Time-dependent deformation functional theory

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We present a constructive derivation of a time-dependent deformation functional theory – a collective variable approach to the nonequilibrium quantum many-body problem. It is shown that the motion of infinitesimal fluid elements (i.e., a set of Lagrangian trajectories) in an interacting quantum system is governed by a closed hydrodynamics equation with the stress force being a universal functional of the Green’s deformation tensor $g_{ij}$. Since the Lagrangian trajectories uniquely determine the current density, this approach can be also viewed as a representation of the time-dependent current density functional theory. To derive the above theory we separate a “convective” and a “relative” motions of particles by reformulating the many-body problem in a comoving Lagrangian frame. Then we prove that a properly defined many-body wave function (and thus any observable) in the comoving frame is a universal functional of the deformation tensor. Both the hydrodynamic and the Kohn-Sham formulations of the theory are presented. In the Kohn-Sham formulation we derive a few exact representations of the exchange-correlation potentials, and discuss their implication for the construction of new nonadiabatic approximations. We also discuss a relation of the present approach to a recent continuum mechanics of the incompressible quantum Hall liquids.

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I. INTRODUCTION

Density functional theory (DFT), pioneered by Hohenberg and Kohn$^1$, and by Kohn and Sham$^2$, is now a standard computational tool for studying ground state properties of various quantum many-body systems$^3$. By construction, DFT, even at the exact level, yields only the ground state energy, and the density distribution. Therefore it can not be considered as a full alternative to the other, e.g., field theoretical many-body methods$^4$. However, the simplicity and the computational power of DFT-based approaches makes them practically the only tool to approach realistic quantum many particle systems at the fully ab initio level. Moreover, from experimental point of view, it is frequently quite sufficient to know just those quantities which are perfectly accessible by DFT methods.

Conceptually DFT belongs to a class of theories of collective variables. The mapping theorems of DFT allow us to formally get rid of the solution of the full many-body Schrödinger equation, and to formulate a closed theory that operates with one, or a few basic collective variables (the ground state density in the original version). In this respect the equilibrium DFT is very similar to the classical hydrostatics$^5$. To find the density $n(x)$ in the classical hydrostatics we need to know the equation of state, e.g., the dependence of pressure on the density, $P(n)$, which is universal for a given substance. Similarly for the calculation of the ground state density in DFT it is enough to know a universal exchange correlation (xc) energy functional $E_{xc}[n]$. Although the exact form of $E_{xc}[n]$ is unknown, efficient practical approximations for it are presently available.

Away from the equilibrium the classical hydrostatics is replaced by the classical hydrodynamics. A similar nonequilibrium extension of DFT, a time-dependent density functional theory (TDDFT), was founded in 1984 by Runge and Gross$^6$. Although TDDFT is still far from the maturity of its static counterpart, it has already gained an enormous popularity in different branches of physics$^7$. A hydrodynamic interpretation of TDDFT has been mentioned in the original paper by Runge and Gross. However, it remained practically out of use for more than 10 years. A comeback of hydrodynamic analogy was caused by attempts$^8,9,10,11$ to go beyond a simple (but formally unjustified) adiabatic local density approximation for the time-dependent xc potential. In the mid-90th it has been realized that nonadiabaticity of density functionals is strongly linked to the spatial nonlocality. In particular, any nonadiabatic xc potential must be strongly nonlocal functional of the density. Otherwise the theory would fail to satisfy a so called harmonic potential theorem$^{12,13}$. An ultimate connection of nonadiabaticity to the spatial nonlocality is frequently referred to as an ultranonlocality of TDDFT.

In the linear response regime a resolution the ultranonlocality problem was proposed by Vignale and Kohn (VK)$^8$. They suggested to switch from TDDFT to a time-dependent current density functional theory (TDCDFT), and to consider the current $j(x,t)$ as a basic variable of the theory. VK have demonstrated that the xc vector potential in linearized TDCDFT can be consistently considered as a local functional of the current. In a subsequent paper Vignale, Ulrich, and Conti (VUC)$^9$ have found an elegant hydrodynamic representation of the VK result – the time derivative of the VK vector potential can be written as a divergence of visco-elastic stress tensor which commonly appears in the linearized...
classical continuum mechanics. Beyond the linear response VUC proposed an ad hoc extension of the nonadiabatic VK functional, which simply adopts the linearized visco-elastic form of the stress tensor for nonlinear dynamics. A similar assumption has been made in a phenomenological approach developed by Kurzweil and Baer. 

A general resolution of the ultranonlocality problem in TDDFT, which has been proposed recently, also extensively relies on ideas and techniques borrowed from the classical continuum mechanics. Physically, the ultranonlocality is related to the convective motion of the electron fluid (in the nonadiabatic theory the particles at a given point of space retain the memory of their previous positions). The key idea of Refs. 16,17 was to eliminate the above source of nonlocality by reformulating the theory in a Lagrangian frame, i.e., in a local reference frame moving with the quantum fluid. Since the convective motion in the Lagrangian frame is absent, a spatially local description of xc effects becomes possible. Hence the general resolution of the long standing ultranonlocality problem can be achieved by properly changing the "point of view": while the xc potential is extremely nonlocal in the laboratory reference frame, it appears to be almost local from the point of view of an observer moving with a flow. The main practical outcome of this idea was a rigorous derivation of a nonadiabatic local approximation for xc potential - the time-dependent local deformation approximation (TDLDeFa)\textsuperscript{17,18}. A connection of a general nonlinear local deformation approximation to the phenomenological current density functional by VUC\textsuperscript{9} has been established in Ref. 19. It turns out that the local current density approximation by VUC corresponds to a small deformation limit of TDLDeFa. Hence the Lagrangian formulation of TDDFT can be considered as a general framework for a description of nonadiabatic xc memory effects. Similar to the local density approximation (LDA) in the static DFT, the TDLDeFa can serve as a basic local approximation in the time-dependent theory.

There are, however, a few important restrictions of the formalism developed in Refs. 16,17. In these works we reformulated the many-body theory and TDDFT in the local comoving frame by making two simplifying assumptions: (i) we considered a many-body system driven by a scalar external potential (therefore an external magnetic field was excluded from the consideration); (ii) we assumed that xc effects can also be described by a scalar xc potential. One of the aims of the present work is to relax both assumptions, and to formulate the theory in a most general form.

Such a generalization is necessary, first of all, for the further refinements and extensions of the simple local deformation approximation. Using the approach restricted to only scalar potentials, we have found that in general the exact stress tensor in the Lagrangian frame (i.e., in the space seen by a comoving observer) is a functional of two collective variables: a symmetric Green's deformation tensor $g_{ij}$, and a skew-symmetric vorticity tensor $F_{ij}$. In the lowest order in spatial derivatives the dependence on the vorticity disappears, and we arrive at the local deformation approximation (TDLDeFa)\textsuperscript{17,18}. If we want to go beyond the local approximation, and construct a gradient extension of TDLDeFa the dependence on $F_{ij}$ must be taken into account, which seems to be extremely demanding technically. In the present paper we show that this dependence is, in a certain sense, trivial and can be singled out by reformulating the theory in terms of vector potentials (both external and exchange-correlation). As a result we get a theory where a properly defined stress tensor is, at the exact level, a universal functional of only one basic variable, the deformation tensor $g_{ij}$. As a matter of fact, this work adds one more member to the family of nonequilibrium DFT-like theories – a time-dependent deformation functional theory.

Another obvious reason for reformulating the theory in terms of vector potentials is the need to describe dynamics of many-body systems in the presence of external magnetic fields. Recently the ideas of the deformation-functional have been successfully applied to a phenomenological derivation of an effective continuum mechanics of fractional quantum Hall liquids\textsuperscript{21,22}. The present work can be considered as a formal justification (at the level of existence theorems) of that approach.

The general idea of this paper is quite similar to that of Ref. 16,17. We formulate the many-body theory in the Lagrangian frame, and then use this formulation to derive a closed theory of a collective variable, the time-dependent deformation functional theory. However, the technique we develop here is essentially different. We show that it is much more transparent and economic to work directly with the many particle wave function, and to formulate the problem of quantum dynamics using a Dirac-Frenkel variational principle. Starting with the quantum mechanical action in the laboratory frame we construct its analog in the comoving frame. Within this approach a theory of a collective variable emerges in a most simple and constructive fashion. We demonstrate that the time-dependent deformation functional theory is a natural intermediate step in solving the many-body problem in the Lagrangian frame. Physically this can be interpreted as follows. The transformation to the comoving frame corresponds to the separation of the convective motion of the fluid, and the motion of particles relatively to the convective flow. The relative motion is described by the many-body wave function $\tilde{\Psi}$ in the Lagrangian space, while the convective motion is determined by a set of trajectories $\mathbf{x}(\xi, t)$ of infinitesimal fluid elements. Accordingly the complete problem splits into two natural parts. First, one solves the many-body problem in the Lagrangian frame. This yields the wave function $\tilde{\Psi}$ as a unique functional of a universal geometric characteristics of the frame – the deformation tensor $g_{ij}$, which plays a role of metric in the Lagrangian space. On the second step we use that solution to find the trajectories
\( \mathbf{x}(\xi, t) \) from a closed hydrodynamics-like equation. The second step is, in fact, the time-dependent deformation functional theory, which we introduce in this paper. The theory is formulated both in the hydrodynamic form, and in a more practical Kohn-Sham form.

The structure of the paper is the following. In Sec. II we illustrate the general formalism using a pedagogical exactly solvable example of one particle quantum dynamics. In this case the quantum problem for the relative motion possesses an analytic solution, and the final time-dependent deformation functional theory is formulated in an explicit form. In the concluding subsection (Sec. III) we extensively discuss the main ideas and the results of Sec. II. This subsection is aimed at preparing a reader to the most general formulation of the theory given in Sec. III. In Sec. IIIA the Dirac-Frenkel variational principle is used to formulate the general many-body problem in the Lagrangian frame. The solution of the quantum problem for the relative motion is analyzed in Sec. IIIB. We prove the basic mapping theorem which states that the many-body wave function in the Lagrangian frame is a universal functional of the deformation tensor. This theorem forms a basis of the time-dependent deformation functional theory that can also be interpreted as an exact quantum continuum mechanics. In Sec. IIIB the Keldysh-contour formalism is employed to derive a closed form of the theory given in Sec. III. In Sec. IV we present a Kohn-Sham formulation of the theory. We introduce \( \chi \) potentials both in the Lagrangian and in the laboratory frame. We also derive a few exact representations of the \( \chi \) potentials in the laboratory frame (since these potentials are of practical interest). Finally, in Sec. V we present our conclusions.

