' , \ldots , \mathbf{x}_N , t \rangle | \mathbf{x} , \mathbf{x}' , \ldots , \mathbf{x}_N , t \rangle. \tag{2.13}
\]

A formal possibility to formulate a closed theory for calculation the density and current distributions follows from the mapping theorem of TDCDFT.\(^{3,4} \) The main statement of this theorem can be formulated as follows. For a given initial state \( \Psi_0 \) a map of the external potentials to the current, \( (U, \mathbf{A}) \rightarrow \mathbf{j} \), is invertible and unique up to a gauge transformation, provided the potentials are analytic in time, and the current density is \( v \)-representable. (Note that here the term “\( v \)-representability” is understood in a broad sense: a current \( \mathbf{j} \) is called \( v \)-representable if it can be produced by some external \( 4 \)-potential \( (U, \mathbf{A}) \).

In fact, the above mapping theorem states that the potentials are unique (modulo gauge transformation) functionals of the initial state and the current density, \( U = U[\Psi_0, \mathbf{j}] \) and \( \mathbf{A} = \mathbf{A}[\Psi_0, \mathbf{j}] \). This immediately implies that the many-body wave function \( \Psi(t) \) and, therefore, any physical observable is also a functional of \( \Psi_0 \) and \( \mathbf{j} \). In particular, inserting the functionals \( \mathbf{A}[\Psi_0, \mathbf{j}] \) and \( \Psi = \Psi[\Psi_0, \mathbf{j}] \) into the definitions of eqn (2.11) and (2.12) we get the exact momentum flow tensor as a unique functional of the initial wave function and the current \( \Pi_{\mu\nu} = \Pi_{\mu\nu}[\Psi_0, \mathbf{j}] \). This functional is universal in a sense that it does not explicitly contain the external potentials, but is uniquely recovered from a given current and an initial state (in the following for the sake of brevity we omit \( \Psi_0 \) in the arguments of the functionals). Substituting the functional \( \Pi_{\mu\nu}[\mathbf{j}] \) into eqn (2.8) we obtain a closed system of equations of motion for \( n(\mathbf{x},t) \) and \( \mathbf{j}(\mathbf{x},t) \). Hence from the system of eqn (2.7)–(2.8) we can in principle determine the dynamics of the density of particles and the density of current avoiding, at least formally, an explicit solution of the full many-body problem. TDCDFT represented in a form of the closed system (2.7)–(2.8) can be viewed as an exact quantum hydrodynamics. It is worth noting that the hydrodynamic formulation of TDCDFT is analogous to the formulation of the static DFT in a form of the direct Hohenberg–Kohn variational principle.\(^{5} \)

A connection of the TDCDFT hydrodynamics to the standard mechanics of fluids\(^{29} \) can be made more obvious if we switch the basic variable from the current \( \mathbf{j} \) to the velocity field \( \mathbf{v} = \mathbf{j}/n \). It is also useful to extract from the full momentum flow tensor \( \Pi_{\mu\nu} \) its exactly known part—the flow of momentum due to convective motion of the fluid, \( mn v_{\mu} v_{\nu} \),

\[
\Pi_{\mu\nu} = mn v_{\mu} v_{\nu} + P_{\mu\nu}, \tag{2.14}
\]

where \( P_{\mu\nu} \) is the stress tensor which is responsible for a local internal force related to a relative motion of particles “inside” an small moving fluid element (see section III below for a more detailed discussion). Using the representation (2.14) and expressing all currents in terms of the velocity field we transform equations of motion (2.7) and (2.8) to the following standard “Navier–Stokes” form

\[
(\partial_t + v \cdot \nabla) n + n \partial_\lambda v_{\lambda} = 0, \tag{2.15}
\]

\[
m(\partial_t + v \cdot \nabla) v_{\mu} - [v \times \mathbf{B}]_{\mu} - E_{\mu} - \frac{1}{n} \partial_\sigma P_{\mu\sigma} = 0. \tag{2.16}
\]

Since the map \( (n, \mathbf{j}) \rightarrow (n, \mathbf{v}) \) is one-to-one we are allowed to replace the functional dependence of the stress tensor on the current by the functional dependence on the velocity field, \( P_{\mu\nu}[\mathbf{v}] \). It is also worth noting that the knowledge of only the current \( \mathbf{j} \) or the velocity \( \mathbf{v} \) is sufficient to recover the density by integrating the continuity equation in the form of (2.7) or (2.7), respectively.

C. Kohan–Sham construction in TDCDFT

Practical applications of any DFT mostly rely on the KS construction,\(^{30} \) which in the present time-dependent setting can be introduced as follows (see, e.g., ref. 22 and 31). Let us consider a fictitious system of \( N \) noninteracting particles in the presence of an electromagnetic field generated by the external \( 4 \)-potential \( (U, \mathbf{A}) \), and by some selfconsistent vector \( \mathbf{A}^{\infty} \) and scalar \( U^{\infty H} = U^{\infty} + U^{H} \) potentials, where \( U^{H} \) is the usual Hartree potential. The dynamics of this system is described by a set of one-particle Schrödinger equations for KS orbitals

\[
\partial_t \phi_j = \frac{1}{m} (i \partial_\lambda + \mathbf{A} + \mathbf{A}^{\infty})^2 \phi_j + (U + U^{\infty H}) \phi_j \tag{2.17}
\]

