

Mapping from current densities to vector potentials in time-dependent current density functional theory

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Under reasonable assumptions the time-dependent particle density $n(\vec{r}, t)$ and the current density $\vec{j}(\vec{r}, t)$ of a many-particle system that evolves under the action of external scalar and vector potentials $V(\vec{r}, t)$ and $\vec{A}(\vec{r}, t)$ and is initially in the quantum state $|\psi(0)\rangle$ can be reproduced in another many-particle system with a different two-particle interaction, subjected to external potentials $V'(\vec{r}, t)$ and $\vec{A}'(\vec{r}, t)$ and starting from an initial state $|\psi'(0)\rangle$, which yields the same density and current as $|\psi(0)\rangle$. Here we show that given the initial state of this other many-particle system, the potentials $V'(\vec{r}, t)$ and $\vec{A}'(\vec{r}, t)$, if they exist, are uniquely determined up to gauge transformations that do not alter the initial state. As a special case, we obtain a simpler proof of the Runge-Gross theorem for time-dependent current density functional theory. This theorem provides a formal basis for the application of time-dependent current density functional theory to transport problems.

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I. INTRODUCTION

Time-dependent density functional theory (TDDFT) attempts to describe the influence of many-body interactions on the time evolution of a quantum many-particle system in terms of an effective local potential that depends on a single collective variable, the particle density $n(\vec{r}, t)$. The possibility of such a description is largely based on a fundamental theorem, proved by Runge and Gross¹ in 1984, which guarantees the invertibility of the mapping from time-dependent potentials $V(\vec{r}, t)$ to time dependent densities, for time evolutions that start from a common initial state $|\psi(0)\rangle$. More precisely, this theorem asserts that two different potentials $V(\vec{r}, t)$ and $V'(\vec{r}, t)$ which are both analytic functions of t in a neighborhood of the initial time $t=0$ and which are *not* trivially related by a gauge transformation (i.e., by the addition of a merely time-dependent constant to the scalar potential), cannot give rise to the same density, starting from the same initial state: therefore $n(\vec{r}, t)$ determines $V(\vec{r}, t)$ uniquely up to a gauge transformation.²

The Runge-Gross theorem has been considerably strengthened a few years ago by the proof of another theorem, which we refer to as the *van Leeuwen's theorem*,³ which states that the time-dependent particle density of a many-particle system that evolves under the action of an external potential $V(\vec{r}, t)$ and is initially in the state $|\psi(0)\rangle$, can be reproduced (under reasonable assumptions) in another many-particle system with a different two-particle interaction, subjected to an external potential $V'(\vec{r}, t)$ and starting from an initial state $|\psi'(0)\rangle$ which yields the same density and divergence of the current density as $|\psi(0)\rangle$. Given the initial state of this other many-particle system, the potential $V'(\vec{r}, t)$ is uniquely determined up to a gauge transformation. The content of the van Leeuwen theorem is particularly interesting in two special cases: (i) if the second many-particle system is noninteracting, then the theorem guarantees the possibility of reproducing the time evolution of the density of an interacting many-particle system in a noninteracting many-particle

system, (ii) if the second many-particle system has the same two-particle interaction as the first, then the theorem becomes equivalent to the Runge-Gross theorem, which is thereby proved in a more direct manner.

Although the TDDFT has been remarkably successful over the 20 years of its history, there are several situations in which it seems useful to reformulate the theory in terms of the particle current density $\vec{j}(\vec{r}, t)$, leading to what is known as time-dependent current density functional theory (TDCDFT).⁴ It has been pointed out that the time-dependent exchange-correlation potential, when regarded as a functional of the density, does not admit a gradient expansion⁴ (this is the so-called “ultranonlocality problem”), whereas the exchange-correlation vector potential of TDCDFT does. For this reason there has been great interest in applying TDCDFT to situations in which the standard TDDFT is known to run into difficulties, such as optical spectra of solids^{5,6} and dielectric properties of polymer chains.⁷ The reformulation of TDDFT in terms of the current density is particularly attractive to those who wish to apply DFT methods to molecular transport problems,⁸ for the TDCDFT gives direct access to the electrical current density. Finally, it should be noted that this theory allows one to dispose of restrictive boundary conditions, such as the one mentioned in Ref. 2.

Efforts to provide a rigorous basis for TDCDFT date back to the pioneering work of Ghosh and Dhara,⁹ where the invertibility (up to a gauge transformation) of the map from scalar and vector potentials $V(\vec{r}, t)$, $\vec{A}(\vec{r}, t)$ to particle density and current density $n(\vec{r}, t)$, $\vec{j}(\vec{r}, t)$ was proved under hypotheses similar to those of the original Runge-Gross theorem. The Ghosh-Dhara proof of this theorem is considerably more complex than the original proof of the Runge-Gross theorem and, furthermore, does not address the issue of representability of the interacting current density evolution in a noninteracting system, which is vital to the existence of a Kohn-Sham equation. In this paper we overcome both limitations by proving the analog of van Leeuwen's theorem in

TDCDFT. The statement of this theorem is as follows.

