Time-dependent deformation functional theory

I. V. Tokatly*
Lehrstuhl für Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstrasse 7/B2, 91058 Erlangen, Germany and Moscow Institute of Electronic Technology, Zelenograd 124498, Russia

(Received 12 December 2006; revised manuscript received 17 January 2007; published 5 March 2007)

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 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 construction of nonadiabatic approximations. We also discuss a relation of the present approach to a recent continuum mechanics of the incompressible quantum Hall liquids.

DOI: 10.1103/PhysRevB.75.125105 PACS number(s): 71.10.−w, 05.30.−d, 47.10.−g, 02.40.−k

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 cannot 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 the 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 $n(\mathbf{x})$ 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 $E_{\mathrm{xc}}[n]$. Although the exact form of $E_{\mathrm{xc}}[n]$ 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 enormous popularity in different branches of physics.[7] A hydrodynamic interpretation of TDDFT was mentioned in the original paper by Runge and Gross. However, it remained practically out of use for more than ten years. A comeback of hydrodynamic analogy was caused by attempts[8–11] to go beyond a simple (but formally unjustified) adiabatic local density approximation for the time-dependent xc potential. In the mid-1990s it was 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 to the ultranonlocality problem was proposed by Vignale and Kohn (VK).[8] They suggested switching from TDDFT to a time-dependent current-density-functional theory (TDCDFT) and considering the current $\mathbf{j}(\mathbf{x},t)$ 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, Ullrich, and Conti[9] (VUC) 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 viscoelastic 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 viscoelastic form of the stress tensor for nonlinear dynamics. A similar assumption has been made in a phenomenological approach developed by Kurzweil and Baer.[14,15]

A general resolution of the ultranonlocality problem in TDDFT, which has been proposed recently,[16,17] also extensively relies on ideas and techniques borrowed from the clas-

sical 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).[17,18] The key idea of Refs. 16 and 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 longstanding 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).[17,18] A connection of a general nonlinear local deformation approximation to the phenomenological current density functional by VUC (Ref. 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 and 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) and (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,[16,17] 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).[17,18] If we want to go beyond the local approximation and construct a gradient extension of TDLDefA,[20] 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 the 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.[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 looks quite similar to that of Refs. 16–18. 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, both the technique we develop here and an emerging physical picture are essentially different. In fact, in this work we present a self-contained derivation of a completely different theory that is universally applicable to any many-body system driven by external time-dependent electric and magnetic fields. First of all, 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 relative 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 $\mathbf{x}(\boldsymbol{\xi},t)$ of infinitesimal fluid elements. Accordingly, the complete problem splits into two natural parts. First, one solves the many-body problem in the Lagrangian frame. The most important property of this problem is that it does not contain any external field. The many-body dynamics is completely determined by the fundamental geometric characteristics of the frame—Green's deformation tensor g_{ij} which plays a role of metric in the Lagrangian space. Hence, the solution of this universal problem yields the wave function $\tilde{\Psi}$ as a unique, universal functional of g_{ij}. On the second step, we use that solution to find the trajectories $\mathbf{x}(\boldsymbol{\xi},t)$ from a closed hydrodynamicslike 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 key observation, which underlies the present theory and which distinguishes it from the earlier formulations,[16–18] is the possibility to separate the convective motion (the collective dynamics) and the universal relative dynamics at the level of the exact many-body theory. This is the central point of our approach, which leads to an emergence of a DFT-like theory in a natural and constructive way. All traditional deri-

vations of DFT/TDDFT, including that of Refs. 17 and 18, rely on the mapping theorems which establish a unique map of the density and/or current to the external potential. In contrast to that, there is no such step in the present formulation of the theory. The role of the common mapping theorems is now played by the theorem that proves the uniqueness of the solution to the universal many-body problem in the Lagrangian frame (see Sec. III B).

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 Sec. II C, we extensively discuss the main ideas and the results of Sec. II. This section is aimed at preparing the reader to the most general formulation of the theory given in Sec. III. In Sec. III A, 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. III B. 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. III C, the Keldysh-contour formalism is employed to derive a closed variational formulation of the theory. We introduce a universal functional $W[g_{ij}^C]$ that plays the role of an effective "elastic" action of the exact quantum continuum mechanics. A relation of this formulation to a recent magnetoelasticity theory of fractional quantum Hall liquid[21,22] is discussed. In Sec. IV, we present a Kohn-Sham formulation of the theory. We introduce xc potentials both in the Lagrangian and in the laboratory frame. We also derive a few exact representations of the xc potentials in the laboratory frame (since just 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 the 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,

$$i\partial_t\Psi(\mathbf{x},t) = H\Psi(\mathbf{x},t), \quad \Psi(\mathbf{x},0) = \Psi_0(\mathbf{x}), \tag{1}$$

where H is the usual one-particle Hamiltonian,

$$H = \frac{1}{2m}[-i\partial_{\mathbf{x}} - \mathbf{A}(\mathbf{x},t)]^2 + U(\mathbf{x},t). \tag{2}$$

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 $S[\Psi^*,\Psi] = \int_0^t \mathcal{L}dt$ with the following Lagrangian:

$$\mathcal{L}[\Psi^*,\Psi] = \int (i\Psi^*\overleftrightarrow{\partial_t}\Psi - \Psi^* H\Psi)d\mathbf{x}, \tag{3}$$

where $\overleftrightarrow{\partial_t}$ is a symmetrized time derivative:[23] $\Psi^*\overleftrightarrow{\partial_t}\Psi = (\Psi^*\partial_t\Psi - \Psi\partial_t\Psi^*)/2$. Using Eq. (2), we represent the Lagrangian [Eq. (3)] in the following explicit form:[24]

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

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 $\mathbf{x}\to\boldsymbol{\xi}$, $\mathbf{x}=\mathbf{x}(\boldsymbol{\xi},t)$, where the function $\mathbf{x}(\boldsymbol{\xi},t)$ is a solution to the following Cauchy problem:

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

Intuitively the function $\mathbf{x}(\boldsymbol{\xi},t)$ 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 $\boldsymbol{\xi}$ has a meaning of the initial point of that trajectory.

The transformation of coordinates $\mathbf{x}\to\boldsymbol{\xi}$ leads to the following replacements in the Lagrangian:

$$d\mathbf{x} \to \sqrt{g}d\boldsymbol{\xi}, \quad \partial_{x^i} \to \frac{\partial\xi^j}{\partial x^i}\partial_{\xi^j}, \quad \partial_t \to \partial_t - \tilde{v}^i\partial_{\xi^j}, \tag{6}$$

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

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

and $\tilde{\mathbf{v}}(\boldsymbol{\xi},t)$ is the velocity vector in the moving frame,

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

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

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

Here, $\tilde{A}_i(\boldsymbol{\xi},t)$ is the external vector potential in the $\boldsymbol{\xi}$ frame,

$$\tilde{A}_i(\boldsymbol{\xi},t) = \frac{\partial x^j}{\partial \xi^i} A_j(\mathbf{x}(\boldsymbol{\xi},t),t). \tag{10}$$

(Raising and lowering of tensor indices are performed according to the usual rules, e.g., $\tilde{v}_i = g_{ij}\tilde{v}^j$.) In the derivation of Eq. (9), we regrouped the terms to obtain a physically expected form of $\tilde{A}_i + m\tilde{v}_i$ in the kinetic energy.

Apparently, the second term in Eq. (9) plays the 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 $\mathbf{x}(\boldsymbol{\xi},t)$ 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

$$L^{\mathrm{cl}}(\boldsymbol{\xi},t) = \frac{m}{2}\tilde{v}^i\tilde{v}_i + \tilde{v}^i\tilde{A}_i - U = \frac{m}{2}(\dot{\mathbf{x}}(t))^2 + \dot{\mathbf{x}}(t)\mathbf{A}(\mathbf{x}(t),t) - U(\mathbf{x}(t),t), \tag{11}$$

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

The Lagrangian of Eq. (9) can be simplified by introducing a transformed wave function $\tilde{\Psi}(\boldsymbol{\xi},t)$,

$$\Psi(\mathbf{x}(\boldsymbol{\xi},t),t) = g^{-1/4} e^{iS_{\mathrm{cl}}(\boldsymbol{\xi},t)} \tilde{\Psi}(\boldsymbol{\xi},t), \tag{12}$$

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

$$S^{\mathrm{cl}}(\boldsymbol{\xi},t) = \int_0^t L^{\mathrm{cl}}(\boldsymbol{\xi},t')dt'. \tag{13}$$

The renormalization factor $g^{-1/4}$ 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 $\tilde{\Psi}(\boldsymbol{\xi},t)$ as a probability density in $\boldsymbol{\xi}$ space.[16,25] 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:

$$\mathcal{L}[\tilde{\Psi}^*,\tilde{\Psi}] = \int d\boldsymbol{\xi}\left\{ i\tilde{\Psi}^* \overleftrightarrow{\partial_t} \tilde{\Psi} - [(i\partial_{\xi^i} - \mathcal{A}_i) g^{-1/4}\tilde{\Psi}^*] \times \frac{\sqrt{g}g^{ij}}{2m}[(-i\partial_{\xi^j} - \mathcal{A}_j) g^{-1/4}\tilde{\Psi}] \right\}. \tag{14}$$