Obviously the density \( n_S \) and the velocity \( \mathbf{v}_S \) of the KS system satisfy the continuity eqn (2.15) and the force balance equation

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of the form of eqn (2.16), but with the stress tensor $P_{\mu\nu}$ and the external Lorentz force being replaced, respectively, by the kinetic stress tensor $T^{SS}_{\mu\nu}$ of the noninteracting KS particles, and by the Lorentz force corresponding to the total effective 4-potential. From the requirement that the KS density and current reproduce the density and the current in the real interacting system we get the following selfconsistency equation connecting the xc potential to the stress tensor functional

$$
\partial_t A^{\mu}_n - [v \times (\partial_k \times A^{\mu})]_\mu + \partial_{\mu} U^{nH} = - \frac{1}{n} \partial_{\nu} \Delta P_{\mu\nu}[v],
$$

where $\Delta P_{\mu\nu}[v] = P_{\mu\nu}[v] - T^{SS}_{\mu\nu}[v]$ is a difference of the stress tensors in the interacting and noninteracting KS systems. Eqn (2.18) can serve as a most general definition of the xc potentials. For a given stress tensor functional (right hand side) it defines the xc 4-potential ($U^{nH}, A^{nH}$) up a gauge transformation.

It is important to stress that the KS construction is only an auxiliary formal device for solving the general collective variable theory in a form of closed equations of motion, eqn (2.7) and (2.8) (or, equivalently, eqn (2.15) and (2.16)), for basic variables—the current/velocity and the density. The situation is very similar to the static DFT where the KS construction serves merely as useful mathematical trick for transforming the fundamental Hohenberg-Kohn variational principle to a system of differential equation for one-particle orbitals.

D Does TDCDFT/TDDFT have a predictive power?

Despite conceptually the traditional formulation of TDCDFT (as well as TDDFT) looks clean and very similar to the static DFT, it may cause some confusions. Let us assume that the stress tensor functional is known. The main goal of the theory is to calculate the current and the density at any instant $t$ by propagating the equations of motion (2.7) and (2.8) starting from the initial time, provided the initial conditions for $j$ and $n$ are given. Apparently the propagation of eqn (2.8) is only possible if $\Pi_{\mu\nu}[j]$ is a retarded functional of the current. In other words at any instant $t$ the stress tensor should only depend on the currents $j(t')$ at previous times $t' < t$. In particular, it should not contain local in time terms which depend on the time derivatives (of any order $r \geq 1$) of the current. However, both the original Runge-Gross proof, and its generalization to TDCDFT by Ghosh and Dhar establish only the uniqueness of the maps $j \rightarrow A$ and $j \rightarrow \Psi$, but do not state anything about the properties of functionals $\Delta[j]$ and $\Psi[j]$. On the other hand if we consider the local momentum conservation law, eqn (2.8), and interpret it as an equation which determines the external 4-potential for a given current, we immediately observe that the external force, and thus the external potential considered as functional of the current does indeed contain a local in time term proportional to $\partial_t j \sim \partial_t j$. Taking this fact naive one may conclude that the functionals $\Psi[j]$ and $\Pi_{\mu\nu}[j]$ should also contain such unwanted terms. Hence the propagation of the basic equation eqn (2.8) (or equivalently eqn (2.16)) becomes problematic. Therefore it appears that TDCDFT/TDDFT does not have a real predictive power.

In a recent paper Maitra et al. clearly demonstrated that the above conclusion is incorrect for the KS formulation of TDDFT. In fact, this is obvious from the van Leeuwen proof of the TDDFT mapping theorem, and its generalization to TDCDFT by Vignale. The construction proposed in ref. 3 and 21 shows that the difference of potentials driving the dynamics two different systems with the same current (e.g., interacting and noninteracting systems in the KS case) is uniquely recovered from the given density/current and has a proper causal structure. Unfortunately this methodology does not allow one, at least directly, to make any definite statement about the retardation properties of the many-body wave function $\Psi[j]$ as a functional of the current and, what is much more important, about the causal structure of the stress tensor functional entering the collective variable theory of eqn (2.15) and (2.16). In section III we show how these questions are resolved within a new constructive reformulation of the theory based on TDDeFT. As a first step in this direction we discuss one more alternative form of the TDCDFT hydrodynamics.

E TDCDFT hydrodynamics in the Lagrangian form

In general TDCDFT is a closed formalism that allows one to describe a convective motion of a quantum many-body system driven by an external field. Usually the convective motion is characterized by the density of particles $n(x,t)$ and the density of current $j(x,t)$ or a velocity field $v(x,t)$. An alternative way to completely characterize the convective motion is commonly referred to as a Lagrangian description. Let us consider the system as a collection of infinitesimal fluid elements (so called “materials”). Every fluid element can be uniquely labeled by a continuous variable $\xi$—its position at the initial time $t = 0$. The Lagrangian description can be viewed as tracking the motion of those infinitesimal elements of the fluid. In other words the convective motion of the system is characterized by a (continuous) set of trajectories $x(\xi, t)$, where the argument $\xi$ indicates the starting point of the trajectory (the unique label of the element). Let us show that in the case of dynamics of a quantum many-body system the map $v(x,t) \rightarrow x(\xi,t)$ is unique and invertible.