## II. GETTING AN IDEA: QUANTUM PARTICLE IN THE LAGRANGIAN FRAME

### A. Quantum mechanics in a local noninertial frame

To illustrate main ideas, and the structure of a general theory developed in Sec. III it is instructive to consider first the simplest case of one quantum particle moving in the presence of external vector and scalar potentials, \( \mathbf{A}(\mathbf{x}, t) \) and \( U(\mathbf{x}, t) \). The system is described by the one particle wave function \( \Psi(\mathbf{x}, t) \) that satisfies the time-dependent Schrödinger equation supplemented with the proper initial condition

\[
\imath \partial_t \Psi(\mathbf{x}, t) = H \Psi(\mathbf{x}, t), \quad \Psi(\mathbf{x}, 0) = \Psi_0(\mathbf{x}),
\]

where \( H \) is the usual one particle Hamiltonian

\[
H = \frac{1}{2m} \left( -\imath \partial_x - A(\mathbf{x}, t) \right)^2 + U(\mathbf{x}, t).
\]

For our purpose it is convenient to reformulate the problem of quantum dynamics using a Dirac-Frenkel variational principle. The Schrödinger equation, Eq. (1), corresponds to the condition for the extremum of the action

\[
S[\Psi^*, \Psi] = \int_0^t \mathcal{L} dt
\]

where \( \mathcal{L}[\Psi^*, \Psi] = \int \left[ i \Psi^* \partial_t \Psi - \Psi^* H \Psi \right] dx, \)

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\]

\[
\mathcal{L} = \int dx \left\{ i \Psi^* \partial_t \Psi - U \Psi^* \Psi - \frac{1}{2m} \left[ (i \partial_{x^i} - A_i) \Psi^* \right] \left[ (i \partial_{x^i} - A_i) \Psi \right] \right\}. \tag{4}
\]

Let us transform the equation of motion, Eq. (1), or, equivalently, the Lagrangian of Eq. (4) to a local noninertial reference frame moving with a given velocity \( \mathbf{v}(\mathbf{x}, t) \). Formally this corresponds to a nonlinear transformation of coordinates \( \mathbf{x} \rightarrow \xi, \mathbf{x} = \mathbf{x}(\xi, t) \), where the function \( \mathbf{x}(\xi, t) \) is a solution to the following Cauchy problem

\[
\frac{\partial \mathbf{x}(\xi, t)}{\partial t} = \mathbf{v}(\mathbf{x}(\xi, t), t), \quad \mathbf{x}(\xi, 0) = \xi. \tag{5}
\]

Intuitively the function \( \mathbf{x}(\xi, t) \) can be viewed as a trajectory of a small element of a fluid with the velocity distribution \( \mathbf{v}(\mathbf{x}, t) \). Accordingly the new spatial coordinate \( \xi \) has a meaning of the initial point of that trajectory.

The transformation of coordinates \( \mathbf{x} \rightarrow \xi \) leads to the following replacements in the Lagrangian

\[
d\mathbf{x} \rightarrow \sqrt{g} d\xi, \quad \partial_{x^i} \rightarrow \frac{\partial \xi^i}{\partial x^j} \partial_{x^j}, \quad \partial_t \rightarrow \partial_t - \mathbf{v}^i \partial_{x^i} \tag{6}
\]

where \( g(\xi, t) = \det g_{ij} \) is the determinant of the induced metric tensor

\[
g_{ij}(\xi, t) = \frac{\partial x^k}{\partial \xi^i} \frac{\partial x^k}{\partial \xi^j} \quad \{ g_{ij} \}^{-1} = g^{ij} = \frac{\partial \xi^i}{\partial x^k} \frac{\partial \xi^j}{\partial x^k} \tag{7}
\]

and \( \mathbf{v}(\xi, t) \) is the velocity field transformed the moving frame:

\[
\tilde{\mathbf{v}}^i(\xi, t) = \frac{\partial \xi^i}{\partial x^j} \mathbf{v}^j(\mathbf{x}(\xi, t), t). \tag{8}
\]

Substituting Eq. (6) into Eq. (4), and using the definitions of Eqs. (7) and (8) we obtain the following transformed Lagrangian

\[
\mathcal{L} = \int \sqrt{g} d\xi \left\{ i \Psi^* \partial_t \Psi + \left[ \frac{m}{2} \mathbf{v}^i \mathbf{v}_i - \mathbf{A}(\mathbf{x}(\xi, t)) - U \right] \Psi^* \Psi - \frac{g^{ij}}{2m} \left[ (i \partial_{\xi^j} - \tilde{A}_j - m \mathbf{v}^j) \Psi^* \right] \left[ (i \partial_{\xi^j} - \tilde{A}_j - m \mathbf{v}^j) \Psi \right] \right\}. \tag{9}
\]

Here \( \tilde{A}_j(\xi, t) \) is the external vector potential in the \( \xi \)-frame:

\[
\tilde{A}_j(\xi, t) = \frac{\partial x^j}{\partial \xi^i} A_i(\mathbf{x}(\xi, t), t). \tag{10}
\]
In the derivation of Eq. (9) we regrouped terms to obtain a physically expected form of $\tilde{A}_i + m\tilde{v}_i$ in the kinetic energy.

Appropriately the second term in Eq. (9) plays a role of an effective scalar potential in the moving reference frame. An important observation is that this term exactly coincides with the classical Lagrangian of a particle moving along the trajectory $\mathbf{x}(\xi, t)$ in the presence of the external fields $\mathbf{A}(\mathbf{x}, t)$ and $U(\mathbf{x}, t)$. Indeed, using Eqs. (8) and (10) we find

$$L^{cl}(\xi, t) = \frac{m}{2} (\dot{\xi})^2 + \mathbf{A}(\mathbf{x}(t), t) \cdot \dot{\mathbf{x}}(t) - U(\mathbf{x}(t), t).$$

where dot denotes the time derivative. Obviously the classical Lagrangian of Eq. (11) parametrically depends on the initial point, $\xi$, of the trajectory.

The Lagrangian of Eq. (10) can be simplified by introducing a transformed wave function $\tilde{\Psi}(\xi, t)$:

$$\tilde{\Psi}(\mathbf{x}(\xi, t), t) = g^{-\frac{1}{4}} e^{iS_{cl}(\xi, t)} \tilde{\Psi}(\xi, t),$$

where $S_{cl}(\xi, t)$ is the classical action that is related to the Lagrangian $L^{cl}$, Eq. (11):

$$S_{cl}(\xi, t) = \int_0^t L^{cl}(\xi, t') dt'.$$

The renormalization factor $g^{-\frac{1}{4}}$ in Eq. (12) accounts for a local change of volume induced by the nonlinear transformation of coordinates. This allows us to preserve the interpretation of the transformed function $\tilde{\Psi}(\xi, t)$ as a probability density in $\xi$-space. The exponential prefactor in Eq. (12) gauges out the effective scalar potential in Eq. (9). Inserting Eq. (12) into Eq. (9) we reduce the Lagrangian to the following compact form

$$\mathcal{L}[\tilde{\Psi}^{*}, \tilde{\Psi}] = \int d\xi \{ i \tilde{\Psi}^{*} \frac{\partial}{\partial \xi} \tilde{\Psi} - [(i\partial_{\xi} - A_{\xi}) g^{-\frac{1}{4}} + \frac{\sqrt{g} g^{ij}}{2m} (i\partial_{\xi} - A_{\xi}) g^{-\frac{1}{4}} \tilde{\Psi}] \}.$$ 

An effective vector potential $\mathbf{A}_i(\xi, t)$ in Eq. (14) is defined as follows

$$\mathbf{A}_i(\xi, t) = \tilde{\mathbf{A}}_i(\xi, t) + \tilde{v}_i(\xi, t) - \partial_{\xi} S^{cl}(\xi, t).$$

The transformed Lagrangian, Eq. (14), can be also represented in a common form of the Dirac-Frenkel functional. It is straightforward to check that Eq. (14) is equivalent (up to irrelevant total derivatives) to the functional

$$\mathcal{L} = \int d\xi \left[ i \tilde{\Psi}^{*} \frac{\partial}{\partial \xi} \tilde{\Psi} - \tilde{\Psi}^{*} \mathcal{H}[g_{ij}, \mathbf{A}_i] \tilde{\Psi} \right].$$

where $\mathcal{H}[g_{ij}, \mathbf{A}_i]$ is the Hamiltonian in the moving frame:

$$\mathcal{H} = g^{-\frac{1}{4}} (i\partial_{\xi} - A_{\xi}) \sqrt{g} g^{ij} (i\partial_{\xi} - A_{\xi}) g^{-\frac{1}{4}}.$$

Hence the transformed Schrödinger equation takes the form

$$i \partial_t \tilde{\Psi}(\xi, t) = \mathcal{H}[g_{ij}, \mathbf{A}_i] \tilde{\Psi}(\xi, t), \quad \tilde{\Psi}(\xi, 0) = \Psi_0(\xi).$$

Equations (18), (17) and (15) completely determine the dynamics of a quantum particle in the local noninertial frame moving with the velocity $\mathbf{v}(\mathbf{x}, t)$. The corresponding Hamiltonian, Eq. (17), contains two types of “external” fields, a tensor field $g_{ij}$, and a vector field $\mathbf{A}_i$. The tensor field $g_{ij}(\xi, t)$ plays a role of an effective metric, which produces a “geodesic” inertia force. This force makes a free particle to move along geodesics in the deformed $\xi$-space. The effective vector potential $\mathbf{A}_i(\mathbf{x}, t)$ is responsible for a combined action of the physical external forces and the rest of inertia forces (i.e., the linear acceleration force, and the generalized Coriolis and centrifugal forces).

To complete the discussion of dynamics in a general noninertial frame, we present two fundamental conservation laws that follow from the equation of motion, Eq. (18) (for a detailed derivation see Appendix). These are the continuity equation

$$\partial_t \tilde{n} + \partial_{\xi k} \tilde{j}^k = 0,$$

and the local momentum balance equation

$$\partial_t \tilde{j}_k - \tilde{j}^i (\partial_{\xi} A_i - \partial_{\xi} A_i) + \tilde{n} \partial_{\xi} A_k + \sqrt{g} \tilde{P}^k_i = 0.$$

In equations (19) and (20) $\tilde{n} = \tilde{\Psi}^2$ is the probability density, and $\tilde{j}^i$ and $\tilde{P}^k_i$ are the current density and the stress tensor, respectively. The operator $\nabla_j$ in Eq. (20) stands for the covariant derivative in a space with metric $g_{ij}$ (see, for example Ref. 26). In particular the stress force, $\nabla_j \tilde{P}^k_i$, in Eq. (20) is the covariant divergence of a second rank tensor:

$$\nabla_j \tilde{P}^k_i = \frac{1}{\sqrt{g}} \partial_{\xi} \sqrt{g} \tilde{P}^k_i - \frac{1}{2} \tilde{P}^{ij} \partial_{\xi} g_{ij}.$$

In Appendix we show that in general the current density and the stress tensor can be expressed in terms of the functional derivatives of the Hamiltonian $\tilde{H}[g_{ij}, \mathbf{A}_i]$ with respect to the vector potential and the metric tensor, respectively:

$$\tilde{j}^k(\xi, t) = - \frac{\delta \tilde{H}[g_{ij}, \mathbf{A}_i]}{\delta A_k(\xi, t)} \tilde{\Psi},$$

$$\tilde{P}^{ij}(\xi, t) = - \frac{2}{\sqrt{g}} \tilde{\Psi} \delta \tilde{H}[g_{ij}, \mathbf{A}_i] \tilde{\Psi}.$$
B. Quantum particle in a comoving frame