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

$$\mathcal{A}_i(\boldsymbol{\xi},t) = \tilde{A}_i(\boldsymbol{\xi},t) + \tilde{v}_i(\boldsymbol{\xi},t) - \partial_{\xi^i} S^{\mathrm{cl}}(\boldsymbol{\xi},t). \tag{15}$$

The transformed Lagrangian [Eq. (14)] can also be 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

$$\mathcal{L} = \int (i\tilde{\Psi}^* \overleftrightarrow{\partial_t} \tilde{\Psi} - \tilde{\Psi}^* \tilde{H}[g_{ij},\mathcal{A}_i]\tilde{\Psi}) d\boldsymbol{\xi}, \tag{16}$$

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

$$\tilde{H} = g^{-1/4}(-i\partial_{\xi^i} - \mathcal{A}_i)\frac{\sqrt{g}g^{ij}}{2m}(-i\partial_{\xi^j} - \mathcal{A}_j) g^{-1/4}. \tag{17}$$

Hence, the transformed Schrödinger equation takes the form

$$i\partial_t \tilde{\Psi}(\boldsymbol{\xi},t) = \tilde{H}[g_{ij},\mathcal{A}_i]\tilde{\Psi}(\boldsymbol{\xi},t), \quad \tilde{\Psi}(\boldsymbol{\xi},0) = \Psi_0(\boldsymbol{\xi}). \tag{18}$$

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 A_i. The tensor field $g_{ij}(\boldsymbol{\xi},t)$ plays the role of an effective metric, which produces a "geodesic" inertia force.[16] This force makes a free particle move along geodesics in the deformed $\boldsymbol{\xi}$ space. The effective vector potential $\mathcal{A}_i(\mathbf{x},t)$ 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).[16]

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 the Appendix). These are the continuity equation,

$$\partial_t \tilde{n} + \partial_{\xi^k}\tilde{j}^k = 0, \tag{19}$$

and the local momentum balance equation,

$$\partial_t \tilde{j}_k - \tilde{j}^i(\partial_{\xi^i}\mathcal{A}_k - \partial_{\xi^k}\mathcal{A}_i) + \tilde{n}\partial_t \mathcal{A}_k + \sqrt{g}\nabla_i \tilde{P}^i_k = 0. \tag{20}$$

In Eqs. (19) and (20), $\tilde{n} = |\tilde{\Psi}|^2$ is the probability density and $\tilde{j}^i$ and $\tilde{P}^i_k$ are the current density and the stress tensor, respectively. The operator ∇_i 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, $\nabla_i \tilde{P}^i_k$, in Eq. (20) is the covariant divergence of a second rank tensor,

$$\nabla_i \tilde{P}^i_k = \frac{1}{\sqrt{g}}\partial_{\xi^i}\sqrt{g}\tilde{P}^i_k - \frac{1}{2}\tilde{P}^{ij}\partial_{\xi^k} g_{ij}. \tag{21}$$

In the 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 $\tilde{H}[g_{ij},\mathcal{A}]$ with respect to the vector potential and the metric tensor, respectively,

$$\tilde{j}^k(\boldsymbol{\xi},t) = -\langle\tilde{\Psi}|\frac{\delta\tilde{H}[g_{ij},\mathcal{A}]}{\delta\mathcal{A}_k(\boldsymbol{\xi},t)}|\tilde{\Psi}\rangle, \tag{22}$$

$$\tilde{P}^{ij}(\boldsymbol{\xi},t) = -\frac{2}{\sqrt{g}}\langle\tilde{\Psi}|\frac{\delta\tilde{H}[g_{ij},\mathcal{A}]}{\delta g_{ij}(\boldsymbol{\xi},t)}|\tilde{\Psi}\rangle. \tag{23}$$

In the case of a single quantum particle, Eqs. (22) and (23) lead to the following explicit representations:

$$\tilde{j}_k = -\frac{i}{2m}(\tilde{\Psi}^*\partial_{\xi^k}\tilde{\Psi} - \tilde{\Psi}\partial_{\xi^k}\tilde{\Psi}^*) - \frac{\tilde{n}}{m}\mathcal{A}_k, \tag{24}$$

$$\tilde{P}_{ij} = \frac{1}{2m}\left[(\hat{K}_i g^{-1/4}\tilde{\Psi})^* (\hat{K}_j g^{-1/4}\tilde{\Psi}) + \text{c.c.} - \frac{g_{ij}}{2\sqrt{g}} \partial_{\xi^k} \sqrt{g} g^{kl} \partial_{\xi^l} \frac{\tilde{\Psi}^* \tilde{\Psi}}{\sqrt{g}} \right], \quad (25)$$

where $\hat{K}_j = -i\partial_{\xi^j} - \mathcal{A}_j$ is the kinematic momentum.

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.[16] One of the most simple and natural choices of such a gauge condition is a requirement of zero current density,

$$\tilde{\mathbf{j}}(\boldsymbol{\xi},t) = 0. \quad (26)$$

This requirement specifies a comoving Lagrangian frame. That is a reference frame moving with the velocity $\mathbf{v}(\mathbf{x},t) = \mathbf{j}(\mathbf{x},t)/n(\mathbf{x},t)$, where $\mathbf{j}$ and n are the current and the density in the laboratory frame. In this case, the new coordinates $\boldsymbol{\xi}$ become the Lagrangian coordinates, while the metric tensor g_{ij} [Eq. (7)] acquires the meaning of Green's deformation tensor.[27] Substituting Eq. (26) in the the continuity equation we observe that in the Lagrangian frame the density distribution is stationary and equals the density at $t=0$, which is fixed by the initial conditions,

$$\tilde{n}(\boldsymbol{\xi},t) = \tilde{n}(\boldsymbol{\xi},0) = n_0(\boldsymbol{\xi}) = |\Psi_0(\boldsymbol{\xi})|^2. \quad (27)$$

Similarly, the local momentum balance equation [Eq. (20)] in the Lagrangian frame is simplified as follows:

$$n_0 \partial_t \mathcal{A}_k + \sqrt{g}\nabla_i \tilde{P}^i_k = 0. \quad (28)$$

Equation (28) reveals a physical significance of the effective vector potential $\mathcal{A}_k$. 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 $\boldsymbol{\xi}$ space.

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

$$-\frac{i}{2m}(\tilde{\Psi}^* \partial_{\xi^k}\tilde{\Psi} - \tilde{\Psi}\partial_{\xi^k}\tilde{\Psi}^*) = \frac{n_0}{m}\mathcal{A}_k. \quad (29)$$

A complete set of equations of motion in the Lagrangian frame consists of three equations. These are the Schrödinger equation [Eq. (18)], the zero-current condition [Eq. (29)], and Eq. (15) that relates the effective vector potential $\mathcal{A}$ to the external fields. The solution of this system yields the wave function $\tilde{\Psi}(\boldsymbol{\xi},t)$ and the trajectory $\mathbf{x}(\boldsymbol{\xi},t)$ 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 $\mathbf{x}(\boldsymbol{\xi},t)$ from Eq. (15) can be brought to a more physical form. The time derivative of Eq. (15) takes the form

$$m\partial_t \tilde{v}_i + \partial_t \tilde{A}_i - \partial_{\xi^i}\left(\frac{m}{2}\tilde{v}^k \tilde{v}_k + \tilde{v}^k \tilde{A}_k - U\right) - \partial_t \mathcal{A}_i = 0. \quad (30)$$

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 $\mathbf{x}(\boldsymbol{\xi},t)$. Indeed, using Eq. (5) and the explicit representations for $\tilde{v}^i$ [Eq. (8)] and for $\tilde{A}_i$ [Eq. (10)], one can straightforwardly reduce Eq. (30) to the following form:

$$m\frac{\partial^2 x^k}{\partial t^2} - \frac{\partial x^i}{\partial t}\left(\frac{\partial A_k}{\partial x^i} - \frac{\partial A_i}{\partial x^k}\right) + \left(\frac{\partial A_k}{\partial t}\right)_{\mathbf{x}} - \frac{\partial U}{\partial x^k} - \frac{\partial \xi^i}{\partial x^k}\frac{\partial \mathcal{A}_i}{\partial t} = 0, \quad (31)$$

where $(\partial A_k/\partial t)_{\mathbf{x}}$ means the time derivative at fixed $\mathbf{x}$. 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:

$$i\partial_t \tilde{\Psi}(\boldsymbol{\xi},t) = \tilde{H}[g_{ij},\mathcal{A}_i]\tilde{\Psi}(\boldsymbol{\xi},t), \quad (32)$$

$$\mathcal{A}_k = -\frac{i}{2n_0}(\tilde{\Psi}^* \partial_{\xi^k}\tilde{\Psi} - \tilde{\Psi}\partial_{\xi^k}\tilde{\Psi}^*), \quad (33)$$

$$m\ddot{x}^k = [\dot{\mathbf{x}} \times \mathbf{B}(\mathbf{x},t)]_k + E_k(\mathbf{x},t) + \frac{\partial \xi^i}{\partial x^k}\partial_t \mathcal{A}_i, \quad (34)$$