For a given velocity $v(x,t)$ the Lagrangian trajectory is solution to the following Cauchy problem

$$
\partial_{\xi} x(\xi,t) = v(x(\xi,t),t), \quad x(\xi,0) = \xi.
$$

It is known (see, for example, ref. 32) that eqn (2.19) has a unique solution $x(\xi,t)$ if the function $v(x,t)$ is continuous and satisfies the Lipschitz condition in spatial variables (i.e. there exists a constant $L > 0$, such that $|v(x) - v(x')| < L|x - x'|$ for any $x$ and $x'$). Apparently the velocity field coming from a physical wave function does satisfy these requirements. Physically the Lipschitz condition prevents generation of folds and shock fronts which are clearly absent at the microscopic level for the Schrödinger dynamics. Hence from a given physical velocity field we uniquely construct a set of Lagrangian trajectories. Every trajectory $x(\xi,t)$ is uniquely determined by its initial point $\xi$, which means that given the initial position $\xi$ of a fluid element we can always find its coordinate $x = x(\xi,t)$ at any instant $t$, and, tracing the trajectory in a reverse order, from a given position $x$ at
time \( t \) one uniquely recovers the initial point of the trajectory, \( \xi = \xi(x, t) \). In a more formal language, the map \( \xi \to x : x = x(\xi, t) \) is unique and invertible. This fact allows us to recover the Eulerian variables, i.e., the velocity field and the density, from given Lagrangian trajectories

\[
v(x, t) = \left[ \frac{\partial \xi}{\partial \xi} \right]_{\xi = \xi(x, t)}, \tag{2.20}
\]

\[
n(x, t) = \left[ \frac{\partial \xi}{\partial \xi} \right]_{\xi = \xi(x, t)}, \tag{2.21}
\]

where \( \xi(x, t) \) is the inverse of \( x(\xi, t) \), \( n(x) \) is the initial density, and \( \sqrt{g(\xi, t)} = J(\xi, t) = \det \left( \frac{\partial x}{\partial \xi} \right) \) is the Jacobian of the transformation of coordinates \( x \to \xi \). Eqn (2.20) is an obvious consequence of eqn (2.19), while eqn (2.21) can be straightforwardly checked by a direct substitution into the continuity eqn (2.15). Therefore the function \( x(\xi, t) \) indeed completely characterizes the convective motion of a system.

The basic equation in the Lagrangian description of collective dynamics is the equation of motion for a fluid element. This equation can be straightforwardly derived from the equation of motion for Eulerian velocity \( v(x, t) \), eqn (2.16), by making the transformation coordinates \( x \to \xi \), i.e., by considering the initial points \( \xi \) of Lagrangian trajectories as independent spatial coordinates. Under this transformation the convective derivative, \( \partial \xi / \partial t \), becomes simply \( \dot{\xi} \), so that the first term in eqn (2.16) transforms to \( m \ddot{x}(\xi, t) \), while the divergence of the stress tensor in the last term in eqn (2.16) becomes a covariant divergence in the space with metrics \( g_{\mu\nu}(\xi, t) \) induced by the transformation from \( x \)-to-\( \xi \)-coordinates. Hence after the transformation of coordinates we arrive at the following equation of motion for a fluid element

\[
m \ddot{x}^\mu - E_\mu(x, t) - \left[ x \times B(x, t) \right]_\mu + \sqrt{g(\xi, t)} \frac{\partial^2 x^\alpha}{\partial \xi^\beta} \frac{\partial \xi^\beta}{\partial x^\alpha} P_{\alpha\beta}[x(\xi, t), t] = 0,
\]

\[
(2.22)
\]

where \( \dot{P}_{\mu\nu}(\xi, t) \) is the original stress tensor \( P_{\alpha\beta}(x, t) \) transformed to the new coordinates according to the standard rules

\[
\dot{P}_{\mu\nu}(\xi, t) = \frac{\partial x^\alpha}{\partial \xi^\mu} \frac{\partial x^\beta}{\partial \xi^\nu} P_{\alpha\beta}(x(\xi, t), t)
\]

\[
(2.23)
\]

The nabla-operator in eqn (2.22) stands for a covariant divergence

\[
\nabla^\mu \dot{P}_{\mu} = \frac{1}{\sqrt{g}} \partial^\mu \sqrt{g} \dot{P}_{\mu} - \frac{1}{2} \dot{P}^{\mu\nu} \partial_{\nu} g_{\mu\nu},
\]

\[
(2.24)
\]

and the metric tensor in the \( \xi \)-space of “initial positions” is defined as follows

\[
g_{\mu\nu}(\xi, t) = \frac{\partial x^\alpha}{\partial \xi^\mu} \frac{\partial x^\beta}{\partial \xi^\nu} [g_{\mu\nu}]^{-1} = g^{\alpha\beta} \frac{\partial ^\mu x^\alpha}{\partial \xi^\mu} \frac{\partial ^\nu x^\beta}{\partial \xi^\nu}
\]

\[
(2.25)
\]

The equation of motion (2.22) has to be solved with the initial conditions \( x(\xi, 0) = \xi \) and \( \dot{x}(\xi, 0) = v_0(\xi) \), where \( v_0(x) \) is the initial velocity distribution calculated from the initial many-body wave function of eqn (2.3).

The first three terms in eqn (2.22) correspond to a classical Newton equation for a particle moving in the external electromagnetic field, while the last, the stress term, takes care of all complicated quantum and many-body effects. Because of the uniqueness and invertibility of the map \( v(x, t) \to x(\xi, t) \) the transformed stress tensor can be considered as a unique functional of the Lagrangian trajectories, \( \dot{P}_{\mu\nu} = \dot{P}_{\mu\nu}[x(\xi, t)] \). Hence eqn (2.22) is a closed equation of motion that, at the formally exact level, completely determines the collective dynamics of the system. This is the basic equation of TDCDFT in the Lagrangian form.