The form of the equations of motion, Eqs. (18) and (15), is invariant under the transformation to an arbitrary local reference frame defined by its velocity – the vector-valued function \( \mathbf{v}(\mathbf{x}, t) \). To specify a particular frame we need to supply the above system of equations by a local “gauge-fixing” condition\(^\text{16}\). One of the most simple and natural choices of such a gauge condition is a requirement of zero current density:

\[
\tilde{j}(\mathbf{\xi}, t) = 0. \tag{26}
\]

This requirement specifies a comoving Lagrangian frame. That is a reference frame moving with the velocity \( \mathbf{v}(\mathbf{x}, t) = j(\mathbf{x}, t)/n(\mathbf{x}, t) \), where \( j \) and \( n \) are the current and the density in the laboratory frame. In this case the new coordinates \( \mathbf{\xi} \) become the Lagrangian coordinates, while the metric tensor \( g_{ij} \), Eq. (7), acquires a meaning of the Green’s deformation tensor\(^2\). Substituting Eq. (26) in the continuity equation we observe that in the Lagrangian frame the density distribution is stationary and equals to the density at \( t = 0 \), which is fixed by the initial conditions

\[
\tilde{n}(\mathbf{\xi}, t) = \tilde{n}(\mathbf{\xi}, 0) = n_0(\mathbf{\xi}) = |\Psi_0(\mathbf{\xi})|^2. \tag{27}
\]

Similarly the local momentum balance equation, Eq. (20), in the Lagrangian frame simplifies as follows

\[
n_0 \partial_{\mathbf{\xi}} A_k + \sqrt{g} \nabla_i \tilde{P}_k^i = 0. \tag{28}
\]

Equation (28) reveals a physical significance of the effective vector potential \( A_k \). It produces a force (an effective electric field) that exactly compensates the local stress force. As a result the net force exerted on every infinitesimal volume element vanishes, which guarantees vanishing current and a stationary density in every point of the Lagrangian \( \mathbf{\xi} \)-space.

Using Eqs. (24) and (27) we can represent the gauge condition of Eq. (26) in the following explicit form

\[
-\frac{i}{2m} (\Psi^* \partial_{\mathbf{\xi}} \tilde{\Psi} - \tilde{\Psi} \partial_{\mathbf{\xi}} \Psi^*) = \frac{n_0}{m} A_k. \tag{29}
\]

A complete set of equations of motion in the Lagrangian frame consists of three equations. These are the Schrödinger equation (18), the zero-current condition (29), and Eq. (15) which relates the effective vector potential \( A \) to the external fields. The solution of this system yields the wave function \( \tilde{\Psi}(\mathbf{\xi}, t) \), and the trajectory, \( \mathbf{x}(\mathbf{\xi}, t) \), of the Lagrangian frame for a given configuration of the external fields, \( \mathbf{A}(\mathbf{x}, t) \) and \( U(\mathbf{x}, t) \).

The problem of finding \( \mathbf{x}(\mathbf{\xi}, t) \) from Eq. (15) can be brought to a more physical form. The time derivative of Eq. (15) takes the form

\[
m \partial_t \tilde{\mathbf{v}} + \partial_{\mathbf{\xi}} \tilde{\mathbf{A}} = -\frac{m}{2} \tilde{\mathbf{v}}^k \tilde{v}_k + \tilde{\mathbf{v}}^k \tilde{A}_k - U = 0. \tag{30}
\]

The first three terms in the left hand side of Eq. (30) correspond to a combination of the external and the inertial forces, while the last term is precisely equal to the local stress force [see Eq. (28)]. Hence Eq. (30) [i. e. the time derivative of Eq. (15)] has a clear meaning of the force balance equation in the comoving frame. On the other hand, it can be considered as an equation of motion for the dynamic variable \( \mathbf{x}(\mathbf{\xi}, t) \). Indeed, using Eq. (5), and the explicit representations for \( \tilde{\mathbf{v}}, \tilde{\mathbf{A}} \), Eq. (8), and for \( \tilde{\mathbf{A}} \), Eq. (10), one can straightforwardly reduce Eq. (30) to the following form

\[
m \frac{\partial^2 \mathbf{x}_k}{\partial t^2} - \frac{\partial \mathbf{x}^i}{\partial t} \left( \frac{\partial A_k}{\partial x^i} - \frac{\partial A_i}{\partial x^k} \right) + \left( \frac{\partial A_k}{\partial t} \right)_x = 0, \tag{31}
\]

where \( \left( \frac{\partial A_k}{\partial t} \right)_x \) means the time derivative at fixed \( x \). Equation (31) is exactly the Newton equation for a classical particle moving in the presence of the external electromagnetic force and the stress force [the last term in the left hand side of Eq. (31)].

Thus the complete system of equations, which determines the quantum dynamics in the Lagrangian frame, can be rewritten as follows

\[
i \partial_t \tilde{\Psi}(\mathbf{\xi}, t) = \tilde{H}[g_{ij}, A_i] \tilde{\Psi}(\mathbf{\xi}, t), \tag{32}
\]

\[
A_k = -\frac{i}{2n_0} (\Psi^* \partial_{\mathbf{\xi}} \tilde{\Psi} - \tilde{\Psi} \partial_{\mathbf{\xi}} \Psi^*), \tag{33}
\]

\[
m \mathbf{x}_k = [\mathbf{x} \times \mathbf{B}(\mathbf{x}, t)]_k + E_k(\mathbf{x}, t) + \frac{\partial \mathbf{x}^i}{\partial x^k} \partial_t A_i, \tag{34}
\]

where \( \mathbf{E}(\mathbf{x}, t) \) and \( \mathbf{B}(\mathbf{x}, t) \) are the external electric and magnetic fields, which are defined in a usual way:

\[
\mathbf{E}(\mathbf{x}, t) = -\partial_t \mathbf{A}(\mathbf{x}, t) - \partial_x U(\mathbf{x}, t), \tag{35}
\]

\[
\mathbf{B}(\mathbf{x}, t) = \partial_{\mathbf{\xi}} \times \mathbf{A}(\mathbf{x}, t). \tag{36}
\]

The system of Eqs. (32)–(34) should be solved with the initial conditions

\[
\tilde{\Psi}(\mathbf{\xi}, 0) = \Psi_0(\mathbf{\xi}), \quad \mathbf{x}(\mathbf{\xi}, 0) = \mathbf{\xi}, \quad \mathbf{x}(\mathbf{\xi}, 0) = \mathbf{v}_0(\mathbf{\xi}), \tag{37}
\]

where \( \mathbf{v}_0(\mathbf{\xi}) \) is the velocity distribution in the initial state \( \Psi_0(\mathbf{\xi}) \). The Hamiltonian \( \tilde{H}[g_{ij}, A_i] \) is defined after Eq. (17), and the metric (deformation) tensor \( g_{ij} \) is connected to the solution, \( \mathbf{x}(\mathbf{\xi}, t) \), of Eq. (34) via Eq. (7).

Interestingly, the whole system of Eqs. (32)–(34) can be obtained from a single variational functional of the following form

\[
\mathcal{L}[\tilde{\Psi}, \mathbf{A}, \mathbf{x}] = \int d\mathbf{\xi} \left\{ i \Psi^* \partial_t \tilde{\Psi} - \tilde{\Psi} \tilde{H}[g_{ij}, A_i] \tilde{\Psi} + n_0(\mathbf{\xi}) \left[ \frac{m}{2} (\mathbf{x})^2 + \mathbf{x} \mathbf{A}(\mathbf{x}, t) - U(\mathbf{x}, t) \right] \right\}. \tag{38}
\]

Apparently the first two conditions for the extremum of Eq. (38), \( \delta \mathcal{L}/\delta \Psi^* = 0 \) and \( \delta \mathcal{L}/\delta \mathbf{A} = 0 \), are equivalent to the Schrödinger equation, Eq. (32), and the zero-current
constraint, Eq. (33), respectively. The third condition, \( \delta \mathcal{L} / \delta x = 0 \), yields the equation

\[
m \dot{x}^k = [\dot{x} \times \mathbf{B}(x,t)]_k + E_k(x,t) - \frac{1}{n_0} \langle \dot{\Psi} | \frac{\delta \mathcal{H}}{\delta x} | \dot{\Psi} \rangle.
\] (39)

By direct calculations one can check the following identity

\[
\langle \dot{\Psi} | \frac{\delta \mathcal{H}}{\delta x} | \dot{\Psi} \rangle = \frac{\partial \xi^i}{\partial x^k} \sqrt{g} \nabla_j \dot{P}_{ij} = -\frac{\partial \xi^i}{\partial x^k} n_0 \partial_k A_i,
\] (40)

where the variational definition of the stress tensor, Eq. (23), and the local momentum balance equation of Eq. (28) have been used. Hence the last term in the right hand side of Eq. (40) is identical to the correct stress force entering the equation of motion for \( x(\xi, t) \), Eq. (34).

The Lagrangian \( \mathcal{L} \), Eq. (38), describes classical dynamics of infinitesimal fluid elements, coupled to constrained quantum dynamics in a space with metric \( g_{ij} \). It is worth noting that the coupling is purely geometric (minimal) – the classical trajectories \( x(\xi, t) \) enter the quantum part of the problem only via the induced metric \( g_{ij}(\xi, t) \), Eq. (7).

The complete set of Eqs. (32)–(34) consists of two parts: (i) the universal, i.e. independent of external fields, quantum problem defined by Eqs. (32), (33), and (ii) the “classical” equation of motion, Eq. (34), for the trajectory of the comoving frame. The universal problem of Eqs. (32), (33) corresponds to quantum dynamics in the space with a given time-dependent metric, subjected to a constraint of zero current density. The solution of this problem (provided it exists and is unique) determines the wave function and the selfconsistent vector potential as universal functionals of the metric tensor, \( \dot{\Psi}[g_{ij}](\xi, t) \), and \( A[g_{ij}](\xi, t) \). Hence the stress force, the stress tensor \( \dot{P}_{ij} \), as well as any other observable are also functionals of the metric (deformation) tensor. Substituting the solution of the universal quantum problem into Eq. (34) we obtain a closed equation of motion for the trajectory \( x(\xi, t) \)

\[
m \dot{x}^k = [\dot{x} \times \mathbf{B}(x,t)]_k + E_k(x,t) - \sqrt{\frac{g_0}{n_0}} \nabla_j \dot{P}_{ij}[g_{ij}].
\] (41)

Equation (41) is easily recognized as an equation of a nonlinear elasticity theory in the Lagrangian formulation of continuum mechanics. In this context the functional dependence of the stress tensor \( \dot{P}_{ij} \) on the deformation tensor \( g_{ij} \) plays a role of the exact equation of state. This equation of state is determined from the solution of the universal quantum problem defined by Eqs. (32), (33).