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,

$$\mathbf{E}(\mathbf{x},t) = -\partial_t \mathbf{A}(\mathbf{x},t) - \partial_{\mathbf{x}} U(\mathbf{x},t), \quad (35)$$

$$\mathbf{B}(\mathbf{x},t) = \partial_{\mathbf{x}} \times \mathbf{A}(\mathbf{x},t). \quad (36)$$

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

$$\tilde{\Psi}(\boldsymbol{\xi},0) = \Psi_0(\boldsymbol{\xi}), \quad \mathbf{x}(\boldsymbol{\xi},0) = \boldsymbol{\xi}, \quad \dot{\mathbf{x}}(\boldsymbol{\xi},0) = \mathbf{v}_0(\boldsymbol{\xi}), \quad (37)$$

where $\mathbf{v}_0(\boldsymbol{\xi})$ is the velocity distribution in the initial state $\Psi_0(\boldsymbol{\xi})$. The Hamiltonian $\tilde{H}[g_{ij},\mathcal{A}_i]$ is defined after Eq. (17), and the metric (deformation) tensor g_{ij} is connected to the solution, $\mathbf{x}(\boldsymbol{\xi},t)$, 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:

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

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

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

By direct calculations one can check the following identity:

$$\langle\tilde{\Psi}|\frac{\delta\tilde{H}}{\delta x^k}|\tilde{\Psi}\rangle=\frac{\partial\xi^i}{\partial x^k}\sqrt{g}\nabla_j\tilde{P}_i^j=-\frac{\partial\xi^i}{\partial x^k}n_0\partial_t\mathcal{A}_i, \tag{40}$$

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 $\mathbf{x}(\boldsymbol{\xi},t)$ [Eq. (34)].

The Lagrangian $\tilde{\mathcal{L}}$ [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 $\mathbf{x}(\boldsymbol{\xi},t)$ enter the quantum part of the problem only via the induced metric $g_{ij}(\boldsymbol{\xi},t)$ [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) and (33) and (ii) the "classical" equation of motion [Eq. (34)] for the trajectory of the comoving frame. The universal problem of Eqs. (32) and (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 self-consistent vector potential as universal functionals of the metric tensor, $\tilde{\Psi}[g_{ij}](\boldsymbol{\xi},t)$ and $\boldsymbol{\mathcal{A}}[g_{ij}](\boldsymbol{\xi},t)$. Hence, the stress force, the stress tensor $\tilde{P}_{ij}$, 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 $\mathbf{x}(\boldsymbol{\xi},t)$,

$$m\ddot{x}^k=[\dot{\mathbf{x}}\times\mathbf{B}(\mathbf{x},t)]_k+E_k(\mathbf{x},t)-\frac{\sqrt{g}}{n_0}\frac{\partial\xi^i}{\partial x^k}\nabla_j\tilde{P}_i^j[g_{ij}]. \tag{41}$$

Equation (41) is easily recognized as an equation of a nonlinear elasticity theory in the Lagrangian formulation of continuum mechanics.[27] In this context, the functional dependence of the stress tensor $\tilde{P}_i^j$ on the deformation tensor g_{ij} plays the 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) and (33).

In the one-particle case, the universal problem of Eqs. (32) and (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 self-consistent vector potential

$$\tilde{\Psi}(\boldsymbol{\xi},t)=\sqrt{n_0(\boldsymbol{\xi})}e^{i\varphi(\boldsymbol{\xi},t)},\quad \mathcal{A}_k(\boldsymbol{\xi},t)=\partial_{\xi^k}\varphi(\boldsymbol{\xi},t) \tag{42}$$

satisfy the system of Eqs. (32) and (33) if the phase $\varphi(\boldsymbol{\xi},t)$ takes the form

$$\varphi=\varphi_0(\boldsymbol{\xi})+\frac{1}{2m}\int_0^t(g^{-1/4}\partial_{\xi^i}\sqrt{g}g^{ij}\partial_{\xi^j}g^{-1/4}\sqrt{n_0})dt', \tag{43}$$

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

$$\tilde{P}_{ij}[g_{ij}]=\frac{1}{m}\left[(\partial_{\xi^i}g^{-1/4}\sqrt{n_0})(\partial_{\xi^j}g^{-1/4}\sqrt{n_0})-\frac{g_{ij}}{4\sqrt{g}}\partial_{\xi^k}\sqrt{g}g^{kl}\partial_{\xi^l}\frac{n_0}{\sqrt{g}}\right]. \tag{44}$$

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 $\boldsymbol{\mathcal{A}}$ [Eq. (42)]. The result takes the form

$$\frac{\sqrt{g}}{n_0}\nabla_j\tilde{P}_k^j=\frac{1}{2m}\partial_{\xi^k}(g^{-1/4}\partial_{\xi^i}\sqrt{g}g^{ij}\partial_{\xi^j}g^{-1/4}\sqrt{n_0}). \tag{45}$$

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:

$$\mathcal{L}_{\mathrm{el}}[\mathbf{x}]=\int d\boldsymbol{\xi}\Big\{n_0\left[\frac{m}{2}(\dot{\mathbf{x}})^2+\dot{\mathbf{x}}A(\mathbf{x},t)-U(\mathbf{x},t)\right] + (\partial_{\xi^i}g^{-1/4}\sqrt{n_0})\frac{\sqrt{g}g^{ij}}{2m}(\partial_{\xi^j}g^{-1/4}\sqrt{n_0})\Big\}. \tag{46}$$

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

C. Overview of the main results and discussion

Let us summarize the 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 $\tilde{\Psi}(\boldsymbol{\xi},t)$,

$\mathbf{x}(\boldsymbol{\xi},t)$, and $\boldsymbol{\mathcal{A}}(\boldsymbol{\xi},t)$. Two of them, the wave function $\tilde{\Psi}(\boldsymbol{\xi},t)$ and the frame's trajectory $\mathbf{x}(\boldsymbol{\xi},t)$ enter the theory as dynamic variables, while the effective vector potential $\boldsymbol{\mathcal{A}}(\boldsymbol{\xi},t)$ 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 $\boldsymbol{\mathcal{A}}$ 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 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 universal 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* (TDDefFT). 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) and (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 latter quantities can be recovered from the former one as follows:

$$n(\mathbf{x},t)=\left[\frac{n_0(\boldsymbol{\xi})}{\sqrt{g(\boldsymbol{\xi},t)}}\right]_{\boldsymbol{\xi}=\boldsymbol{\xi}(\mathbf{x},t)}, \tag{47}$$

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

where $\boldsymbol{\xi}(\mathbf{x},t)$ 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)–(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 TDDefFT 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

$$H=H_0+H_{\text{int}}, \tag{49}$$

where H_0 corresponds to the sum of one particle contributions and H_{int} is the interaction Hamiltonian,

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

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

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

$$\mathcal{L}[\Psi^*,\Psi]=\int(i\Psi^*\overleftrightarrow{\partial_t}\Psi-\Psi^*H\Psi)\prod_{\alpha=1}^{N}d\mathbf{x}_\alpha. \tag{52}$$

The next step is to make a transformation to the comoving Lagrangian frame. Formally this corresponds to the transformation of coordinates $\mathbf{x}_\alpha\mapsto\boldsymbol{\xi}_\alpha:\mathbf{x}_\alpha=\mathbf{x}(\boldsymbol{\xi}_\alpha,t)$, $\alpha=1,\ldots,N$, where the function $\mathbf{x}(\boldsymbol{\xi},t)$ is the trajectory of a fluid element, which is defined by Eq. (5). In addition, we introduce a renormalized many-body wave function $\tilde{\Psi}(\boldsymbol{\xi}_1,\ldots,\boldsymbol{\xi}_N,t)$ in the new frame,

$$\Psi(\mathbf{x}(\boldsymbol{\xi}_1,t),\ldots,\mathbf{x}(\boldsymbol{\xi}_N,t),t)=\prod_{\alpha=1}^{N}g^{-1/4}(\boldsymbol{\xi}_\alpha,t)e^{iS_{\text{cl}}(\boldsymbol{\xi}_\alpha,t)}\tilde{\Psi}(\boldsymbol{\xi}_1,\ldots,\boldsymbol{\xi}_N,t), \tag{53}$$

where $iS_{\text{cl}}(\boldsymbol{\xi},t)$ 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 the calculations also straightforwardly follows the line of the previous section. That is 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 $\tilde{\mathcal{L}}[\tilde{\Psi}^*,\tilde{\Psi},\boldsymbol{\mathcal{A}},\mathbf{x}]$ that describes the dynamics of N-particle system in the comoving frame,

$$\tilde{\mathcal{L}} = \int [i\tilde{\Psi}^* \overleftrightarrow{\partial_t} \tilde{\Psi} - \tilde{\Psi}^* \tilde{H}[g_{ij}, \boldsymbol{\mathcal{A}}]\tilde{\Psi}] \prod_{\alpha=1}^{N} d\boldsymbol{\xi}_\alpha + \int n_0(\boldsymbol{\xi}) \left[\frac{m}{2}(\dot{\mathbf{x}})^2 + \dot{\mathbf{x}}\mathbf{A}(\mathbf{x},t) - U(\mathbf{x},t) \right] d\boldsymbol{\xi}, \quad (54)$$

where $n_0(\boldsymbol{\xi}) = N \int \Pi_{\alpha=2}^{N} d\boldsymbol{\xi}_\alpha |\Psi_0(\boldsymbol{\xi}, \boldsymbol{\xi}_2, \ldots, \boldsymbol{\xi}_N)|^2$ is the initial density distribution.