On the first sight the representation of TDCDFT hydrodynamics in the Lagrangian form of eqn (2.22) does not bring anything fundamentally new. This is indeed true if one follows a route outlined in this section: starting from the traditional formulation of the TDCDFT mapping theorem and via the Eulerian equation of motion for the density and the current. However, in the next section we will see that using the ideas of the Lagrangian description one can reformulate the whole theory, including all basic theorems, in a constructive way that also ends up with the equation of motion (2.22), but provides us with a clearly constrained search-like procedure for calculating the basic stress tensor functional.

### III. Time-dependent deformation functional theory

#### A Many-body theory in a comoving reference frame

Conceptually TDCDFT is a reduced theory aimed at describing only the convective motion of the system without a detailed knowledge of the full dynamics of all microscopic degrees of freedom. Therefore it looks natural to start the construction of such a theory by separating the “convective” degrees of freedom at the very beginning, i.e. at the level of the full microscopic many-body theory. The Lagrangian description is perfectly suited for this purpose. Since in this formalism the convective dynamics is characterized by the motion of fluid elements, it can be easily separated from the microscopic dynamics of quantum particles by transforming the many-body theory to a local noninertial reference frame moving along the Lagrangian trajectories.

At the formal level one proceeds as follows. Consider a reference frame defined by some (unspecified for the moment) velocity field \( v(x, t) \) which is required to be continuous and Lipschitz in spatial variables. By solving the Cauchy problem of eqn (2.19) with the above velocity in the right hand side we get the local trajectories \( x(\xi, t) \) of the frame. The transformation of the theory to the new reference frame corresponds to a transformation of coordinates \( x_j \to \xi_j \), with \( x_j(\xi_j, t) \) being the transformation function, i.e., \( x_j = x_j(\xi_j, t) \), in the many-body Schrödinger eqn (2.1). It is convenient to define the many-body wave function \( \Psi(\xi_1, \ldots, \xi_N, t) \) in the new frame as follows

\[
\Psi(\xi_1, \ldots, \xi_N, t) = \prod_{j=1}^N \psi_j(\xi_j, t) e^{-i S(\xi_j, t)} \Psi(x(\xi_1, t), \ldots, x(\xi_N, t), t),
\]

(3.26)
where \( S_{\nu}(\xi, t) \) is the classical action of a particle moving along the trajectory \( x(\xi, t) \)

\[
S_{\nu}(\xi, t) = \int_{0}^{t} \left[ \frac{m}{2} \left( x(t) \right)^{2} + \dot{x}(t)A(x(t), t) - U(x(t), t) \right] \, dt.
\]

Eqn (3.26) is a relatively straightforward generalization of the transformation to a homogeneously accelerated frame, which is used, for example, in the proofs of a harmonic potential theorem. The exponential prefactor accounts for the phase

\[
\exp \left( i \frac{\hbar}{m} \int_{0}^{t} L(t) \, dt \right)
\]

The Schroedinger eqn (3.28), the definition of the effective vector potential (3.30), and the zero current condition (3.32) constitute a closed system of equations that determine dynamics of the many-body system in the comoving reference frame. In principle one can eliminate the effective vector potential from this system by substituting \( \mathcal{A}(\xi, t) \) from eqn (3.32) into eqn (3.30) and (3.28). As a result we will get a system of two first order (in time) differential equations for two functions—(i) the trajectory \( x(\xi, t) \) which describes the convective motion on the system, and (ii) the transformed wave function \( \Psi(\xi_1, \ldots, \xi_N, t) \) describing the rest of microscopic degrees of freedom in the frame moving with the convective flow. The equations have to be solved with the initial conditions eqn (3.31) for \( \Psi(t) \) and \( x(\xi, 0) = \xi \) for the Lagrangian trajectory. The system of eqn (3.28), (3.30) and (3.32) is equivalent to the original linear Schroedinger eqn (2.1). Therefore we can guarantee that there exists a unique solution of the corresponding initial value problem.

\section{A “constrained search” formulation of TDDefFF}

Let us discuss possible procedures for solving the system of eqn (3.28), (3.30) and (3.32), but first it is useful to rewrite it in a more physical and clear form.

First of all, we note that because eqn (3.30) contains the classical action \( S_{\nu}(\xi, t) \) of eqn (2.37), it is nonlocal in time. It is convenient to remove this nonlocality by differentiating eqn (3.30) with respect to \( t \). Taking the derivative we reduce eqn (3.30) to the following form

\[
\tilde{\Psi}(\xi_1, \ldots, \xi_N, 0) = \Psi_{0}(\xi_1, \ldots, \xi_N).
\]

Eqn (2.22)–(3.31) completely determine dynamics of the quantum \( N \)-particle system in an arbitrary local noninertial frame.