In the one particle case the universal problem of Eqs. (32), (33) is exactly solvable. Therefore the exact quantum equation of state can be found in an explicit form. Indeed, it is easy to see that the following wave function and the selfconsistent vector potential

\[
\dot{\Psi}(\xi, t) = \sqrt{n_0(\xi)} e^{i\varphi(\xi, t)}, \quad A_k(\xi, t) = \partial_k \varphi(\xi, t)
\] (42)

satisfy the system of Eqs. (32), (33) if the phase \( \varphi(\xi, t) \) takes the form

\[
\varphi = \varphi_0(\xi) + \frac{1}{2m} \int_0^t \left[ g^{-\frac{1}{2}} \partial_l \sqrt{g} g^{ij} \partial_l g^{-\frac{1}{2}} \sqrt{n_0} \right] dt'
\] (43)

where \( n_0(\xi) \) and \( \varphi_0(\xi) \) are the density and the phase of the initial state: \( \Psi_0(\xi) = \sqrt{n_0} e^{i\varphi_0} \). Substituting the wave function, Eq. (42), into Eq. (25) we find the stress tensor functional (the quantum equation of state):

\[
\dot{P}_{ij}[g_{ij}] = \frac{1}{2m} \left[ \left( \partial_l g^{-\frac{1}{2}} \right) \left( \partial_l g^{ij} \right) - \frac{g_{ij}}{4g} \right] \partial_k \sqrt{g} \sqrt{n_0} \partial_l n_0
\] (44)

The corresponding stress force, which enters the “elastic” equation of motion, Eq. (41), can be calculated by taking either the covariant divergence of the stress tensor, Eq. (44), or the time derivative of the vector potential \( A \), Eq. (42). The result takes the form

\[
\nabla_0 \dot{P}_{ij} = \frac{1}{2m} \partial_k \left[ g^{-\frac{1}{2}} \partial_l g^{ij} \partial_l g^{-\frac{1}{2}} \sqrt{n_0} \right]
\] (45)

It is worth mentioning that the equation of motion, Eq. (41), with the stress force of Eq. (45) can be interpreted as the Lagrangian formulation of the one particle quantum fluid dynamics (see, for example, Ref. 28).

To complete the formal consideration of the one particle dynamics, we note that Eq. (41) with the stress tensor of Eq. (44) corresponds to the Euler-Lagrange equation for the following “elastic” Lagrangian

\[
\mathcal{L}_{el}[x] = \int d\xi \left\{ \frac{m}{2} \left( \dot{x}^2 \right) + x A(x,t) - U(x,t) \right\} + \left( \partial_l g^{-\frac{1}{2}} \sqrt{n_0} \sqrt{g} \right) \frac{g_{ij} \partial_l n_0}{2m} \right\}
\] (46)

The last term in Eq. (46) plays a role of a quantum elastic energy. As it should be, the elastic energy depends on \( x(\xi, t) \) only via the Green’s deformation tensor \( g_{ij}(\xi, t) \).

C. Overview of the main results and discussion

Let us summarize main results of the present section. Starting from the usual Dirac-Frenkel variational principle, we derived a complete set of Eqs. (32)–(34), which describes quantum dynamics in the comoving Lagrangian frame. This set of equations is generated by a generalized Dirac-Frenkel functional, Eq. (38), that depends on three functions \( \dot{\Psi}(\xi, t) \), \( x(\xi, t) \), and \( A(\xi, t) \). Two of them, the wave function \( \dot{\Psi}(\xi, t) \), and the frame’s trajectory \( x(\xi, t) \), enter the theory as dynamic variables, while the effective vector potential \( A(\xi, t) \) is responsible for the zero-current constraint. This constraint ensures that our reference frame is indeed Lagrangian (comoving), i.e. a special frame where one observes no current, and a stationary density distribution. In fact, the force produced
by the vector potential \( \mathbf{A} \) exactly compensates the stress force thus providing a physical mechanism of the vanishing current density [see Eq. (28)].

The structure of the basic Lagrangian, Eq. (38), is extremely simple and transparent. It describes the dynamics of two coupled subsystems. These are: (i) the classical system of infinitesimal fluid elements labeled by their initial positions \( \boldsymbol{\xi} \), and moving along trajectories \( \mathbf{x}(\boldsymbol{\xi}, t) \); and (ii) the quantum system placed in a space with metric \( g_{ij}(\boldsymbol{\xi}, t) \), and subjected to the zero-current constraint. The two systems are coupled via Eq. (7) that identifies the metric \( g_{ij}(\boldsymbol{\xi}, t) \) (entering the quantum problem) with the Green’s deformation tensor generated by the classical trajectories \( \mathbf{x}(\boldsymbol{\xi}, t) \).

One of the most important observations is that the constrained quantum problem, Eqs. (32) and (33), does not contain any physical external potential, but depends only on the metric (deformation) tensor. In that sense the quantum problem in the Lagrangian frame is universal—it defines the wave function as a functional of the deformation tensor, \( \tilde{\Psi}(\boldsymbol{\xi}, t) = \tilde{\Psi}[g_{ij}](\boldsymbol{\xi}, t) \). As a result any observable in the comoving frame is also a universal functional of \( g_{ij} \). It is, therefore, natural to call this formalism a time-dependent deformation functional theory (TDDeFT). The physical observable of primary importance is the stress tensor \( \tilde{P}_{ij} \) as it determines the stress force in the equation of motion for the fluid elements. The existence of the universal functional \( \tilde{P}_{ij}[g_{ij}] \) [i.e. the existence of the solution to the universal problem of Eqs. (32), (33)] allows us to formulate a closed hydrodynamics-type equation for the only collective variable, the trajectory \( \mathbf{x}(\boldsymbol{\xi}, t) \). It should be noted that the knowledge of \( \mathbf{x}(\boldsymbol{\xi}, t) \) is equivalent to the knowledge of the time-dependent density \( n(\mathbf{x}, t) \), and velocity \( \mathbf{v}(\mathbf{x}, t) \) in the laboratory frame. The later quantities can be recovered from the former one as follows

\[
n(\mathbf{x}, t) = \frac{n_0(\boldsymbol{\xi}(\mathbf{x}, t))}{\sqrt{g(\boldsymbol{\xi}, t)}}, \quad (47)
\]

\[
\mathbf{v}(\mathbf{x}, t) = \left[ \frac{\partial \mathbf{x}(\boldsymbol{\xi}, t)}{\partial t} \right]_{\boldsymbol{\xi} = \mathbf{x}(\mathbf{x}, t)} \quad (48)
\]

where \( \mathbf{x}(\boldsymbol{\xi}, t) \) is the inverse of \( \mathbf{x}(\boldsymbol{\xi}, t) \).

In the present section we considered the simplest, but still nontrivial case of one particle quantum dynamics. An illustrative power of this example is related to the possibility to exactly solve the universal quantum problem in the Lagrangian frame, and to find the universal functionals, \( \tilde{\Psi}[g_{ij}](\boldsymbol{\xi}, t) \) and \( \tilde{P}_{ij}[g_{ij}](\boldsymbol{\xi}, t) \), in the explicit form [see Eqs. (42)-(43) and Eq. (44), respectively]. The exact solution of the universal problem is no longer possible if more than one particle is present. However, as we will see in the next section, both the general idea of TDDeFT and the formal structure of the theory remain basically unchanged in the most general case of an interacting quantum many-body system.

### III. TIME-DEPENDENT DEFORMATION FUNCTIONAL THEORY

#### A. Quantum many-body theory in the comoving frame

Let us consider a system of \( N \) identical particles interacting via a two-body potential \( V(|\mathbf{x} - \mathbf{x}'|) \). The system is described by the \( N \)-body wave function \( \Psi(\mathbf{x}_1, \ldots, \mathbf{x}_N, t) \) that satisfies the time-dependent Schrödinger equation with the Hamiltonian

\[
H = H_0 + H_{\text{int}}, \quad (49)
\]

where \( H_0 \) corresponds to the sum of one particle contributions, and \( H_{\text{int}} \) is the interaction Hamiltonian:

\[
H_0 = \sum_{\alpha=1}^{N} \left[ \frac{-i\partial_{\mathbf{x}_\alpha} - A(\mathbf{x}_\alpha, t))^2}{2m} + U(\mathbf{x}_\alpha, t) \right], \quad (50)
\]

\[
H_{\text{int}} = \frac{1}{2} \sum_{\alpha, \beta} V(|\mathbf{x}_\alpha - \mathbf{x}_\beta|). \quad (51)
\]

Following the route outlined in Sec. II, we restate the problem in a form of the variational principle with the following Lagrangian

\[
\mathcal{L}[\Psi^*, \Psi] = \int \left[ i\Psi^* \dot{\Psi} - \Psi^* H \Psi \right] \prod_{\alpha=1}^{N} d\mathbf{x}_\alpha. \quad (52)
\]

The next step is to make a transformation to the comoving Lagrangian frame. Formally this corresponds to the transformation of coordinates \( \mathbf{x}_\alpha \rightarrow \xi_\alpha: \mathbf{x}_\alpha = \mathbf{x}(\xi_\alpha, t), \alpha = 1, \ldots, N \), where the function \( \mathbf{x}(\xi, t) \) is the trajectory of a fluid element, which is defined by Eq. (5). In addition, we introduce a renormalized many-body wave function \( \tilde{\Psi}(\xi_1, \ldots, \xi_N, t) \) in the new frame:

\[
\Psi(\mathbf{x}(\xi_1, t), \ldots, \mathbf{x}(\xi_N, t), t) = \prod_{\alpha=1}^{N} g^{-\frac{1}{2}}(\xi_\alpha, t) e^{iS_\alpha(\xi_\alpha, t)} \times \tilde{\Psi}(\xi_1, \ldots, \xi_N, t), \quad (53)
\]

where \( iS_\alpha(\xi, t) \) is the classical action defined after Eq. (13). Equation (53) is a direct generalization of Eq. (12) for the \( N \)-particle system. The rest of calculations also straightforwardly follows the line of the previous section. Namely, we substitute Eq. (53) into the Lagrangian, Eq. (52), perform the above mentioned transformation of coordinates, and successively repeat all intermediate steps described in Sec. II. As a result we arrive at the following generalized Dirac-Frenkel functional \( \tilde{\mathcal{L}}[\tilde{\Psi}^*, \tilde{\Psi}, \mathbf{A}, \mathbf{x}] \) that describes the dynamics of \( N \)-particle system in the comoving frame,

\[
\tilde{\mathcal{L}} = \int \left[ i\tilde{\Psi}^* \partial_t \tilde{\Psi} - \tilde{\Psi}^* \tilde{H}[g_{ij}, \mathbf{A}] \tilde{\Psi} \right] \prod_{\alpha=1}^{N} d\xi_\alpha
+ \int n_0(\xi) \left[ \frac{m}{2} \left( \ddot{x}_A(\mathbf{x}, t) - U(\mathbf{x}, t) \right) \right] d\xi \quad (54)
\]
defines the many body wave function as a solution to this problem, provided it exists and unique, DefFT. It implies the existence of the exact nonequilibrium of this functional is the key statement of TD-DFT, Eqs. (58) and (59), constitute a closed Eq. (60) can be represented in three equivalent forms, the stress tensor in the Lagrangian frame can be found in \[ \mathbf{\sigma}_{ij} \] of solutions to the universal quantum problem, Eqs. (58), (59) independently of the third \( g \) is a unique solution, provided the external fields \( \mathbf{A} \) and \( U \), and the initial state \( \Psi_0 \) are given. It is, however, not obvious that given metric \( g_{ij} \) we can solve the universal problem of Eqs. (58), (59) for analytic and v-representable metrics \( g \). As in the previous works on “geometric” TDDFT, the present formulation of the many-body theory opens up a possibility to approach the problem in an alternative and, possibly, more natural and internally consistent way.