Equation (54) has precisely the same structure as the one-particle Lagrangian of Eq. (38). The only difference is that the Hamiltonian $\tilde{H}[g_{ij}, \boldsymbol{\mathcal{A}}]$ in Eq. (54) corresponds to a system of N interacting particles in the space with metric g_{ij}. Accordingly, $\tilde{H}[g_{ij}, \boldsymbol{\mathcal{A}}]$ contains two terms,

$$\tilde{H}[g_{ij}, \boldsymbol{\mathcal{A}}] = \tilde{H}_0[g_{ij}, \boldsymbol{\mathcal{A}}] + \tilde{H}_{\text{int}}[g_{ij}]. \quad (55)$$

The first term $\tilde{H}_0$ is a sum of N one-particle Hamiltonians,

$$\tilde{H}_0[g_{ij}, \boldsymbol{\mathcal{A}}] = \sum_{\alpha=1}^{N} g_\alpha^{-1/4} \hat{K}_{\alpha,i} \frac{\sqrt{g_\alpha} g_\alpha^{ij}}{2m} \hat{K}_{\alpha,j} g_\alpha^{-1/4}, \quad (56)$$

where $\hat{K}_{\alpha,j} = -i\partial_{\xi_\alpha^j} - \mathcal{A}_j(\boldsymbol{\xi}_\alpha, t)$ and $g_\alpha^{ij} = g^{ij}(\boldsymbol{\xi}_\alpha, t)$. The second term $\tilde{H}_{\text{int}}$ in Eq. (55) describes a pairwise interparticle interaction in the Lagrangian frame,

$$\tilde{H}_{\text{int}}[g_{ij}] = \frac{1}{2} \sum_{\alpha,\beta} V(l_{\boldsymbol{\xi}_\alpha \boldsymbol{\xi}_\beta}), \quad (57)$$

where $l_{\boldsymbol{\xi}_\alpha \boldsymbol{\xi}_\beta}$ is the length of geodesic that connects points $\boldsymbol{\xi}_\alpha$ and $\boldsymbol{\xi}_\beta$ in the space with metrics g_{ij}.

Apparently, the physical significance of the Lagrangian [Eq. (54)] remains unchanged. It describes the classical system of fluid elements, which is geometrically coupled to the constrained quantum N-body system in the space with metrics g_{ij}. The Euler-Lagrange equations take the form

$$i\partial_t \tilde{\Psi}(\boldsymbol{\xi}_1, \ldots, \boldsymbol{\xi}_N, t) = \tilde{H}[g_{ij}, \mathcal{A}_i]\tilde{\Psi}(\boldsymbol{\xi}_1, \ldots, \boldsymbol{\xi}_N, t), \quad (58)$$

$$\mathcal{A}_k(\boldsymbol{\xi}, t) = -\frac{iN}{2n_0(\boldsymbol{\xi})} \Im \int \prod_{\alpha=2}^{N} d\boldsymbol{\xi}_\alpha \tilde{\Psi}^*(\boldsymbol{\xi}, \boldsymbol{\xi}_2, \ldots, \boldsymbol{\xi}_N, t) \partial_{\xi^k} \tilde{\Psi} \times (\boldsymbol{\xi}, \boldsymbol{\xi}_2, \ldots, \boldsymbol{\xi}_N, t), \quad (59)$$

$$m\ddot{x}^k = [\dot{\mathbf{x}} \times \mathbf{B}(\mathbf{x},t)]_k + E_k(\mathbf{x},t) - \frac{\sqrt{g}}{n_0} \frac{\partial \xi^i}{\partial x^k} \nabla_j \tilde{P}_i^j, \quad (60)$$

where $\tilde{P}^{ij}(\boldsymbol{\xi}, t)$ is the expectation value of the stress tensor operator [see Eq. (23)]. An explicit expression for the stress tensor in the Lagrangian frame can be found in Refs. 16 and 17. It is worth recalling that the stress force in Eq. (60) can be represented in three equivalent forms [Eq. (40)].

The most important property of the set of Eqs. (58)–(60) is that the equations of constrained quantum dynamics [Eqs. (58) and (59)] constitute a closed universal problem, which depends only on the initial state $\Psi_0(\boldsymbol{\xi}_1, \ldots, \boldsymbol{\xi}_N)$ and on the metric tensor $g_{ij}(\boldsymbol{\xi}, t)$. The solution to this problem, provided it exists and is unique, defines the many-body wave function as a universal functional of Ψ_0 and g_{ij}, i.e., $\tilde{\Psi}[\Psi_0, g_{ij}](\boldsymbol{\xi}_1, \ldots, \boldsymbol{\xi}_N, t)$. The existence of this functional is the key statement of TDDefFT. It implies the existence of the exact nonequilibrium equation of state, $\tilde{P}^{ij} = \tilde{P}^{ij}[g_{ij}]$, and thus allows us to formulate a closed theory of one vector-valued collective variable—the trajectory function $\mathbf{x}(\boldsymbol{\xi}, t)$. This theory can be interpreted as the exact quantum continuum mechanics.

B. The universal problem and mapping theorems of TDDefFT

The complete system of Eqs. (58)–(60) is simply a reformulation of the original linear Schrödinger equation with the Hamiltonian [Eq. (49)]. Therefore, Eqs. (58)–(60) possess a unique solution, provided the external fields $\mathbf{A}$ and U and the initial state Ψ_0 are given. It is, however, not obvious that, given the metric g_{ij}, we can solve the universal problem of Eqs. (58) and (59) independently of the third equation [Eq. (60)]. The problem of well possedness of the nonlinear Cauchy problem defined by Eqs. (58) and (59) for a given $g_{ij}(\boldsymbol{\xi}, t)$ is equivalent to the problem of the existence of TDDefFT.

In Sec. II B, we have demonstrated that in the one-particle case, the universal problem of Eqs. (58) and (59) [for $N=1$, they reduce to Eqs. (32) and (33)] admits an exact analytic solution. Hence, in this particular case, the universal functional $\tilde{\Psi}[\Psi_0, g_{ij}]$ (and thus TDDefFT) does indeed exist. The simplest way to argue in favor of TDDefFT in the general case of $N>1$ is to refer to the Runge-Gross theorem[6] or to its generalizations.[29] In fact, just this argumentation was used in the previous works on "geometric" TDDFT.[17,18] 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 TDDefFT formally translates to the problem of the existence and uniqueness of solutions to the universal quantum problem [Eqs. (58) and (59)]. This problem defines a map $g_{ij} \mapsto \tilde{\Psi}$, which also assumes a map $g_{ij} \mapsto \boldsymbol{\mathcal{A}}$, and implies the existence of the generalized equation of state. Substituting the constraint of Eq. (59) into Eq. (58), we observe that the latter 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.[30] In this paper, we adopt common simplifying assumptions,[6,7,29,31] and prove the uniqueness of the solution to Eqs. (58) and (59) for analytic and v-representable metrics $g_{ij}(\boldsymbol{\xi}, t)$. 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,

$$g_{ij}(t) = \delta_{ij} + \sum_{k=1}^{\infty} \frac{g_{ij}^{(k)}}{k!} t^k, \tag{61}$$

where $g_{ij}^{(k)} = \partial_t^k g_{ij}(0)$. 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 of Eq. (5). Similarly, one can expand the wave function $\tilde{\Psi}(t)$,

$$\tilde{\Psi}(t) = \Psi_0 + \sum_{k=1}^{\infty} \frac{\tilde{\Psi}^{(k)}}{k!} t^k. \tag{62}$$