Since our aim is to reformulate the theory in a particular frame moving with a physical flow (this frame is called comoving, or Lagrangian) we need to impose an additional local condition to specify the required frame. By the definition, in the comoving frame the current density is zero everywhere and at all times, while the density of particles stays stationary and equal to the initial density distribution \( n_{0}(\xi) \). Hence the most natural frame-fixing condition is the requirement of zero transformed current density \( \tilde{J}(\xi, t) = 0 \). Explicitly this condition reads

\[
m_{\nu}(\xi, t) = \frac{i}{\hbar} \lim_{\xi \rightarrow \xi} \left( \partial_{\xi} - \partial_{\xi} \right) \tilde{\rho}(\xi, t, t).
\]

where \( \tilde{\rho}(\xi, t, t) \) is the one particle reduced density matrix calculated from the transformed wave function

\[
\rho(x, x', t) = N \int \prod_{j=2}^{N} d\xi_{j} \Psi^{\dagger}(\xi, \xi_{2}, \ldots, \xi_{N}, t) \Psi(\xi', \xi_{2}, \ldots, \xi_{N}, t).
\]

The frame-fixing condition (3.32) simply states that in the comoving frame a “paramagnetic” current (the right hand side of (3.32)) is exactly cancelled by the “diamagnetic” contribution (the left hand side of (3.32)).

The Schrodinger eqn (3.28), the definition of the effective vector potential (3.30), and the zero current condition (3.32) constitute a closed system of equations that determine dynamics of the many-body system in the comoving reference frame. In principle one can eliminate the effective vector potential from this system by substituting \( \mathcal{A}(\xi, t) \) from eqn (3.32) into eqn (3.30) and (3.28). As a result we will get a system of two first order (in time) differential equations for two functions—(i) the trajectory \( x(\xi, t) \) which describes the convective motion on the system, and (ii) the transformed wave function \( \Psi(\xi_1, \ldots, \xi_N, t) \) describing the rest of microscopic degrees of freedom in the frame moving with the convective flow. The equations have to be solved with the initial conditions eqn (3.31) for \( \Psi(t) \) and \( x(\xi, 0) = \xi \) for the Lagrangian trajectory. The system of eqn (3.28), (3.30) and (3.32) is equivalent to the original linear Schroedinger eqn (2.1). Therefore we can guarantee that there exists a unique solution of the corresponding initial value problem.

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\[
m_{\nu} = E_{\nu}(x, t) + [\hat{x} \times B(x, t)]_{\nu} + \frac{\partial E_{\nu}}{\partial x} \partial_{\nu} \mathcal{A},
\]

which is exactly the classical Newtonian equation for a particle moving in the external electromagnetic field and, in addition, in the “electric” field generated by the effective vector potential \( \mathcal{A} \).

Comparing eqn (3.34) with eqn (2.22) we immediately observe that these two equation become identical if the time derivative of the effective vector potential would be equal to the covariant divergence of the stress tensor. To see that this is indeed the case we consider the local force balance equation that follows from the many-body Schrodinger eqn (2.38) in the local noninertial frame. Apparently the force balance equation should be of the general form of eqn (2.8), but with the usual divergence of the momentum flow tensor replaced by covariant divergence of the stress tensor in the \( \xi \)-space. Namely,

\[
\partial_{\nu} \tilde{J}_{\mu} - \tilde{J}^{\mu} (\partial_{\nu} \mathcal{A}_{\mu} - \partial_{\nu} \mathcal{A}_{\nu} + \tilde{n} \partial_{\nu} \mathcal{A}_{\nu} + \sqrt{g} \nabla_{\nu} \tilde{P}_{\mu} = 0.
\]

\section{C Numerical solution}

The solution of the system of eqns (3.28), (3.30) and (3.32) is related to the problem of finding the trajectory \( x(\xi, t) \) and the wave function \( \Psi(\xi_1, \ldots, \xi_N, t) \) which satisfy these equations.

\section{D The original TDDefFF code}

The original TDDefFF code is based on the explicit numerical solution of the system of eqns (3.28), (3.30) and (3.32) by using explicit integration methods such as Runge-Kutta.

\section{E Comparing TDDefFF code and the new code}

The new code is based on the implicit numerical solution of the system of eqns (3.28), (3.30) and (3.32) by using implicit integration methods such as trapezoidal rule.

\section{F The new code compared to the original TDDefFF code}

The new code is more efficient than the original TDDefFF code.

\section{G Conclusion}

The new code is more efficient than the original TDDefFF code.

\section{H Future work}

Future work includes the development of a more efficient code and the comparison with other methods.
where the stress tensor in the space with metric $g_{\mu\nu}$ can be conveniently determined from the following universal formula,

$$
\hat{P}_{\mu}(\xi, t) = \frac{2}{\sqrt{g}} \langle \Psi | \hat{H}[g_{\mu\nu}, \mathcal{A}] | \Psi \rangle \equiv \langle \Psi | \hat{P}_{\mu}[g_{\mu\nu}, \mathcal{A}] | \Psi \rangle
$$

(3.36)

with the Hamiltonian defined by eqn (3.29). An explicit form of the stress tensor operator $\hat{P}_{\mu}$, entering eqn (3.36) can be found, for example, in ref. 27. At the moment the important point is that $\hat{P}_{\mu}[g_{\mu\nu}, \mathcal{A}]$ is an explicitly known and local in time functional of the metric tensor and the effective vector potential. Since in the comoving frame the transformed current density $\hat{j}$ is zero, only the last two terms survive in eqn (3.35). Therefore in our frame of interest the force balance equation reduces to the following identity

$$
\partial_t \mathcal{A}_{\mu} = -\frac{\sqrt{g}}{n_0} \nabla_{\mu} \hat{P}_{\nu}\n_
u
$$

(3.37)

Inserting this identity into eqn (3.34) we exactly recover the basic equation of hydrodynamics in the Lagrangian description, eqn (2.22). The important progress is that the stress tensor in this equation is now defined entirely in terms of the fundamental fields entering the many-body problem in the comoving frame. Hence we have transformed eqn (3.30) to a transparent physical form and demonstrated that it is indeed the correct equation of motion for the fluid elements.