As we have already mentioned, within the present formalism the question of existence of TDDFT formally translates to the problem of the existence and uniqueness of solutions to the universal quantum problem, Eqs. (58), (59). This problem defines a map \( g_{ij} \rightarrow \Psi \), which also assumes a map \( g_{ij} \rightarrow \mathbf{A} \), and implies the existence of the generalized equation of state. Substituting the constraint of Eq. (59) into Eq. (58) we observe that the later becomes a nonlinear Schrödinger equation (NSE) with a special type of cubic nonlinearity. A rigorous analysis of the Cauchy problem for this NSE will be presented in a separate publication. In this paper we adopt common in TDDFT field simplifying assumptions, and prove the uniqueness of the solution to Eqs. (58), (59) for analytic and v-representable metrics \( g_{ij} \). As usual we call an observable v-representable if it can be produced in a given physical system by applying some external potentials. In the present context a metric (deformation) tensor \( g_{ij} \) is v-representable if it is defined by Eqs. (7) and (5), where \( \mathbf{v}(\mathbf{x}, t) \) is a physical velocity generated by some external potentials \( \mathbf{A}(\mathbf{x}, t) \) and \( U(\mathbf{x}, t) \).

Let us assume that the deformation tensor is analytic in \( t \). Hence it possesses a Taylor expansion with a finite formulation of a closed theory of one vector-valued collective variable – the trajectory function \( \mathbf{x}(\xi, t) \). This theory can be interpreted as the exact quantum continuum mechanics.

B. The universal problem and mapping theorems of TDDFT

The complete system of Eqs. (58)-(60) is simply a reformulation of the original linear Schrödinger equation with the Hamiltonian (49). Therefore Eqs. (58)-(60) possess a unique solution, provided the external fields \( \mathbf{A} \) and \( U \), and the initial state \( \Psi_0 \) are given. It is, however, not obvious that given metric \( g_{ij} \) we can solve the universal problem of Eqs. (58), (59) independently of the third equation, Eq. (60). The problem of well-posedness of the nonlinear Cauchy problem defined by Eqs. (58), (59) for a given \( g_{ij} \) is equivalent to the problem of existence of TDDFT.

In Sec. II B we have demonstrated that in the one particle case the universal problem of Eqs. (58), (59) [for \( N = 1 \) they reduce to Eqs. (32), (33)] admits an exact analytic solution. Hence in this particular case the universal functional \( \tilde{\Psi}[\Psi_0, g_{ij}] \) (and thus TDDFT) does indeed exist. The simplest way to argue in favor TDDFT in the general case of \( N > 1 \) is to refer to the Runge-Gross theorem, or to its generalizations. In fact, just this argumentation was used in the previous works on “geometric” TDDFT. The present formulation of the many-body theory opens up a possibility to approach the problem in an alternative and, possibly, more natural and internally consistent way.

As we have already mentioned, within the present formalism the question of existence of TDDFT formally translates to the problem of the existence and uniqueness of solutions to the universal quantum problem, Eqs. (58), (59). This problem defines a map \( g_{ij} \rightarrow \Psi \), which also assumes a map \( g_{ij} \rightarrow \mathbf{A} \), and implies the existence of the generalized equation of state. Substituting the constraint of Eq. (59) into Eq. (58) we observe that the later becomes a nonlinear Schrödinger equation (NSE) with a special type of cubic nonlinearity. A rigorous analysis of the Cauchy problem for this NSE will be presented in a separate publication. In this paper we adopt common in TDDFT field simplifying assumptions, and prove the uniqueness of the solution to Eqs. (58), (59) for analytic and v-representable metrics \( g_{ij} \). As usual we call an observable v-representable if it can be produced in a given physical system by applying some external potentials. In the present context a metric (deformation) tensor \( g_{ij} \) is v-representable if it is defined by Eqs. (7) and (5), where \( \mathbf{v}(\mathbf{x}, t) \) is a physical velocity generated by some external potentials \( \mathbf{A}(\mathbf{x}, t) \) and \( U(\mathbf{x}, t) \).

Let us assume that the deformation tensor is analytic in \( t \). Hence it possesses a Taylor expansion with a finite
radius of convergence,
\[ g_{ij}(t) = \delta_{ij} + \sum_{k=1}^{\infty} \frac{g_{ij}^{(k)}}{k!} t^k, \quad (61) \]
where \( g_{ij}^{(k)} = \partial^k g_{ij}(0) \). The first term in the right hand side of Eq. (61) is the initial metric tensor \( g_{ij}^{(0)} = g_{ij}(0) = \delta_{ij} \), which follows from the initial condition to Eq. (5). Similarly one can expand the wave function \( \Psi(t) \)
\[ \Psi(t) = \Psi_0 + \sum_{k=1}^{\infty} \frac{\Psi^{(k)}}{k!} t^k \quad (62) \]
Now we substitute Eq. (59) into Eq. (58), and insert the expansions Eqs. (61) and (62) into the resulting nonlinear Schrödinger equation. Collecting terms with the same power of \( t \) we transform Eq. (59) to the following set of equations for the derivatives \( \Psi^{(k)} \)
\[ \Psi^{(k)}(t) = -iF^{(k-1)}, \quad k = 1, 2, \ldots \quad (63) \]
where \( F^{(k)} \) denote the coefficients for the Taylor expansion of the right hand side of Eq. (58). Since Eq. (59), which relates \( A \) to \( \Psi \), is local in time, the nonlinear operator in the right hand side of Eq. (58) also locally depends on the wave function. This implies that the \( k \)th Taylor coefficient \( F^{(k)} \) contains derivatives \( \Psi^{(p)} \) only with \( p \leq k \). Hence Eq. (63) can be schematically represented as follows
\[ \Psi^{(1)} = -iF^{(0)}[g_{ij}^{(0)}; \Psi_0], \]
\[ \Psi^{(2)} = -iF^{(1)}[g_{ij}^{(0)}, g_{ij}^{(1)}; \Psi_0, \Psi^{(1)}], \]
\[ \Psi^{(k)} = -iF^{(k-1)}[g_{ij}^{(0)}, \ldots, g_{ij}^{(k-1)}; \Psi_0, \ldots, \Psi^{(k-1)}], \]
\[ \ldots \]

Applying this system can be solved recursively starting from the first equation. The solution uniquely defines a map: \( \{g_{ij}^{(k)}, \Psi_0 \} \rightarrow \{\Psi^{(k)} \} \). Substituting the coefficients \( \Psi^{(k)} \) into the Taylor expansion, Eq. (62), we obtain the time-dependent wave function as a unique functional of the metric tensor and the initial state: \( \Psi[g_{ij}, \Psi_0](t) \). Importantly, this is true only if the Taylor series of Eq. (62) converges, i.e., if the solution to our nonlinear problem exists, which can not be taken for granted in general. In this paper we follow the common practice and make an additional assumption of v-representability of the metric, which guarantees an a priori existence of the solution and thus a convergence of the Taylor series.

The above results constitute a constructive prove of following uniqueness theorem: For an analytic and v-representable Green’s deformation tensor \( g_{ij} \), the wave function \( \Psi(t) \) in the Lagrangian frame is a unique functional of \( g_{ij} \) and the initial state \( \Psi_0 \). In other words, the map \( g_{ij}, \Psi_0 \rightarrow \Psi(t) \) is unique.

This theorem is analogous to the Runge-Gross theorem in TDDFT. In particular it proves the existence of the exact nonequilibrium equation of state, \( \tilde{P}^{ij} = \tilde{P}^{ij}[g_{ij}] \), and the existence of a closed theory of only one collective variable – the trajectory \( \mathbf{x}(\xi, t) \). Since the deformation tensor is a unique functional of the velocity, the above uniqueness theorem can be also viewed as a proof of the velocity-to-wave function mapping that forms a basis of TDCDFT.

The presented proof of \( g_{ij} \rightarrow \tilde{\Psi}(t) \) mapping is closely related to constructive proofs of the mapping theorems in TDDFT and TDCDFT by van Leeuwen\textsuperscript{31} and Vignale\textsuperscript{29}, respectively. In fact, the formal statement of the problem in Refs. 31 and 29 is very similar to our system of Eqs. (58), (59). In either proof one solves the many-body Schrödinger equation, supplemented by a constraint – the force balance equation – that relates the potential to a collective variable of interest (the density in Ref. 31, or the current in Ref. 29). The structure of the recursive calculation of the Taylor coefficients is basically the same in all the proofs. However, in the present formulation of the theory the proof becomes almost trivial due to a complete (both in time and in space) locality of the constraint, Eq. (59). We note that the proof of the Vignale’s theorem can also be essentially simplified by reformulating the problem in a similar local fashion\textsuperscript{32}. It is also important to note that neither proof attempts to address a question of convergence of the resulting unique Taylor series for the potential and/or the wave function. Therefore, strictly speaking, the v-representability problem remains unresolved in any nonlinearized version of TDDFT, in spite occasional statements to the contrary in the literature.

C. Keldysh-contour formulation of the exact quantum continuum mechanics

In the previous section we have proved that the wave function \( \Psi(\xi_1, \ldots, \xi_N, t) \) and the effective vector potential \( A(\xi, t) \) are universal functionals of the Green’s deformation tensor \( g_{ij}(\xi, t) \). Hence the stress tensor \( \tilde{P}_{ij} \) in the Lagrangian frame is also a universal functional of \( g_{ij} \). In general the stress tensor \( \tilde{P}_{ij} \) is proportional to the expectation value of the partial variational derivative \( \delta\tilde{H}[g_{ij}, A]/\delta g_{ij} \) at fixed \( A \) [see Eq. (23)]. However, in the Lagrangian frame the current density vanishes, which implies the following identity \( j^k = \langle \delta\tilde{H}[g_{ij}, A]/A_k \rangle \equiv 0 \). Thus in the Lagrangian frame \( \tilde{P}_{ij} \) can be also defined via the total variational derivative of the Hamiltonian with respect to the metric
\[ \tilde{P}^{ij}[g_{ij}](\xi, t) = -\frac{2}{\sqrt{g}} \langle \tilde{\Psi}[g_{ij}] \delta\tilde{H}[g_{ij}]/\delta g_{ij}(\xi, t) \tilde{\Psi}[g_{ij}] \rangle, \quad (64) \]
where \( \tilde{H}[g_{ij}] \equiv \tilde{H}[g_{ij}, A[g_{ij}]] \). Equation (64) relates the exact nonequilibrium equation of state to the solution of
the universal quantum problem, Eqs. (58), (59). Substituting this equation of state into Eq. (60) we obtain a formally closed equation of the exact quantum continuum mechanics (in the Lagrangian formalism)

\[ m\ddot{x}^k = [x \times B(x, t)]_k + E_k(x, t) - \frac{\sqrt{g}}{n_0} \frac{\partial \xi^i}{\partial x^k} \nabla_j \tilde{P}^j_{ij} [g_{ij}] \]  

(65)

By solving this equation with initial conditions \( x(\xi, 0) = \xi \) and \( \dot{x}(\xi, 0) = v_0(\xi) \) we get a set of trajectories \( x(\xi, t) \) for a given configuration of the external fields. The knowledge of these trajectories allows us to uniquely determine the density, Eq. (47), and the velocity, Eq. (48), in the laboratory frame.