Now, we substitute Eq. (59) into Eq. (58) and insert expansions (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 $\tilde{\Psi}^{(k)}$:

$$\tilde{\Psi}^{(k)} = -iF^{(k-1)}, \quad k = 1,2, \ldots, \tag{63}$$

where $F^{(k)}$ denote the coefficients for the Taylor expansion of the right-hand side of Eq. (58). Since Eq. (59), which relates $\boldsymbol{\mathcal{A}}$ to $\tilde{\Psi}$, 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 kth Taylor coefficient $F^{(k)}$ contains derivatives $\tilde{\Psi}^{(p)}$ only with $p \leqslant k$. Hence, Eq. (63) can be schematically represented as follows:

$$\tilde{\Psi}^{(1)} = -iF^{(0)}[g_{ij}^{(0)}; \Psi_0],$$

$$\tilde{\Psi}^{(2)} = -iF^{(1)}[g_{ij}^{(0)}, g_{ij}^{(1)}; \Psi_0, \tilde{\Psi}^{(1)}],$$

$$\cdots,$$

$$\tilde{\Psi}^{(k)} = -iF^{(k-1)}[g_{ij}^{(0)}, \ldots, g_{ij}^{(k-1)}; \Psi_0, \ldots, \tilde{\Psi}^{(k-1)}],$$

$$\cdots.$$

Apparently, this system can be solved recursively starting from the first equation. The solution uniquely defines a map: $\{g_{ij}^{(k)}, \Psi_0\} \mapsto \{\tilde{\Psi}^{(k)}\}$. Substituting the coefficients $\tilde{\Psi}^{(k)}$ 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: $\tilde{\Psi}[g_{ij}, \Psi_0](t)$. Importantly, this is true only if the Taylor series of Eq. (62) converges, i.e., if the solution to our nonlinear problem exists, which cannot 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 proof of the following *uniqueness theorem*: For an analytic and v-representable Green's deformation tensor g_{ij}, the wave function $\tilde{\Psi}(t)$ in the Lagrangian frame is a unique functional of g_{ij} and the initial state Ψ_0. In other words, the map g_{ij}, $\Psi_0 \mapsto \tilde{\Psi}(t)$ 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 $\mathbf{x}(\boldsymbol{\xi}, t)$. 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 $g_{ij} \mapsto \tilde{\Psi}(t)$ mapping is closely related to constructive proofs of the mapping theorems in TDDFT and TDCDFT by van Leeuwen[31] and Vignale,[29] respectively. In fact, the formal statement of the problem in Refs. 31 and 29 is very similar to our system of Eqs. (58) and (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 Vignale's theorem can be also essentially simplified by reformulating the problem in a similar local fashion.[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 of 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 $\tilde{\Psi}(\boldsymbol{\xi}_1, \ldots, \boldsymbol{\xi}_N, t)$ and the effective vector potential $\boldsymbol{\mathcal{A}}(\boldsymbol{\xi}, t)$ are universal functionals of Green's deformation tensor $g_{ij}(\boldsymbol{\xi}, t)$. 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 $\delta \tilde{H}[g_{ij}, \boldsymbol{\mathcal{A}}] / \delta g_{ij}$ at fixed $\boldsymbol{\mathcal{A}}$ [see Eq. (23)]. However, in the Lagrangian frame, the current density vanishes, which implies the following identity $j^k = \langle \delta \tilde{H}[g_{ij}, \boldsymbol{\mathcal{A}}] / \mathcal{A}_k \rangle \equiv 0$. 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,

$$\tilde{P}^{ij}[g_{ij}](\boldsymbol{\xi}, t) = -\frac{2}{\sqrt{g}} \langle \tilde{\Psi}[g_{ij}] | \frac{\delta \tilde{H}[g_{ij}]}{\delta g_{ij}(\boldsymbol{\xi}, t)} | \tilde{\Psi}[g_{ij}] \rangle, \tag{64}$$

where $\tilde{H}[g_{ij}] \equiv \tilde{H}[g_{ij}, \boldsymbol{\mathcal{A}}[g_{ij}]]$. Equation (64) relates the exact nonequilibrium equation of state to the solution of the universal quantum problem [Eqs. (58) and (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),

$$m\ddot{x}^k = [\dot{\mathbf{x}} \times \mathbf{B}(\mathbf{x},t)]_k + E_k(\mathbf{x},t) - \frac{\sqrt{g}}{n_0}\frac{\partial \xi^i}{\partial x^k}\nabla_j \tilde{P}_i^j[g_{ij}]. \quad (65)$$

By solving this equation with initial conditions $\mathbf{x}(\boldsymbol{\xi},0)=\boldsymbol{\xi}$ and $\dot{\mathbf{x}}(\boldsymbol{\xi},0)=\mathbf{v}_0(\boldsymbol{\xi})$, we get a set of trajectories $\mathbf{x}(\boldsymbol{\xi},t)$ 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. III B. In spite of an apparent "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. That is, there exists an action functional $S[\mathbf{x}(\boldsymbol{\xi},t)]$ that generates the equation of motion [Eq. (65)]. In Sec. II B, 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:

$$\langle\tilde{\Psi}|\frac{\delta\tilde{H}[g_{ij}]}{\delta g_{ij}}|\tilde{\Psi}\rangle = \frac{\delta}{\delta g_{ij}}\langle\tilde{\Psi}|\tilde{H}[g_{ij}]|\tilde{\Psi}\rangle \equiv \frac{\delta E[g_{ij}]}{\delta g_{ij}}, \quad (66)$$

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 and/or 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 noninstantaneous 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.[33]

The existence of the map g_{ij}, $\Psi_0 \mapsto \tilde{\Psi}(t)$, assumes the existence of a unitary evolution operator $U[g_{ij}](t,0)$,

$$|\tilde{\Psi}(t)\rangle = U[g_{ij}](t,0)|\Psi_0\rangle, \quad (67)$$

$$U[g_{ij}](t,0) = T\exp\left[-i\int_0^t \tilde{H}[g_{ij}](t')dt'\right], \quad (68)$$

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:

$$\tilde{P}^{ij} = -\frac{2}{\sqrt{g}}\langle\Psi_0|U(0,t)\frac{\delta\tilde{H}[g_{ij}]}{\delta g_{ij}}U(t,0)|\Psi_0\rangle. \quad (69)$$

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

$$W[g_{ij}^-,g_{ij}^+] = i\ln\langle\Psi_0|U^+(0,\infty)U^-(\infty,0)|\Psi_0\rangle, \quad (70)$$

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) and (59)], with the metric $g_{ij}^\pm(\boldsymbol{\xi},t)$. 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.[33] The contour C consists of two branches: the "forward" $(-)$ branch that goes from 0 to ∞ and the "back" $(+)$ branch going from ∞ to the initial time, $t=0$. Using this notion one can represent the generating functional W [Eq. (70)] in the following compact form:

$$W[g_{ij}^C] = i\ln\langle\Psi_0|T_C e^{-i\int_C \tilde{H}[g_{ij}^C](t)dt}|\Psi_0\rangle, \quad (71)$$

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:

$$\tilde{P}^{ij}[g_{ij}] = -\frac{2}{\sqrt{g}}\left.\frac{\delta W[g_{ij}^C]}{\delta g_{ij}^C}\right|_{g_{ij}^C=g_{ij}(t)}. \quad (72)$$

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

$$g_{ij}^C = \frac{\partial x_C^k}{\partial \xi^i}\frac{\partial x_C^k}{\partial \xi^j}. \quad (73)$$

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 $\mathbf{x}_C$,

$$-n_0\tilde{F}_k^{\mathrm{str}} = \sqrt{g}\frac{\partial \xi^i}{\partial x^k}\nabla_j\tilde{P}_i^j[g_{ij}] = \left.\frac{\delta W[g_{ij}^C]}{\delta x_C^k}\right|_{\mathbf{x}_C=\mathbf{x}(\boldsymbol{\xi},t)}. \quad (74)$$

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

$$S_C[\mathbf{x}_C] = \int_C dt\int d\boldsymbol{\xi} n_0\left[\frac{m}{2}(\dot{\mathbf{x}}_C)^2 + \dot{\mathbf{x}}_C\mathbf{A}(\mathbf{x}_C,t) - U(\mathbf{x}_C,t)\right] - W[g_{ij}^C]. \quad (75)$$

Indeed, the stationarity condition for the action $S_C[\mathbf{x}_C]$,

$$\left.\frac{\delta S_C[\mathbf{x}_C]}{\delta \mathbf{x}_C}\right|_{\mathbf{x}_C=\mathbf{x}(\boldsymbol{\xi},t)} = 0, \quad (76)$$

recovers the correct form of the hydrodynamics equation of motion [Eq. (65)] for the trajectory $\mathbf{x}(\boldsymbol{\xi},t)$.

The variational formulation [Eqs. (75) and (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 functional $W[g_{ij}]$ based on fundamental symmetries of a given physical system. Recently, this approach has been used to derive a hydrodynamics theory of strongly correlated many-body states in the fractional quantum Hall regime.[21] 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 that the variational formulation of TDDefFT 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 TDDFT was proposed by van Leeuwen[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 and 35. van Leeuwen's formulation of TDDFT 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 TDDefFT relies only on the real-time uniqueness theorem presented in Sec. III B.