Using the results of eqn (3.34) and (3.37) we can write down the following final system of equations describing the dynamics of the full many-body system

$$
\partial_t \hat{\Psi}(\xi_1, \ldots, \xi_N, t) = \hat{H}[g_{\mu\nu}, \mathcal{A}]\hat{\Psi}(\xi_1, \ldots, \xi_N, t) \tag{3.38}
$$

$$
\mathcal{A}((\xi, t)) = \frac{i}{2n_0(\xi)} \lim_{\xi' \to \xi} (\partial_\xi - \partial_{\xi'}) \hat{\rho}(\xi', \xi', t) \tag{3.39}
$$

$$
m\hat{\Sigma}^\mu = E_\mu(x, t) + [\hat{\mathbf{B}}(x, t)]_{\mu} - \frac{\sqrt{g}}{n_0} \nabla_{\mu} \hat{P}_{\nu}\n_\nu \tag{3.40}
$$

where the Hamiltonian $\hat{H}[g_{\mu\nu}, \mathcal{A}]$, the reduced density matrix $\hat{\rho}(\xi', \xi', t)$, and the stress tensor $\hat{P}_{\mu}[g_{\mu\nu}, \mathcal{A}]$ are defined after eqn (3.29), (3.33), and (3.36), respectively. The metric tensor $g_{\mu\nu}(\xi, t)$ entering eqn (3.38) and (3.40) is related to the Lagrangian trajectory via eqn (2.25).

Importantly, the system of eqn (3.38)–(3.40) is mathematically equivalent to the original linear many-body Schrödinger eqn (2.1). In fact, everything we did to derive eqn (3.38)–(3.40) from eqn (2.1) was an identical change of variables aimed at separating the “convective” and the “relative” motions of quantum particles. However after this identical transformation the structure of the many-body theory becomes quite remarkable. The key observation is that the physical external fields enter only the equation of motion for the fluid elements, eqn (3.40), while the many-body dynamics, which is governed by eqn (3.38) and (3.39), depends only on the fundamental geometric characteristic of the comoving frame—the metric tensor $g_{\mu\nu}(\xi, t)$. Formally eqn (3.38) and (3.39) describe the dynamics of $N$ quantum particles driven by a given time-dependent metric and constrained by the requirement of zero current density. This constrained many-body problem can be equivalently represented in a form of a Dirac–Frenkel variational principle with the following action functional

$$
S[\Psi, \mathcal{A}] = \int_0^T dt \langle i(\hat{\Psi}^\dagger \partial_t |\hat{\Psi}\rangle - \langle \hat{\Psi}^\dagger [\hat{H}[g_{\mu\nu}, \mathcal{A}], \hat{\Psi}\rangle \rangle. \tag{3.41}
$$

Indeed, the conditions for the extremum of this action,

$$
\frac{\delta S[\Psi, \mathcal{A}]}{\delta \Psi^\dagger} = 0, \quad \frac{\delta S[\Psi, \mathcal{A}]}{\delta \mathcal{A}} = 0, \tag{3.42}
$$

are identical to eqn (3.38) and (3.39), respectively. From the variational formulation we clearly see the effective vector potential is simply a Lagrange multiplier that ensures the zero current constraint.

The formulation of the many-body part of the problem in a form of the variational principle can be viewed as a time-dependent analog of the Levy–Lieb constrained search formulation of the static DFT
date{38} (see also ref. 37). By finding an extremizer of the functional (3.41), or, equivalently, by solving the constrained many-body problem of eqn (3.38) and (3.39) for a given metric of the form (2.25) we get the wave function $\Psi$ and the Lagrange multiplier $\mathcal{A}$ as universal functionals of the metric tensor: $\Psi = \Psi[g_{\mu\nu}]$ and $\mathcal{A} = \mathcal{A}[g_{\mu\nu}]$. Substitution of these functionals in to eqn (3.36) gives the universal stress tensor functional $\hat{P}_{\mu}[g_{\mu\nu}]$. Thus eqn (3.40) becomes a closed equation of motion for fluid elements, which determines the Lagrangian trajectories of the system. As all basic quantities are functionals of the metric tensor, which is exactly the Green’s deformation tensor of the classical elasticity theory,

$$
\frac{\delta S[\Psi, \mathcal{A}]}{\delta \mathcal{A}} = 0, \quad \frac{\delta S[\Psi, \mathcal{A}]}{\delta \mathcal{A}} = 0, \tag{3.42}
$$

which is natural to call this approach the time-dependent deformation functional theory (TDDfT).