The existence of a closed continuum mechanics defined by Eq. (65) is a generic fact, which follows from the uniqueness theorem of Sec. IIB. In spite of an apparently “classical” form of Eq. (65), it exactly describes the dynamics of a quantum many-body system. All quantum and correlation effects are encoded in the equation of state – the functional dependence of the stress tensor on the deformation tensor.

The question we address in this section concerns a principal possibility to formulate the exact continuum mechanics in a form of a closed variational principle. Namely, is there exists an action functional \( S[x(\xi, t)] \) that generates the equation of motion, Eq. (64). In Sec. IIB we have explicitly constructed such a functional for the exactly solvable one particle case. The corresponding Lagrangian is given by Eq. (46) that defines a simple, purely elastic, i.e., local in time, theory. A formal reason for this is the following identity

\[ \langle \tilde{\Psi} | \frac{\delta \tilde{H}[g_{ij}]}{\delta g_{ij}} | \tilde{\Psi} \rangle = \frac{\delta}{\delta g_{ij}} \langle \tilde{\Psi} | \tilde{H}[g_{ij}] | \tilde{\Psi} \rangle = \frac{\delta E[g_{ij}]}{\delta g_{ij}}, \]  

(66)

where \( E[g_{ij}] \) is the energy functional, which turns out to be local in time [see the last term in Eq. (46)]. Therefore in the one particle case the stress tensor is equal to the variational derivative of the energy functional, exactly as it is in the classical elasticity theory. (We note in brackets that the space-nonlocality, i.e. the presence of gradients in \( E[g_{ij}] \), is responsible for quantum effects).

In a many/few-particle system the identity of Eq. (66) does not hold. In general, for a system of \( N > 1 \) particles the stress tensor is not a functional derivative of any functional. Physically this is related to a relative motion of particles, which produces a non-instantaneous response of the system to a dynamic change of the metric. Nonetheless a variational formulation of the theory is still possible if one doubles the number of degrees of freedom by considering the evolution along a Keldysh contour \( C \).

The existence of the map \( g_{ij}, \Phi_0 \rightarrow |\tilde{\Psi}(t)\rangle \) assumes the existence of a unitary evolution operator \( U[g_{ij}](t, 0) \)

\[ |\tilde{\Psi}(t)\rangle = U[g_{ij}](t, 0)|\Phi_0\rangle, \]  

(67)

\[ U[g_{ij}](t, 0) = T \exp \left\{ -i \int_0^t \tilde{H}[g_{ij}](t')dt' \right\}, \]  

(68)

where \( T \) stands for the usual chronological ordering. Using Eqs. (67) and (68) we can rewrite the definition of the stress tensor, Eq. (64), as follows

\[ \tilde{P}^{ij} = -\frac{2}{\sqrt{g}} \langle \Phi_0 | U(0, t) \frac{\delta \tilde{H}[g_{ij}]}{\delta g_{ij}} U(t, 0) | \Phi_0 \rangle. \]  

(69)

Let us introduce two different deformation tensors, \( g_{ij}^-(t) \), and \( g_{ij}^+(t) \), and construct the following generating functional

\[ W[g_{ij}^-, g_{ij}^+] = i \ln \langle \Phi_0 | U^+(t, 0) U^-(0, t) | \Phi_0 \rangle, \]  

(70)

where \( U^\pm(t, 0) = U[g_{ij}^\pm](t, 0) \) is the evolution operator obtained from the solution of the universal problem, Eqs. (58), (59), with the metric \( g_{ij}^\pm(\xi, t) \). The stress tensor, Eq. (69), is recovered by differentiating \( W[g_{ij}^-, g_{ij}^+] \) with respect to \( g_{ij}^- \), and setting \( g_{ij}^- = g_{ij}^+ = g_{ij} \). Formally the operator \( U^+(0, \infty) U^-(\infty, 0) \) in Eq. (70) describes a propagation from the initial time to infinity, and then back to \( t = 0 \). This can be viewed as a propagation along a closed Keldysh contour \( C \). The contour \( C \) consists of two branches: the “forward” (−) branch that goes from \( t = 0 \) to \( \infty \), and the “back” (+) branch going from \( \infty \) to the initial time, \( t = 0 \). Using this notion one can represent the generating functional \( W \), Eq. (70), in the following compact form

\[ W[g_{ij}^C] = i \ln \langle \Phi_0 | T e^{-i \int_C \tilde{H}[g_{ij}^C](t)dt} | \Phi_0 \rangle, \]  

(71)

where \( T_C \) orders times along the Keldysh contour, and \( g_{ij}^C \) takes the values \( g_{ij}^- \), and \( g_{ij}^+ \) on the forward, and back branches, respectively. The physical stress tensor, Eq. (69), is given by the following functional derivative

\[ \tilde{P}^{ij}[g_{ij}] = -\frac{2}{\sqrt{g}} \frac{\delta W[g_{ij}^C(\xi, t)]}{\delta g_{ij}^-} \bigg|_{g_{ij}^- = g_{ij}(t)}. \]  

(72)

The notation \( g_{ij}^C = g_{ij}(t) \) means that we set metric tensors on either branch equal to the physical deformation tensor \( g_{ij}(\xi, t) \). Let us introduce the contour trajectory \( x_C(\xi, t) \) that generates the contour deformation tensor

\[ g_{ij}^C = \frac{\partial x_C^k}{\partial \xi^i} \frac{\partial x_C^l}{\partial \xi^j}. \]  

(73)

Using Eqs. (72) and (73) one can show that the stress force entering Eq. (65) is the functional derivative of the generating functional \( W \) with respect to \( x_C \)

\[ -n_0 F_k^{\text{str}} = \sqrt{g} \frac{\partial \xi^i}{\partial x_C^k} \tilde{P}^j_{ij} [g_{ij}] = \frac{\delta W[g_{ij}^C]}{\delta x_C^k} \bigg|_{x_C = x(\xi, t)} \]  

(74)

Equation (74) naturally suggests the following form of the Keldysh action functional

\[ S_C[x_C] = \int_C dt \int d\xi n_0 \left[ \frac{m}{2} (\dot{x}_C)^2 + x_C A(x_C, t) \right] - U(x_C, t) - W[g_{ij}^C]. \]  

(75)
Indeed, the stationarity condition for the action $S_C[x_C]$, 

$$\frac{\delta S_C[x_C]}{\delta x_C} \bigg|_{x_C = x(\xi, t)} = 0,$$  

reovers the correct form of the hydrodynamics equation of motion, Eq. (65), for the trajectory $x(\xi, t)$.

The variational formulation, Eqs. (75), (76), of the exact quantum continuum mechanics is the main result of the present section. From the practical point of view, the very existence of the action functional, Eq. (75), is already a very useful statement. In particular it justifies an application of many powerful methods of the classical continuum mechanics to dynamics of quantum many-body systems. One of those methods is a construction of an effective elastic functionals $W[g_{ij}]$ based on fundamental symmetries of a given physical system. This approach has been used to derive a hydrodynamics theory of strongly correlated many-body states in the fractional quantum Hall regime\textsuperscript{23}. One of the basic assumptions made in Ref. 21 was the existence of the action functional of the form of Eq. (75). The results of the present section provide a rigorous justification of that approach. In the next section we will show the variational formulation of TDDfFT also offers a convenient tool for the definition of xc potentials in the Kohn-Sham scheme.

A few years ago a Keldysh-contour formulation of TDDfFT was proposed by van Leeuwen\textsuperscript{34,35} to resolve the causality problem of the original Runge-Gross theory. Despite certain similarities, our construction is fundamentally different from that of Refs. 34,35. The van Leeuwen’s formulation of TDDfFT requires the existence of the Keldysh-contour analog of the Runge-Gross mapping theorem, which has not been proved up to now. In contrast to that, the present approach to TDDfFT relies only on the real-time uniqueness theorem presented in Sec. IIIB.

**IV. A TIME-DEPENDENT KOHN-SHAM CONSTRUCTION**

In general the exact stress tensor $\tilde{P}_{ij}[g_{ij}]$ as well as the effective energy functional $W[g_{ij}^{\text{xc}}]$ contain both kinetic and interaction contributions. In some systems, such as strongly correlated collective quantum Hall states, or one-dimensional Luttinger liquids, it is natural to consider the functional $\tilde{P}_{ij}[g_{ij}]$ (or $W[g_{ij}^{\text{xc}}]$) as a single entity. This approach was successfully employed in our recent studies of the fractional quantum Hall liquids and liquid crystals\textsuperscript{21,22,36}. However, in the most of less exotic many-body systems, e. g., in atoms, molecules or solids, it is useful to extract at least a part of the kinetic contribution to the universal functionals, and to consider it separately from the rest. The Kohn-Sham (KS) construction is a special tool for such a separation – it allows one to calculate exactly the noninteracting part of the kinetic stress functionals.

The time-dependent KS construction in TDDfFT can be introduced as follows. Let us consider a system of $N$ noninteracting KS particles moving in the presence of effective potentials, $A_S = A + A_{\text{xc}}$ and $U_S = U + U_{\text{xc}}$. Here $A(x, t)$ and $U(x, t)$ are the external fields, while $A_{\text{xc}}(x, t)$ and $U_{\text{xc}}(x, t)$ are selfconsistent xc potentials that are adjusted to reproduce a collective variable of interest in the physical interacting system. In the Lagrangian formulation of TDDfFT the proper collective variable is the trajectory $x(\xi, t)$. In the KS system the equation of motion for $x(\xi, t)$, takes the form

$$m\ddot{x} = \dot{x} \times B_S(x, t) + E_S(x, t) + \tilde{F}^{\text{str}}_S[x],$$  

where $\tilde{F}^{\text{str}}_S[x]$ is the kinetic stress tensor that is related to the kinetic stress tensor, $\tilde{P}_{S,ij}[g_{ij}]$, of noninteracting KS particles:

$$\tilde{F}^{\text{str}}_S[k] = -\frac{\sqrt{g}}{n_0} \frac{\partial e_i}{\partial x^k} \nabla_j \tilde{P}_{S,ij}[g_{ij}].$$  

In Eq. (77) $E_S(x, t)$ and $B_S(x, t)$ are, respectively, the electric, and the magnetic fields associated to the effective potentials $A_S(x, t)$ and $U_S(x, t)$. The functional $\tilde{P}_{S,ij}[g_{ij}]$ is obtained from the solution of the universal problem, Eqs. (58), (59), for a noninteracting system (i. e., with $H_{\text{int}}[g_{ij}] = 0$). To determine the xc potentials one has to compare Eq. (77) with the corresponding equation for the real interacting system, Eq. (65). Apparently they coincide if the force produced by the xc potentials equals to the difference of stress forces in the interacting and the noninteracting systems

$$E_{\text{xc},k}(x, t) + [\dot{x} \times B_{\text{xc}}(x, t)]_k = -\frac{\sqrt{g}}{n_0} \frac{\partial e_i}{\partial x^k} \nabla_j \tilde{P}_{\text{xc},ij}[g_{ij}],$$  

where $\tilde{P}_{\text{xc},ij}[g_{ij}](\xi, t) = \tilde{P}_{S,ij}[g_{ij}](\xi, t) - \tilde{P}^{\text{str}}_S[g_{ij}](\xi, t)$ is the xc stress tensor functional, and the xc electric and magnetic fields are defined as follows

$$E_{\text{xc}}(x, t) = -\partial_x A_{\text{xc}}(x, t) - \partial_x U_{\text{xc}}(x, t),$$  

$$B_{\text{xc}}(x, t) = \partial_x \times A_{\text{xc}}(x, t).$$  

Equations (79)–(81) define the xc potentials up to a gauge transformation.