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 $W[g_{ij}^C]$ 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 $W[g_{ij}^C]$) as a single entity. This approach was successfully employed in our recent studies of the fractional quantum Hall liquids and liquid crystals.[21,22,36] However, in most of the 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 TDDefFT can be introduced as follows. Let us consider a system of N noninteracting KS particles moving in the presence of effective potentials, $\mathbf{A}_S=\mathbf{A}+\mathbf{A}_{\rm xc}$ and $U_S=U+U_{\rm xc}$. Here, $\mathbf{A}(\mathbf{x},t)$ and $U(\mathbf{x},t)$ are the external fields, while $\mathbf{A}_{\rm xc}(\mathbf{x},t)$ and $U_{\rm xc}(\mathbf{x},t)$ are self-consistent xc potentials that are adjusted to reproduce a collective variable of interest in the physical interacting system. In the Lagrangian formulation of TDDefFT, the proper collective variable is the trajectory $\mathbf{x}(\boldsymbol{\xi},t)$. In the KS system, the equation of motion for $\mathbf{x}(\boldsymbol{\xi},t)$ takes the form

$$m\ddot{\mathbf{x}}=\dot{\mathbf{x}}\times\mathbf{B}_S(\mathbf{x},t)+\mathbf{E}_S(\mathbf{x},t)+\tilde{\mathbf{F}}_S^{\rm str}[\mathbf{x}], \tag{77}$$

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

$$\tilde{F}_{S,k}^{\rm str}[\mathbf{x}]=-\frac{\sqrt{g}}{n_0}\frac{\partial\xi^i}{\partial x^k}\nabla_j\tilde{P}_{Si}^j[g_{ij}]. \tag{78}$$

In Eq. (77), $\mathbf{E}_S(\mathbf{x},t)$, and $\mathbf{B}_S(\mathbf{x},t)$ are, respectively, the electric and the magnetic fields associated with the effective potentials $\mathbf{A}_S(\mathbf{x},t)$ and $U_S(\mathbf{x},t)$. The functional $\tilde{P}_{S,ij}[g_{ij}]$ is obtained from the solution of the universal problem [Eqs. (58) and (59)] for a noninteracting system (i.e., with $\tilde{H}_{\rm int}[g_{ij}]=0$). 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 the difference of stress forces in the interacting and the noninteracting systems,

$$E_{{\rm xc},k}(\mathbf{x},t)+[\dot{\mathbf{x}}\times\mathbf{B}_{\rm xc}(\mathbf{x},t)]_k=-\frac{\sqrt{g}}{n_0}\frac{\partial\xi^i}{\partial x^k}\nabla_j\tilde{P}_{{\rm xc},i}^j[g_{ij}], \tag{79}$$

where $\tilde{P}_{{\rm xc},i}^j[g_{ij}](\boldsymbol{\xi},t)=\tilde{P}_i^j[g_{ij}](\boldsymbol{\xi},t)-\tilde{P}_{S,i}^j[g_{ij}](\boldsymbol{\xi},t)$ is the xc stress tensor functional, and the xc electric and magnetic fields are defined as follows:

$$\mathbf{E}_{\rm xc}(\mathbf{x},t)=-\partial_t\mathbf{A}_{\rm xc}(\mathbf{x},t)-\partial_{\mathbf{x}}U_{\rm xc}(\mathbf{x},t), \tag{80}$$

$$\mathbf{B}_{\rm xc}(\mathbf{x},t)=\partial_{\mathbf{x}}\times\mathbf{A}_{\rm xc}(\mathbf{x},t). \tag{81}$$

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 $\boldsymbol{\xi}=\boldsymbol{\xi}(\mathbf{x},t)$, where $\boldsymbol{\xi}(\mathbf{x},t)$ is the inverse of $\mathbf{x}(\boldsymbol{\xi},t)$. The result of this procedure for Eq. (79) takes the form

$$\partial_t A_{{\rm xc},k}-[\mathbf{v}\times(\partial_{\mathbf{x}}\times\mathbf{A}_{\rm xc})]_k+\partial_k U_{\rm xc}=\frac{1}{n}\partial_j P_{{\rm xc},jk}, \tag{82}$$

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

$$P_{{\rm xc},ij}(\mathbf{x},t)=\frac{\partial\xi^k}{\partial x^i}\frac{\partial\xi^l}{\partial x^j}\tilde{P}_{kl}[g_{ij}](\boldsymbol{\xi}(\mathbf{x},t),t). \tag{83}$$

Equation (82) recovers the force definition of the xc potentials introduced in Ref. 16. The most important 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, $\tilde{P}_{{\rm xc},ij}(\boldsymbol{\xi},t)$, is a unique functional of only one basic variable—Green's deformation tensor g_{ij}. The transformed xc stress tensor $P_{{\rm xc},ij}(\mathbf{x},t)$ [Eq. (83)], which determines xc potentials in the laboratory frame, already depends not only on g_{ij} but also on the function $\boldsymbol{\xi}(\mathbf{x},t)$ itself. However, the dependence on $\boldsymbol{\xi}(\mathbf{x},t)$ is trivial [in the prefactor and in the argument in Eq. (83)] and can be accounted for exactly, provided the universal functional $\tilde{P}_{{\rm xc},ij}[g_{ij}](\boldsymbol{\xi},t)$ 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 $W[g_{ij}^C]$. Indeed, us-

ing Eq. (74), we can rewrite Eq. (79) in the following form:

$$\mathbf{E}_{\mathrm{xc}}+\dot{\mathbf{x}}\times\mathbf{B}_{\mathrm{xc}}=-\frac{1}{n_0}\left.\frac{\delta W_{\mathrm{xc}}[g_{ij}^C]}{\delta\mathbf{x}_C}\right|_{\mathbf{x}_C=\mathbf{x}(\boldsymbol{\xi},t)}, \tag{84}$$

where $W_{\mathrm{xc}}[g_{ij}^C]=W[g_{ij}^C]-W_S[g_{ij}^C]$ 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., generalized gradient approximation (GGA)-like] of various approximations. It reduces the problem to approximating a global scalar functional $W_{\mathrm{xc}}[g_{ij}^C]$, which seems to be a simpler task. Importantly, the very form of Eq. (84) already guarantees many exact constraints. For instance, any functional $W_{\mathrm{xc}}[g_{ij}^C]$ yields the xc force that is equal to the divergence of a 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 $W_{\mathrm{xc}}[g_{ij}^C]$, 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 $\boldsymbol{\xi}=\boldsymbol{\xi}(\mathbf{x},t)$. As a result, the right-hand side of Eq. (83) is recovered.

The W functional of TDDefFT 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,[8] as well as its extension by VUC,[9] corresponds to the following quadratic functional:

$$W_{\mathrm{xc}}^{\mathrm{VK}}[g_{ij}^C]=\frac{1}{8}\int d\boldsymbol{\xi}\int_C dtdt'\left\{2\mu_{\mathrm{xc}}^C(t-t')\delta g_{ij}^C(t)\delta g_{ij}^C(t')+\left[K_{\mathrm{xc}}^C(t-t')-\frac{2}{3}\mu_{\mathrm{xc}}^C(t-t')\right]\delta g_{ii}^C(t)\delta g_{jj}^C(t')\right\}, \tag{85}$$

where $\delta g_{ij}=g_{ij}-\delta_{ij}$ is the linearized strain tensor, while $K_{\mathrm{xc}}^C(t-t')$ and $\mu_{\mathrm{xc}}^C(t-t')$ 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 δg_{ij}.

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

$$W_{\mathrm{xc}}^{\mathrm{LDefA}}[g_{ij}^C]=\int d\boldsymbol{\xi}\int_C dtE_{\mathrm{xc}}[g_{ij}^C(\boldsymbol{\xi},t)], \tag{86}$$

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

$$E_{\mathrm{xc}}(g_{ij})=\sum_{\mathbf{p}}\left[g^{ij}\frac{p_ip_j}{2m}f_{\mathrm{xc}}(p;n_0)+\frac{1}{2\sqrt{g}}\bar{V}(\sqrt{g^{ij}p_ip_j})g_2(p;n_0)\right]. \tag{87}$$

In this equation, $\bar{V}(q)$ is the Fourier component of the interaction potential, $f_{\mathrm{xc}}(p;n_0)$ 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 $f_{\mathrm{xc}}(p;n_0)$ and $g_2(p;n_0)$ are calculated for a homogeneous system with the density $n_0(\boldsymbol{\xi})$. In the limit of small deformations, when g_{ij} slightly deviates from δ_{ij}, the nonlinear elastic approximation defined by Eqs. (86) and (87) reduces to the high-frequency limit of VK approximation [Eq. (85)]. It is worth noting that the derivation of the nonadiabatic local deformation approximation within the present formalism is identical to that given in Refs. 17 and 18. Therefore, we do not reproduce it here. However, it should be emphasized that the present formulation makes it possible to go beyond the simplest local approximation by deriving the GGA-like extensions of xc deformation functionals.