The direct solution of eqn (3.40) with a known functional $\hat{P}_{\mu}[g_{\mu\nu}]((\xi, t))$ gives the description of the convective motion in terms of the Lagrangian picture. Alternatively we can transform $\hat{P}_{\mu}[g_{\mu\nu}]((\xi, t))$ to the laboratory frame to recover the tensor $\hat{P}_{\mu}[v(x, t)]$

$$
P_{\mu}[v](x, t) = \frac{\partial x^\mu}{\partial x^\nu} \frac{\partial x^\nu}{\partial x^\nu} \hat{P}_{\nu}[g_{\mu\nu}](\xi(x, t), t))((\xi(x, t), t), \tag{3.43}
$$

which can be used either in the hydrodynamic formulation of eqn (2.7)–(2.8) or to calculate the $xc$ potentials for the KS formulation of TDDCfT, eqn (2.17)–(2.18). Finally, since in the laboratory frame the function $\xi(x, t)$ (the initial point of the trajectory that arrives to $x$ at time $t$) can be found from the equation

$$
[v_{\xi} + v(x, t)\partial_\xi]\xi(x, t) = 0, \quad \xi(x, t) = x \quad \tag{3.44}
$$

the stress tensor determined by eqn (3.43) is indeed a universal functional of the Eulerian velocity $v(x, t)$.

Therefore we recovered the full formal structure of the traditional TDDCfT, but at the fundamentally new level of understanding. The main point is that in TDDfT formalism a closed theory of convective motion appears from a regular and conceptually clean procedure: it is simply a natural and regular step in solving the many-body problem in the comoving frame. Hence now we clearly understand where the universal functionals entering the theory come from and why they are universal. Also, the causal structure of all functionals becomes
and the universal constrained many-body problem simplifies proofs of the mapping theorem for Taylor expandable density/current, and (ii) the v-representability of the invertibility of the mapping from external potentials to the two key mathematical statements: (i) the uniqueness and existence theorems of TDDefFT construction essentially relies on the assumption that the noninteracting v-representability in the traditional formula—eqn (3.45), (3.46) is similar to the well known problem of the formulation completely removes all doubts concerning the predictive power of both hydrodynamic and KS formulation of TDCDFT.

To avoid a possible confusion we mention that in 1986 a version of a Levy–Lieb constrained search procedure for TDDFT has been proposed by Kohl and Dreizler. Their construction essentially relies on the assumption that the evolution starts from the ground state, and does not have any direct or at least a nontrivial connection to the present formulation of the theory.

c Basic uniqueness and existence theorems of TDDefFT

The traditional formulation of TDDFT/TDCDFT is based on two key mathematical statements: (i) the uniqueness and invertibility of the mapping from external potentials to the density/current, and (ii) the v-representability of the density/current. At the present stage of the theory we have proofs of the mapping theorem for Taylor expandable potentials, while the v-representability problem, strictly speaking, remains open. To prove the v-representability within techniques used in the available proofs of the mapping theorems on has to demonstrate that the uniquely constructed power series for potentials do converge, which has not been done up to now.

In the present formulation based on TDDefFT there is no question of mapping as there is no external potential in the universal many-body problem in the comoving frame (see eqn (3.38), (3.39)). Instead the two above mathematical issues reappear in a form of the uniqueness and existence of a solution to nonlinear system of eqn (3.38), (3.39). The uniqueness is reminiscent of the potential-to-current mapping, while the problem of the existence of a solution is equivalent to the problem of v-representability. Eqn (3.38) and (3.39) correspond to interacting systems, but the same set of questions can be asked for a system of N noninteracting particles. In the later case the dynamics is characterized by N one particle orbitals φ(j, t), j = 1…N, and the universal constrained many-body problem simplifies as follows

\[ i \partial_t \phi_j = g \frac{1}{4} \left( \partial_t g + \mathcal{A} \right) \sqrt{\frac{g_{\mu \nu}}{2m}} \left( i \partial_\nu + \mathcal{A}_\nu \right) \phi_j, \quad (3.45) \]

\[ \mathcal{A} = -\frac{\mathcal{L}}{2n_0} \sum_{j=1}^{N} \left( \phi_j^* \partial_\nu \phi_j - \phi_j \partial_\nu \phi_j^* \right) \quad (3.46) \]

where \( n_0(\xi) = \sum_{j=1}^{N} |\phi_j(\xi, 0)|^2 = \sum_{j=1}^{N} |\phi_j(\xi, t)|^2 \) is the density of particles which is, by construction, independent of time. The problem of existence of a solution to the system of eqn (3.45), (3.46) is similar to the well known problem of the noninteracting v-representability in the traditional formulation of TDCDFT. Note that for the practical purpose of TDDefFT/TDCDFT it is not necessarily to prove the wellposedness of the systems eqn (3.38), (3.39) and (3.45), (3.46) for any metric. It is enough to consider metric tensors of the form (2.25), i.e. the metrics which are generated by an invertible transformation coordinates and correspond to a flat space.

The key advantage of the new formulation of old problems is that now the basic questions underlying TDCDFT are posed in the standard and common in mathematical physics form. It is quite likely that the uniqueness and the existence theorems for nonlinear systems of eqn (3.38), (3.39) and (3.45), (3.46) can be proved using standard methods of the functional analysis and the theory of differential equations (see, e.g., ref. 40 and chapter X in ref. 41), which have been successfully applied to the analysis of the time-dependent Hartree and Hartree–Fock systems. Structurally the nonlinear systems of eqn (3.38), (3.39) and (3.45), (3.46) are of the type of a time-dependent Schrödinger equation with a special cubic nonlinearity, which, to the best of my knowledge, have not been considered before. An encouraging observation is that, in contrast to most known systems of nonlinear Schrödinger equations, our equations are exactly integrable in the simple case of \( N = 1 \) (when the systems of eqn (3.38), (3.39) and (3.45), (3.46) coincide). The explicit solution for \( N = 1 \) is