In practical application it is much more convenient to work with the KS system (i. e., to solve the time-dependent KS equations) in the laboratory frame. Therefore we need to transform the definition of xc potentials from the Lagrangian frame back to the laboratory one. This is done simply by setting $\xi = \xi(x, t)$, where $\xi(x, t)$ is the inverse of $x(\xi, t)$. The result of this procedure for Eq. (79) takes the form

$$\partial_t A_{\text{xc},k} - (v \times (\partial_x A_{\text{xc}}))_k + \partial_k U_{\text{xc}} = \frac{1}{n} \partial_j P_{\text{xc},jk}$$  

where $P_{\text{xc},ij}(x, t)$ is the xc stress tensor in the laboratory frame, which is related to $\tilde{P}_{\text{xc},ij}[g_{ij}](\xi, t)$ as follows

$$P_{\text{xc},ij}(x, t) = \frac{\partial \xi^k}{\partial x^i} \frac{\partial \xi^l}{\partial x^j} \tilde{P}_{kl}[g_{ij}](\xi(x, t), t).$$


Equation (82) recovers the force definition of the xc potentials introduced in Ref. 16. The most important new result of the present general approach is the functional dependence on the collective variables. We have proved that the stress tensor in the Lagrangian frame, \( \overline{P}_{xc,ij}(\xi, t) \), is a unique functional of only one basic variable — the Green’s deformation tensor \( g_{ij} \). The transformed xc stress tensor \( \overline{P}_{xc,ij}(x, t) \), Eq. (83), which determines xc potentials in the laboratory frame, already depends not only on \( g_{ij} \), but also on the function \( \xi(x, t) \) itself. However, the dependence on \( \xi(x, t) \) is trivial [in the prefactor, and in the argument in Eq. (83)], and can be accounted for exactly, provided the universal functional \( \overline{P}_{xc,ij}(g_{ij})(\xi, t) \) is known.

Another practically important outcome is the possibility to define the xc force, and thus the xc potentials, via a functional derivative of the scalar functional \( W_{xc}^{\xi}(g_{ij}) \). Indeed, using Eq. (74) we can rewrite Eq. (79) in the following form

\[
E_{xc} + \dot{x} \times B_{xc} = -\frac{1}{n_0} \frac{\delta W_{xc}^{\xi}(g_{ij})}{\delta \xi_C} \bigg|_{\xi_C = \xi(x, t)} \tag{84}
\]

where \( W_{xc}^{\xi}(g_{ij}) = W_{xc}(g_{ij}) - W_{S}(g_{ij}) \) is the difference of W-functionals in the interacting, and noninteracting systems. The variational definition of the xc potentials, Eq. (84), should be more convenient for phenomenological construction (e. g. GGA-like) of various approximations. It reduces the problem to approximating a global scalar functional \( W_{xc}^{\xi}(g_{ij}) \), which seems to be a simpler task. Importantly, the very form of Eq. (84) already guarantees many exact constraints. For instance, any functional \( W_{xc}^{\xi}(g_{ij}) \) yields the xc force that is equal to the divergence of the symmetric second rank tensor, which automatically ensures the zero net force, and the zero net torque conditions. It is worth outlining that the variational definition of the xc potentials, Eq. (84), is possible only in the Lagrangian frame. Given a functional \( W_{xc}^{\xi}(g_{ij}) \), the xc force in the laboratory frame is obtained as follows. One first calculates the variational derivative in the right hand side of Eq. (84), and then makes the transformation to the laboratory frame by setting \( \xi = \xi(x, t) \). As a result the right hand side of Eq. (83) is recovered.

The W-functional of TDDFtF also offers a convenient tool for a compact, unified, and transparent representation of all currently known approximations in TDDFT/TDCDFT. For example, the local VK approximation\(^a\), as well as its extension by VUC\(^b\), corresponds to the following quadratic functional

\[
W_{xc}^{VK}(g_{ij}) = \frac{1}{8} \int d\xi \int dt dt' \left\{ 2\mu_{xc}(t-t')\delta g_{ij}(t)\delta g_{ij}(t') + \left[ K_{xc}(t-t') - \frac{2}{\overline{P}_{xc}(t-t')^2} \right] \delta g_{ij}(t)\delta g_{ij}(t') \right\}, \tag{85}
\]

where \( \delta g_{ij} = g_{ij} - \delta_{ij} \) is the linearized strain tensor, while \( K_{xc}(t-t') \) and \( \mu_{xc}(t-t') \) are, respectively, the nonadiabatic xc bulk and shear moduli of the homogeneous system, defined on the Keldysh contour. The VK approximation given by Eq. (85) is valid in the limit of small \( \delta_{ij} \).

A nonlinear elastic local deformation approximation (LDefA) introduced in Ref. 17 is generated by a completely local W-functional of the following form

\[
W_{xc}^{LDefA}(g_{ij}) = \int d\xi \int dt E_{xc}(g_{ij}^C(\xi, t)), \tag{86}
\]

where the nonadiabatic xc energy density \( E_{xc}(g_{ij}) \) is defined as follows

\[
E_{xc}(g_{ij}) = \sum_p \left\{ \frac{1}{2} \frac{\tilde{V}(\sqrt{g_{ij}^C p_p})}{\sqrt{g_{ij}^C}} g_2(p; n_0) \right\}. \tag{87}
\]

In this equation \( \tilde{V}(q) \) is the Fourier component of the interaction potential, \( f_{xc}(p; n_0) \) is the correlation part of the one particle distribution function, and \( g_2(p; n_0) \) is the Fourier component of the pair correlation function. Both \( f_{xc}(p; n_0) \) and \( g_2(p; n_0) \) are calculated for a homogeneous system with the density \( n_0(\xi) \). In the limit of small deformations, when \( g_{ij} \) slightly deviates from \( \delta_{ij} \), the nonlinear elastic local deformation approximation defined by Eqs. (86), (87) reduces to the high-frequency limit of VK approximation, Eq. (85).

For comparison we also show the functional \( W_{xc}^{Ad}(g_{ij}) \) that corresponds to the adiabatic local density approximation (ALDA):

\[
W_{xc}^{Ad}(g_{ij}) = \int d\xi \int dt \sqrt{g(\xi, t)} E_{xc}^{hom}(n_0(\xi)), \tag{88}
\]

where \( E_{xc}^{hom}(n) \) is the usual ground state xc energy density of the homogeneous system.

Finally we derive one more exact representation of the xc force. Namely, we relate \( A_{xc} \) and \( U_{xc} \) to the effective vector potential \( \mathbf{A} \) that enters the universal problem of Eqs. (58), (59). According to the momentum balance equation in the Lagrangian frame, Eq. (28), [see also the identity of Eq. (40)], the divergence of the stress tensor is equal to the time derivative of the effective vector potential \( \mathbf{A} \). Hence the xc force in the Lagrangian frame, Eq. (79), can be also represented as follows

\[
E_{xc,k}(x, t) + [\dot{x} \times B_{xc}(x, t)]_k = \frac{\partial \mathbf{A}_C^C}{\partial x_k} \partial_t A_{xc,i}(\xi, t), \tag{89}
\]

where \( A_{xc}(\xi, t) = \mathbf{A}(\xi, t) - \mathbf{A}_0(\xi, t) \) is the difference of the effective vector potentials in the interacting and noninteracting systems with the same metric \( g_{ij} \). The right hand side of Eq. (89) needs to be transformed to the laboratory frame. Let us first use the standard transformation rule to define an effective vector potential, \( A_{xc}^L(x, t) \), in the laboratory frame

\[
A_{xc,i}(\xi, t) = \frac{\partial x^j}{\partial \xi^i} A_{xc,j}^L(x(\xi, t), t). \tag{90}
\]
Substituting Eq. (90) in the right hand side of Eq. (89) we find for the stress force

\[
\frac{\partial \xi^i}{\partial t} \partial_i A_{xc,i}(\xi, t) = \partial_i A'_{xc,i}(\xi, t) + \frac{\partial \xi_i}{\partial v^i} \frac{\partial^2 v_j}{\partial v^i} A'_{xc,j} = \partial_i A'_{xc,i}(\xi, t) + \frac{\partial v_i}{\partial t} A'_{xc,i}(\xi, t) + \frac{\partial v_i}{\partial x^k} A'_{xc,i}(\xi, t)
\]

(91)

where we used the definition of the velocity, Eq. (5). Inserting the result of Eq. (91) into Eq. (89) we obtain the following equation for the xc potentials in the laboratory frame

\[
\partial_t A_{xc} - v \times (\partial_x \times A_{xc}) + \partial_x U_{xc} = -\partial_t A'_{xc} + v \times (\partial_x \times A'_{xc}) - \partial_x (vA'_{xc}).
\]

(92)

This equation determines the xc potentials, \(A_{xc}(x, t)\) and \(U_{xc}(x, t)\), up to an arbitrary gauge transformation. One of possible solutions to Eq. (92) takes the form

\[
A_{xc}(x, t) = -A'_{xc}(x, t),
\]

(93)

\[
U_{xc}(x, t) = -v(x, t)A'_{xc}(x, t).
\]

(94)

Therefore there is a particular mixed gauge in which the xc potentials are locally expressed in terms of the effective vector potential \(A_{xc}\). The convenience of the exact representation given by Eqs. (93), (94) is that it directly relates the xc potentials, which enter the KS equations, to the solution of the universal quantum problem, Eqs. (58), (59). Equations (93) and (94) can be useful for the analysis of the exact properties of KS potentials, such as symmetries, scaling properties, etc.

V. CONCLUSION

In this paper we presented a self-contained, constructive derivation of the time-dependent deformation functional theory (TDDFT). The main idea of our approach to the time-dependent many-body problem is a separation of the convective and relative motions of quantum particles. Technically these two types of motion are separated by the transformation to the comoving Lagrangian reference frame. The convective motion is described by a set of trajectories \(x(\xi, t)\) of infinitesimal fluid elements, where \(\xi\) is the initial position (the Lagrangian coordinate) of a given element. The motion of particles relatively to the convective flow is determined by the many-body wave function \(\tilde{\Psi}\) in the comoving frame. Since the convective motion is singled out by the above transformation, the number of degrees of freedom entering the quantum many-body problem is reduced. Formally the dynamics of the wave function \(\tilde{\Psi}\) is constrained by a local “gauge” condition of zero current density. The most important property of this constrained quantum problem is that it does not contain external fields. It is completely determined by the fundamental geometric characteristics of the Lagrangian frame – the Green’s deformation tensor \(g_{ij}\) that enters the equations of motion as a metric tensor. Hence the many-body problem for the relative motion appears to be universal. This problem, naturally defines the wave function as a universal functional of the deformation tensor, \(\tilde{\Psi}[g_{ij}]\). Therefore the expectation value of any observable in the Lagrangian frame is also a functional of the deformation tensor. In particular this is true for the stress force entering the equation of motion for the Lagrangian trajectories \(x(\xi, t)\). Thus the trajectories and hence the whole convective motion of an arbitrary quantum many-body system can be found from a closed hydrodynamics-like theory. We call this theory TDDFT since the deformation tensor is the basic variable entering all relevant universal functionals.