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

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

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

Finally, we derive one more exact representation of the xc force. That is, we relate $\mathbf{A}_{\mathrm{xc}}$ and U_{xc} to the effective vector potential $\boldsymbol{\mathcal{A}}$ that enters the universal problem of Eqs. (58) and (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 $\boldsymbol{\mathcal{A}}$. Hence, the xc force in the Lagrangian frame [Eq. (79)] can be also represented as follows:

$$E_{\mathrm{xc},k}(\mathbf{x},t)+[\dot{\mathbf{x}}\times\mathbf{B}_{\mathrm{xc}}(\mathbf{x},t)]_k=\frac{\partial\xi^i}{\partial x^k}\partial_t\mathcal{A}_{\mathrm{xc},i}(\boldsymbol{\xi},t), \tag{89}$$

where $\boldsymbol{\mathcal{A}}_{\mathrm{xc}}(\boldsymbol{\xi},t)=\boldsymbol{\mathcal{A}}(\boldsymbol{\xi},t)-\boldsymbol{\mathcal{A}}_S(\boldsymbol{\xi},t)$ 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, $\boldsymbol{\mathcal{A}}'_{\mathrm{xc}}(\mathbf{x},t)$, in the laboratory frame,

$$\mathcal{A}_{\mathrm{xc},i}(\boldsymbol{\xi},t)=\frac{\partial x^j}{\partial\xi^i}\mathcal{A}'_{\mathrm{xc},j}(\mathbf{x}(\boldsymbol{\xi},t),t). \tag{90}$$

Substituting Eq. (90) in the the right-hand side of Eq. (89), we find for the stress force,

$$\frac{\partial\xi^i}{\partial x^k}\partial_t\mathcal{A}_{\mathrm{xc},i}(\boldsymbol{\xi},t)=\partial_t\mathcal{A}'_{\mathrm{xc},k}|_{\boldsymbol{\xi}}+\frac{\partial\xi^i}{\partial x^k}\frac{\partial^2x^j}{\partial t\partial\xi^i}\mathcal{A}'_{\mathrm{xc},j}=\partial_t\mathcal{A}'_{\mathrm{xc},k}|_{\mathbf{x}}+v^j\frac{\partial\mathcal{A}'_{\mathrm{xc},k}}{\partial x^j}+\frac{\partial v^j}{\partial x^k}\mathcal{A}'_{\mathrm{xc},j}, \tag{91}$$

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:

$$\partial_t \mathbf{A}_{\mathrm{xc}} - \mathbf{v} \times (\partial_{\mathbf{x}} \times \mathbf{A}_{\mathrm{xc}}) + \partial_{\mathbf{x}} U_{\mathrm{xc}} = -\partial_t \boldsymbol{\mathcal{A}}'_{\mathrm{xc}} + \mathbf{v} \times (\partial_{\mathbf{x}} \times \boldsymbol{\mathcal{A}}'_{\mathrm{xc}}) - \partial_{\mathbf{x}}(\mathbf{v}\boldsymbol{\mathcal{A}}'_{\mathrm{xc}}). \quad (92)$$

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

$$\mathbf{A}_{\mathrm{xc}}(\mathbf{x},t) = -\boldsymbol{\mathcal{A}}'_{\mathrm{xc}}(\mathbf{x},t), \quad (93)$$

$$U_{\mathrm{xc}}(\mathbf{x},t) = -\mathbf{v}(\mathbf{x},t)\boldsymbol{\mathcal{A}}'_{\mathrm{xc}}(\mathbf{x},t). \quad (94)$$

Therefore, there is a particular mixed gauge in which the xc potentials are locally expressed in terms of the effective vector potential $\boldsymbol{\mathcal{A}}_{\mathrm{xc}}$. The convenience of the exact representation given by Eqs. (93) and (94) is that it directly relates the xc potentials, which enter the KS equations, to the solution of the universal quantum problem [Eqs. (58) and (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 (TDDefFT). 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 $\mathbf{x}(\boldsymbol{\xi},t)$ of infinitesimal fluid elements, where $\boldsymbol{\xi}$ is the initial position (the Lagrangian coordinate) of a given element. The motion of particles relative 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—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 $\mathbf{x}(\boldsymbol{\xi},t)$. Thus, the trajectories and hence the whole convective motion of an arbitrary quantum many-body system can be found from a closed hydrodynamicslike theory. We call this theory TDDefFT since the deformation tensor is the basic variable entering all relevant universal functionals. The most interesting and unusual property of the present approach is that a DFT-like theory emerges in a constructive fashion. It appears as a natural and unavoidable step in solving the quantum many-body problem in a comoving Lagrangian frame.

The set of Lagrangian trajectories $\mathbf{x}(\boldsymbol{\xi},t)$ and the current density $\mathbf{j}(\mathbf{x},t)$ are in a one-to-one correspondence. Therefore, our theory can, in principle, be viewed as a particular realization of TDCDFT. However, it is also legitimate, and perhaps even more natural, to consider TDDefFT as an independent member of the family of time-dependent DFT-like theories, such as TDDFT by Runge and Gross[6] and TDCDFT proposed by Vignale and Kohn.[8]

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, TDDefFT provides the most natural and unified framework for interpreting all currently known local nonadiabatic approximations.[8,9,14,15,17,18,20] In this paper, we concentrated on fundamental issues of the theory and did not attempt to derive new approximations for xc functionals. We have, however, made a step forward in this direction. We introduced a scalar W functional and derived a number of exact representations for the xc potentials (see Sec. IV), which should result in further progress in constructing new practical nonadiabatic functionals. One of the most promising directions is to go beyond the time-dependent local deformation approximation derived in Refs. 17 and 18 (beyond VK approximation in the linear regime). An attempt to apply the formalism of Ref. 17 to construct a GGA extension of the VK linear functional has been recently made by Tao and Vignale.[20] The present formulation of the theory is definitely much better suited for the derivation of similar extensions.

APPENDIX: 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 $g_{ij}(\boldsymbol{\xi},t)$ and subjected to an external field that is generated by the four-potential $\mathcal{A}_0(\boldsymbol{\xi},t)$ and $\mathcal{A}(\boldsymbol{\xi},t)$. The dynamics of the N-body wave function $\Psi(\boldsymbol{\xi}_1,\ldots,\boldsymbol{\xi}_N,t)$ is governed by the time-dependent Schrödinger equation with the following Hamiltonian:

$$H = \sum_{\alpha=1}^{N} g_\alpha^{-1/4}[i\partial_{\xi_\alpha^i} + \mathcal{A}_i(\boldsymbol{\xi}_\alpha)]\frac{\sqrt{g_\alpha} g_\alpha^{ij}}{2m}[i\partial_{\xi_\alpha^j} + \mathcal{A}_j(\boldsymbol{\xi}_\alpha)]g_\alpha^{-1/4} + \sum_{\alpha=1}^{N} \mathcal{A}_0(\boldsymbol{\xi}_\alpha) + \frac{1}{2}\sum_{\alpha,\beta} V(l_{\boldsymbol{\xi}_\alpha \boldsymbol{\xi}_\beta}), \quad (A1)$$

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

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

$$S[\Psi,\mathcal{A}_0,\boldsymbol{\mathcal{A}},g_{ij}] = \int dt \prod_{\alpha=1}^{N} d\boldsymbol{\xi}_\alpha \Psi^*(i\overleftrightarrow{\partial_t} - H)\Psi. \quad (A2)$$

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 direct substitution, we find the following transformation:

$$\Psi' = \Psi e^{i\Sigma_\alpha \phi(\xi_\alpha, t)}, \tag{A3}$$

$$\mathcal{A}_0' = \mathcal{A}_0 - \partial_t \phi(\boldsymbol{\xi}, t), \quad \mathcal{A}_i' = \mathcal{A}_i + \partial_{\xi^i} \phi(\boldsymbol{\xi}, t), \tag{A4}$$

$$g_{ij}'(\boldsymbol{\xi}, t) = g_{ij}(\boldsymbol{\xi}, t), \tag{A5}$$

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

$$S[\Psi', \mathcal{A}_0', \boldsymbol{\mathcal{A}}', g_{ij}'] = S[\Psi, \mathcal{A}_0, \boldsymbol{\mathcal{A}}, g_{ij}]. \tag{A6}$$

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

$$\delta S|_{\text{extr}} = \int dt d\boldsymbol{\xi} \left(-\frac{\delta S}{\delta \mathcal{A}_0} \partial_t \phi + \frac{\delta S}{\delta \mathcal{A}_i} \partial_{\xi^i} \phi \right) = 0. \tag{A7}$$

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 δS [Eq. (A7)]. The requirement that Eq. (A7) is fulfilled for any ϕ yields the continuity equation,

$$\partial_t n + \partial_{\xi^i} j^i = 0, \tag{A8}$$

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

$$n = -\frac{\delta S}{\delta \mathcal{A}_0} = \langle \Psi | \frac{\delta H}{\delta \mathcal{A}_0} | \Psi \rangle, \tag{A9}$$

$$j^i = \frac{\delta S}{\delta \mathcal{A}_i} = -\langle \Psi | \frac{\delta H}{\delta \mathcal{A}_i} | \Psi \rangle. \tag{A10}$$