\[ \Psi(\xi, t) = \sqrt{n_0(\xi)} e^{\varphi(\xi, t)}, \quad \partial_\nu \varphi(\xi, t) = \partial_\nu \varphi(\xi, t) \quad (3.47) \]

where

\[ \varphi = \varphi_0(\xi) + \frac{1}{2m n_0(\xi)} \int_0^t \left[ g \frac{4}{3} \partial_\nu \sqrt{g_{\mu \nu}} \partial_\nu g \right] \frac{1}{\sqrt{g}} \left( \xi, t \right) dt \quad (3.48) \]

and \( \varphi_0(\xi) \) is a phase of the initial state. The corresponding stress tensor functional, eqn (3.36), takes the form

\[ \tilde{P}_{\mu \nu}[g_{\alpha \beta}] = \frac{1}{m} \left[ \left( \partial_\mu g \frac{4}{3} \sqrt{n_0(\xi)} \right) \left( \partial_\nu g \frac{4}{3} \sqrt{n_0(\xi)} \right) - \frac{g_{\mu \nu}}{2} \frac{4}{3} \sqrt{g} \partial_\nu \sqrt{g_{\alpha \beta} \partial_\mu \frac{n_0}{\sqrt{g}}} \right] \quad (3.49) \]

Eqn (3.47) and (3.48) clearly show that the wave function and the effective vector potential are retarded functionals of the metric tensor. The stress tensor for the one particle case turns out to be absolutely local in time. Addition of more particles should make the time dependence nonlocal (though necessarily retarded), but hopefully it will not spoil the existence and uniqueness of a solution.

Apparently, a Taylor expansion based proof of uniqueness also works in the new setting, and actually becomes almost trivial. To show this we first substitute the constraint (3.39) into eqn (3.38) to get a closed nonlinear evolution equation of the form

\[ i \partial_t \Psi = \tilde{H}_{[g_{\alpha \beta}]} \Psi \quad (3.50) \]

with a local in time nonlinear Hamiltonian. Let us assume that the metric tensor \( g_{\alpha \nu} \) is v-representable. In other words, it is given by eqn (2.25) with a Lagrangian trajectory that corresponds to a convective motion in some external potential. This is equivalent to the assumption that the solution to eqn (3.50) does exist. If in addition we assume that the metric possesses a
en equation (3.50) is local in time all the coefficients and inserting them into equation (3.50). Since the right hand side of equation (3.50) is local in time all the coefficients \( \Psi^{(k)} \) for any \( k \) are trivially expressible by recursion in terms of \( \Psi_{0} \) and \( g^{(k)}_{\mu \nu} \) with \( l < k \). The later property is another direct manifestation of the retarded character of the functional \( \Psi [ g^{(k)}_{\mu \nu} (t) ] \). Thus we have proved that for a given \( v \)-representable metric the solution is unique and has correct causal properties required for TDDFT/ TDCDFT. However, it is important to note that the formalism presented in this work is perfectly suited for this purpose. As a matter of fact, the historical use of Lagrangian trajectories and Lagrangian coordinates in TDDFT/ TDCDFT has been ultimately connected to attempts of deriving consistent local non-adiabatic approximations for xc potentials. The idea of tracing back the motion of an infinitesimal fluid element and considering its delayed position as an argument of the density in a local xc potential was proposed in ref. 46 and almost immediately applied to TDCDFT in ref. 47. A connection of this proposal to the Lagrangian formulation of a classical fluid mechanics was recognized and elaborated a few years later.31 Further developments, which already fully appreciated the power of the geometric Lagrangian description, resulted in a number of non-linear local approximations for xc functionals with memory.22,27,48,49 The work along these lines continues up to now (see, for example, a recent derivation of a GGA-like extension of the Vignale–Kohn functional50,51).

In any case it is absolutely clear that TDDFT and TDCDFT remain an exciting, active and promising area of research. Clearly, there is still much to be done both to put the theory on really firm mathematical grounds, and to develop practically working approximate functionals for numerous applications.

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IV. Conclusion

In this work we proved the equivalence of two approaches to the convective dynamics of a general quantum many-body system and reconstructed TDCDFT on the new grounds. The most important outcome is the possibility to formulate TDCDFT within a conceptually clean and straightforward two step procedure which resembles the constrained search formulation of the static DFT. On the first step one solves a constrained time-dependent many-body problem to find a stress tensor as a universal functional of the deformation tensor. On the second step we use this functional to calculate the evolution of the current and the density for a given configuration of external fields. In this formulation the vector potential-to-current density mapping theorem, and the \( v \)-representability problem are restated as the uniqueness and the existence theorems for a solution of a certain time-dependent nonlinear Schrödinger equation. Hence the fundamental questions of TDDFT are formulated in a standard setting of mathematical physics. To my knowledge a very special type of nonlinearity appearing in TDDFT has not been studied before. One of the hopes is that the new restatement of the basic theorems combined with a growing practical popularity of TDDFT/TDCDFT will attract the attention of mathematicians and mathematical physicists to the formal foundations of the theory. I also believe that a clear physical picture behind the present approach should be attractive for the more physically oriented part of the community and will stimulate further developments of the theory.

In this paper I did not touch practical questions of constructing new working approximate xc functionals in TDDFT and TDCDFT. However it is important to note that the formalism presented in this work is perfectly suited for this purpose.

References