The set of Lagrangian trajectories \(x(\xi, t)\) and the current density \(j(x, t)\) are in a one-to-one correspondence. Therefore our theory can in principle be viewed as a particular realization of TDDFT. However it is also legitimate, and perhaps even more natural, to consider TDDFT as an independent member of the family of time-dependent DFT-like theories, such as TDDFT by Runge and Gross, and TDCDFT proposed by Vignale and Kohl. An apparent advantage of the deformation-based formalism is the existence of a well founded local approximation for xc potentials in the KS formulation of the theory. In fact, TDDFT provides the most natural and unified framework for interpreting all currently known local nonadiabatic approximations. The exact representations for the xc potentials derived in Sec. IV should result in the further progress in constructing new practical nonadiabatic functionals.

APPENDIX A: LOCAL SYMMETRIES AND CONSERVATION LAWS

In this Appendix we derive two local conservation laws for a \(N\)-body system placed in the space with metric \(g_{ij}(\xi, t)\), and subjected to an external field that is generated by the four-potential \(A_0(\xi, t)\), \(A(\xi, t)\). The dynamics of the \(N\)-body wave function \(\Psi(\xi_1, \ldots, \xi_N, t)\) is governed by the time-dependent Schrödinger equation with the following Hamiltonian

\[
H = \sum_{\alpha=1}^{N} g_{ij}^{-1} [i \partial_{\xi_i} + A_i(\xi_\alpha)] \sqrt{g_{ij}} g_{ij}^{ij} [i \partial_{\xi_i} + A_j(\xi_\alpha)] g_{ij}^{-1} + \sum_{\alpha=1}^{N} A_0(\xi_\alpha) + \frac{1}{2} \sum_{\alpha, \beta} V(\xi_\alpha, \xi_\beta)
\]

(91)

where \(g_{ij}^{ij} = g^{ij}(\xi_\alpha, t)\) and \(l_{\xi_\alpha, \xi_\beta}\) is the length of geodesic that connects points \(\xi_\alpha\) and \(\xi_\beta\).

Below we derive local balance equations from local symmetries of the Dirac-Frenkel action functional (for a similar derivation see also Ref. 37):

\[
S[\tilde{\Psi}, A_0, A, g_{ij}] = \int dt \prod_{\alpha=1}^{N} d\xi_\alpha \tilde{\Psi}^* \left( i \frac{\partial}{\partial t} - H \right) \tilde{\Psi}. \quad (A2)
\]
In particular the local gauge invariance of $S$ is responsible for the local conservation of the number of particles, while the general coordinate invariance of the action yields the local momentum balance equation.

Let us consider the gauge invariance first. By a direct substitution we find that the following transformation

$$
\Psi' = \Psi e^{i \sum_\alpha \phi (\xi, t)},
$$

(A3)

$$
\mathcal{A}_0' = A_0 - \partial_\xi \phi (\xi, t), \quad \mathcal{A}_i' = A_i + \partial_\xi \phi (\xi, t),
$$

(A4)

$$
g'_{ij} (\xi, t) = g_{ij} (\xi, t),
$$

(A5)

where $\phi (\xi, t)$ is an arbitrary function, leaves the action $S$ unchanged, i.e.,

$$
S [\Psi', \mathcal{A}_0', \mathcal{A}_i', g_{ij}'] = S [\Psi, \mathcal{A}_0, \mathcal{A}_i, g_{ij}].
$$

(A6)

Inserting the infinitesimal version ($\phi \to 0$) of Eqs. (A3)–(A5) into Eq. (A6) we get the following condition

$$
\delta S |_{\text{extr}} = \int dt d\xi \left( - \frac{\delta S}{\delta A_0} \partial_\xi \phi + \frac{\delta S}{\delta \mathcal{A}_i} \partial_\xi \phi \right) = 0
$$

(A7)

As usual we take the variation of the action at the extremal “trajectory” that is defined by the equation $\delta S/\delta \Psi = 0$. Therefore the change of the wave function, Eq. (A3), does not contribute to $\delta S$, Eq. (A7). The requirement that Eq. (A7) is fulfilled for any $\phi$ yields the continuity equation

$$
\partial_t n + \partial_\xi j^i = 0,
$$

(A8)

where the density $n (\xi, t)$ and the current $j^i (\xi, t)$ are defined as follows

$$
n = - \frac{\delta S}{\delta A_0} = \langle \Psi | \frac{\delta H}{\delta A_0} | \Psi \rangle,
$$

(A9)

$$
j^i = \frac{\delta S}{\delta \mathcal{A}_i} = - \langle \Psi | \frac{\delta H}{\delta \mathcal{A}_i} | \Psi \rangle.
$$

(A10)

Similarly the momentum balance equation follows from the invariance of the action $S$, Eq. (A2), under a general nonsingular transformation of coordinates, $\xi' = \xi (\xi, t)$, where $\xi' (\xi, t)$ is an arbitrary (invertible) function. The transformation of fields, which leaves the action invariant, is the following

$$
\Psi' (\{\xi' \}_{\beta = 1}^N, t) = \prod_{\alpha=1}^{N} \left| \frac{\partial \xi'_{\alpha}}{\partial \xi_{\alpha}} \right|^{-1/2} \Psi (\{\xi_{\beta} \}_{\beta = 1}^N, t),
$$

(A11)

$$
g'_{ij} (\xi', t) = \frac{\partial \xi'^k}{\partial \xi^\alpha} \frac{\partial \xi'^\rho}{\partial \xi^\beta} g_{kp} (\xi, t),
$$

(A12)

$$
\mathcal{A}_0' (\xi', t) = \frac{\partial \xi'^i}{\partial \xi^\alpha} A_0 (\xi, t) - m g'_{ij} (\xi', t) \frac{\partial \xi'^n}{\partial t},
$$

(A13)

$$
\mathcal{A}_i' (\xi', t) = A_0 (\xi, t) + \mathcal{A}_i (\xi, t) \frac{\partial \xi'^i}{\partial t} + \frac{m}{2} g'_{ij} (\xi', t) \frac{\partial \xi'^i}{\partial t} \frac{\partial \xi'^j}{\partial t},
$$

(A14)

where $\xi'_{\alpha} = \xi' (\xi_{\alpha}, t)$. Let us consider an infinitesimal transformation of coordinates, which is generated by the function $\xi' = \xi + \eta (\xi, t)$, $\eta \to 0$. The corresponding change of the action (at the extremal) takes the form

$$
\int dt d\xi \left( \frac{\delta S}{\delta g_{ij}} \partial_\xi g_{ij} + \frac{\delta S}{\delta A_0} \delta A_0 + \frac{\delta S}{\delta \mathcal{A}_i} \delta \mathcal{A}_i \right) = 0
$$

(A15)

In equation (A15) $\delta g_{ij}$, $\delta A_0$, and $\delta \mathcal{A}_i$ are given by the infinitesimal version of Eqs. (A12)–(A14):

$$
\delta g_{ij} = - \eta^k \partial_\xi g_{ij} - g_{ik} \partial_\xi \eta^k - g_{jk} \partial_\xi \eta^k,
$$

(A16)

$$
\delta \mathcal{A}_i = - \eta^k \partial_\xi \mathcal{A}_i - A_k \partial_\xi \eta^k - m g_{ik} \partial_\xi \eta^k,
$$

(A17)

$$
\delta A_0 = - \eta^k \partial_\xi A_0 + A_k \partial_\xi \eta^k.
$$

(A18)

Inserting Eqs. (A16)–(A18) into Eq. (A15), and integrating by parts we obtain the following condition of the general coordinate invariance of the action:

$$
\partial_\xi \left( m g_{ik} \frac{\delta S}{\delta \mathcal{A}_i} - A_k \frac{\delta S}{\delta A_0} \right) + \partial_{\xi'} \left( 2 g_{kj} \frac{\delta S}{\delta g_{ij}} + A_{\xi} \frac{\delta S}{\delta A_0} \right) - \frac{\delta S}{\delta A_0} \partial_\xi + A_k \partial_\xi \eta^k = 0.
$$

(A19)

Equation (A19) can be further simplified as follows

$$
m \partial_\xi j_k - j^i (\partial_\xi \mathcal{A}_i - \partial_\xi \mathcal{A}_i) + n \partial_\xi A_k + n \partial_\xi \mathcal{A}_0 + \partial_{\xi'} \left( 2 g_{kj} \frac{\delta S}{\delta g_{ij}} \right) - \frac{\delta S}{\delta g_{ij}} \partial_\xi g_{ij} = 0,
$$

(A20)

where we have used the continuity equation, Eq. (A8), and the definitions of the density, and the current, Eqs. (A9) and (A10). The last two terms in the left hand side of Eq. (A20) are easily recognized as a covariant divergence the following symmetric second rank tensor

$$
P^{ij} = \frac{2}{\sqrt{g}} \frac{\delta S}{\delta g_{ij}} = - \frac{2}{\sqrt{g}} \langle \Psi | \frac{\delta H}{\delta g_{ij}} | \Psi \rangle.
$$

(A21)

Indeed, using the definition of Eq. (A21) we find

$$
\partial_{\xi'} \left( 2 g_{kj} \frac{\delta S}{\delta g_{ij}} \right) - \frac{\delta S}{\delta g_{ij}} \partial_\xi g_{ij} = \sqrt{g} \left( \frac{1}{\sqrt{g}} \partial_\xi \sqrt{g} P_k^i - \frac{1}{2} P^{ij} \partial_\xi g_{ij} \right) \equiv \sqrt{g} \nabla_i P_k^i
$$

Therefore the condition of the general coordinate invariance, Eq. (20), takes the standard form of the local momentum balance equation

$$
m \partial_\xi j_k - j^i (\partial_\xi \mathcal{A}_i - \partial_\xi \mathcal{A}_i) + n \partial_\xi A_k + n \partial_\xi \mathcal{A}_0 + \sqrt{g} \nabla_i P_k^i = 0.
$$

(A22)

Apparently the tensor $P^{ij}$ defined after Eq. (A21) plays a role of the physical stress tensor.
We use a symmetrized time derivative, $\Psi^* \frac{\partial}{\partial t} \Psi$, instead of a more common asymmetric form, $\Psi^* \frac{\partial}{\partial t} \Psi$, for purely technical reasons. It does not change the equations of motion, but significantly simplifies the transformation to a general noninertial reference frame.

Throughout this paper we use Latin indexes, $i, j, k$, etc., to label Cartesian axes. Additional Greek indexes will be used in Sec. III for labeling particles in the many-body system. We also employ the standard convention of summation over repeated Latin indexes.

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