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

$$\Psi'(\{\boldsymbol{\xi}_\beta'\}_{\beta=1}^N, t) = \prod_{\alpha=1}^N \left| \frac{\partial \boldsymbol{\xi}_\alpha}{\partial \boldsymbol{\xi}_\alpha'} \right|^{1/2} \Psi(\{\boldsymbol{\xi}_\beta\}_{\beta=1}^N, t), \tag{A11}$$

$$g_{ij}'(\boldsymbol{\xi}', t) = \frac{\partial \xi^k}{\partial \xi'^i} \frac{\partial \xi^p}{\partial \xi'^j} g_{kp}(\boldsymbol{\xi}, t), \tag{A12}$$

$$\mathcal{A}_k'(\boldsymbol{\xi}', t) = \frac{\partial \xi^i}{\partial \xi'^k} \mathcal{A}_i(\boldsymbol{\xi}, t) - m g_{ij}'(\boldsymbol{\xi}', t) \frac{\partial \xi'^i}{\partial t}, \tag{A13}$$

$$\mathcal{A}_0'(\boldsymbol{\xi}', t) = \mathcal{A}_0(\boldsymbol{\xi}, t) + \mathcal{A}_i'(\boldsymbol{\xi}', t) \frac{\partial \xi'^i}{\partial t} + \frac{m}{2} g_{ij}'(\boldsymbol{\xi}', t) \frac{\partial \xi'^i}{\partial t} \frac{\partial \xi'^j}{\partial t}, \tag{A14}$$

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

$$\int dt d\boldsymbol{\xi} \left(\frac{\delta S}{\delta g_{ij}} \delta g_{ij} + \frac{\delta S}{\delta \mathcal{A}_0} \delta \mathcal{A}_0 + \frac{\delta S}{\delta \mathcal{A}_i} \delta \mathcal{A}_i \right) = 0. \tag{A15}$$

In Eq. (A15), δg_{ij}, $\delta \mathcal{A}_0$, and $\delta \mathcal{A}_i$ are given by the infinitesimal version of Eqs. (A12)–(A14),

$$\delta g_{ij} = -\eta^k \partial_{\xi^k} g_{ij} - g_{ik} \partial_{\xi^j} \eta^k - g_{jk} \partial_{\xi^i} \eta^k, \tag{A16}$$

$$\delta \mathcal{A}_i = -\eta^k \partial_{\xi^k} \mathcal{A}_i - \mathcal{A}_k \partial_{\xi^i} \eta^k - m g_{ik} \partial_t \eta^k, \tag{A17}$$

$$\delta \mathcal{A}_0 = -\eta^k \partial_{\xi^k} \mathcal{A}_0 + \mathcal{A}_k \partial_t \eta^k. \tag{A18}$$

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

$$\partial_t \left(m g_{ik} \frac{\delta S}{\delta \mathcal{A}_i} - \mathcal{A}_k \frac{\delta S}{\delta \mathcal{A}_0} \right) + \partial_{\xi^i} \left(2 g_{kj} \frac{\delta S}{\delta g_{ij}} + \mathcal{A}_k \frac{\delta S}{\delta \mathcal{A}_0} \right) - \frac{\delta S}{\delta \mathcal{A}_0} \partial_{\xi^k} \mathcal{A}_0 - \frac{\delta S}{\delta \mathcal{A}_i} \partial_{\xi^k} \mathcal{A}_i - \frac{\delta S}{\delta g_{ij}} \partial_{\xi^k} g_{ij} = 0. \tag{A19}$$

Equation (A19) can be further simplified as follows:

$$m \partial_t j_k - j^i (\partial_{\xi^i} \mathcal{A}_k - \partial_{\xi^k} \mathcal{A}_i) + n \partial_t \mathcal{A}_k + n \partial_{\xi^k} \mathcal{A}_0 + \partial_{\xi^i} \left(2 g_{kj} \frac{\delta S}{\delta g_{ij}} \right) - \frac{\delta S}{\delta g_{ij}} \partial_{\xi^k} g_{ij} = 0, \tag{A20}$$

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

$$P^{ij} = \frac{2}{\sqrt{g}} \frac{\delta S}{\delta g_{ij}} = -\frac{2}{\sqrt{g}} \langle \Psi | \frac{\delta H}{\delta g_{ij}} | \Psi \rangle. \tag{A21}$$

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

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

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

$$m \partial_t j_k - j^i (\partial_{\xi^i} \mathcal{A}_k - \partial_{\xi^k} \mathcal{A}_i) + n \partial_t \mathcal{A}_k + n \partial_{\xi^k} \mathcal{A}_0 + \sqrt{g} \nabla_i P_k^i = 0. \tag{A22}$$

Apparently, the tensor P^{ij} defined after Eq. (A21) plays a role of the physical stress tensor.

*Electronic address: ilya.tokatly@physik.uni-erlangen.de

[1] P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964).
[2] W. Kohn and L. J. Sham, Phys. Rev. **140**, A1133 (1965).
[3] R. M. Dreizler and E. K. U. Gross, *Density-Functional Theory* (Springer, Berlin, 1990).
[4] A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Prentice-Hall, Englewood Cliffs, NJ, 1963).
[5] In the semiclassical limit DFT reduces to the Thomas-Fermi theory, which is the hydrostatics of the electron gas.
[6] E. Runge and E. K. U. Gross, Phys. Rev. Lett. **52**, 997 (1984).
[7] *Time-Dependent Density Functional Theory*, Lecture Notes in Physics Vol. 706, edited by M. A. L. Marques, F. Noguiera, A. Rubio, K. Burke, C. A. Ullrich, and E. K. U. Gross (Springer, Berlin, 2006).
[8] G. Vignale and W. Kohn, Phys. Rev. Lett. **77**, 2037 (1996).
[9] G. Vignale, C. A. Ullrich, and S. Conti, Phys. Rev. Lett. **79**, 4878 (1997).
[10] E. K. U. Gross and W. Kohn, Phys. Rev. Lett. **55**, 2850 (1985); **57**, 923(E) (1986).
[11] J. F. Dobson, M. J. Bünner, and E. K. U. Gross, Phys. Rev. Lett. **79**, 1905 (1997).
[12] J. F. Dobson, Phys. Rev. Lett. **73**, 2244 (1994).
[13] G. Vignale, Phys. Rev. Lett. **74**, 3233 (1995).
[14] Y. Kurzweil and R. Baer, J. Chem. Phys. **121**, 8731 (2004).
[15] Y. Kurzweil and R. Baer, Phys. Rev. B **72**, 035106 (2005).
[16] I. V. Tokatly, Phys. Rev. B **71**, 165104 (2005).
[17] I. V. Tokatly, Phys. Rev. B **71**, 165105 (2005).
[18] I. V. Tokatly, Lect. Notes Phys. **706**, 123 (2006).
[19] C. A. Ullrich and I. V. Tokatly, Phys. Rev. B **73**, 235102 (2006).
[20] J. Tao and G. Vignale, Phys. Rev. Lett. **97**, 036403 (2006).
[21] I. V. Tokatly, Phys. Rev. B **74**, 035333 (2006).
[22] I. V. Tokatly, Phys. Rev. B **73**, 205340 (2006).
[23] We use a symmetrized time derivative, $\Psi^* \overleftrightarrow{\partial_t} \Psi$, instead of a more common asymmetric form, $\Psi^* \partial_t \Psi$, for purely technical reasons (Ref. 37). It does not change the equations of motion, but significantly simplifies the transformation to a general noninertial reference frame.
[24] Throughout this paper we use Latin indices, i,j,k, etc., to label Cartesian axes. Additional Greek indices 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 indices.
[25] B. Podolsky, Phys. Rev. **32**, 812 (1928).
[26] B. A. Dubrovin, A. T. Fomenko, and S. P. Novikov, *Modern Geometry—Methods and Applications* (Springer-Verlag, New York, 1984), Vol. 1.
[27] *Physical Acoustics*, edited by W. P. Masson (Academic, New York, 1964), Vol. 1.
[28] P. Holland, Ann. Phys. **315**, 505 (2005).
[29] G. Vignale, Phys. Rev. B **70**, 201102(R) (2004).
[30] I. V. Tokatly and G. V. Nesterenko (unpublished).
[31] R. van Leeuwen, Phys. Rev. Lett. **82**, 3863 (1999).
[32] I. V. Tokatly (unpublished).
[33] L. V. Keldysh, Sov. Phys. JETP **20**, 1018 (1965).
[34] R. van Leeuwen, Phys. Rev. Lett. **80**, 1280 (1998).
[35] R. van Leeuwen, Int. J. Mod. Phys. B **15**, 1969 (2001).
[36] I. V. Tokatly and G. Vignale, Phys. Rev. Lett. **98**, 026805 (2007).
[37] D. Son and M. Wingate, Ann. Phys. **321**, 197 (2006).