Theorem. Consider a many-particle system described by the time-dependent Hamiltonian

$$\hat{H}(t) = \sum_i \left[\frac{1}{2m} [\hat{p}_i + \vec{A}(\hat{r}_i, t)]^2 + V(\hat{r}_i, t) \right] + \sum_{i < j} U(\hat{r}_i - \hat{r}_j), \quad (1)$$

where $V(\vec{r}, t)$ and $\vec{A}(\vec{r}, t)$ are given external scalar and vector potentials, which are analytic functions of time in a neighborhood of $t=0$, and $U(\hat{r}_i - \hat{r}_j)$ is a translationally invariant two-particle interaction. Let $n(\vec{r}, t)$ and $\vec{j}(\vec{r}, t)$ be the particle density and current density that evolve under \hat{H} from a given initial state $|\psi(0)\rangle$. Then, under reasonable assumptions discussed below, the same density and current density can be obtained from another many-particle system, with Hamiltonian

$$\hat{H}'(t) = \sum_i \left[\frac{1}{2m} [\hat{p}_i + \vec{A}'(\hat{r}_i, t)]^2 + V'(\hat{r}_i, t) \right] + \sum_{i < j} U'(\hat{r}_i - \hat{r}_j), \quad (2)$$

starting from an initial state $|\psi'(0)\rangle$ which yields the same density and current density as $|\psi(0)\rangle$ at time $t=0$. The potentials $V'(\vec{r}, t)$ and $\vec{A}'(\vec{r}, t)$ are uniquely determined by $V(\vec{r}, t)$, $\vec{A}(\vec{r}, t)$, $|\psi(0)\rangle$, and $|\psi'(0)\rangle$, up to gauge transformations of the form

$$\begin{aligned} V'(\vec{r}, t) &\rightarrow V(\vec{r}, t) - \frac{\partial \Lambda(\vec{r}, t)}{\partial t}, \\ \vec{A}'(\vec{r}, t) &\rightarrow \vec{A}(\vec{r}, t) + \vec{\nabla} \Lambda(\vec{r}, t), \end{aligned} \quad (3)$$

where Λ is an arbitrary regular function of \vec{r} and t , which satisfies the initial condition $\Lambda(\vec{r}, 0)=0$. The proof of this theorem is presented in the next section, and its physical implications are discussed in Sec. III.

II. PROOF

As a first step let us observe that, given a set of potentials $V(\vec{r}, t)$, $\vec{A}(\vec{r}, t)$, one can always make a gauge transformation of the form (3) that eliminates the scalar potential at all times. To this end, one simply chooses $\Lambda(\vec{r}, t)$ to be the solution of the differential equation

$$\frac{\partial \Lambda(\vec{r}, t)}{\partial t} = V(\vec{r}, t) \quad (4)$$

with an initial condition $\Lambda(\vec{r}, 0)=0$. We will henceforth assume that such a transformation has been done in both the unprimed and primed systems so that the scalar potentials V and V' are zero at all times.

The current density operator in the unprimed system is given by

$$\hat{j}(\vec{r}, t) = \frac{1}{2} \sum_i \{ \hat{v}_i(t), \delta(\vec{r} - \hat{r}_i) \}, \quad (5)$$

where $\{\hat{A}, \hat{B}\} \equiv (\hat{A}\hat{B} + \hat{B}\hat{A})$ denotes the *anticommutator* of two operators \hat{A} and \hat{B} , and the velocity operator of the i th particle is given by

$$\hat{v}_i = \frac{1}{m} [\hat{p}_i + \vec{A}(\hat{r}_i, t)], \quad (6)$$

where $\hat{p}_i = -i\hbar(\partial/\partial\hat{r}_i)$ is the canonical momentum operator. Notice that the velocity operator depends explicitly on time via the vector potential. A completely analogous expression can be written, of course, for the current density of the primed system, the only difference being the replacement of the velocity operator \hat{v}_i by \hat{v}'_i , which is given by Eq. (6) with \vec{A} replaced by \vec{A}' .

Let us denote by $\vec{j}(\vec{r}, t)$ and $n(\vec{r}, t)$ the expectation values of the current density and density operators in the quantum state that evolves from the initial state $|\psi(0)\rangle$ under the Hamiltonian \hat{H} . It is not difficult to verify that $\vec{j}(\vec{r}, t)$ obeys the equation of motion

$$\begin{aligned} \frac{d\vec{j}(\vec{r}, t)}{dt} &= \frac{\partial \vec{j}(\vec{r}, t)}{\partial t} + \frac{i}{\hbar} \langle [\hat{H}(t), \vec{j}(\vec{r}, t)] \rangle = \frac{n(\vec{r}, t)}{m} \frac{\partial \vec{A}(\vec{r}, t)}{\partial t} - \frac{\vec{j}(\vec{r}, t)}{m} \\ &\quad \times [\vec{\nabla} \times \vec{A}(\vec{r}, t)] + \frac{\vec{\mathcal{F}}(\vec{r}, t)}{m} + \vec{\nabla} \cdot \vec{\sigma}(\vec{r}, t), \end{aligned} \quad (7)$$

where $\partial \vec{A}(\vec{r}, t)/\partial t$ and $\vec{\nabla} \times \vec{A}(\vec{r}, t)$ are, respectively, the external electric and the magnetic fields, $\vec{\mathcal{F}}(\vec{r}, t)$ is the internal force density, and $\vec{\sigma}(\vec{r}, t)$ is a stress tensor. The last two quantities are defined as follows:

$$\vec{\mathcal{F}}(\vec{r}, t) = - \left\langle \sum_i \delta(\vec{r} - \hat{r}_i) \sum_{j \neq i} \vec{\nabla}_{\hat{r}_i} U(\hat{r}_i - \hat{r}_j) \right\rangle \quad (8)$$

and

$$\sigma_{\alpha\beta}(\vec{r}, t) = - \left\langle \frac{1}{4} \sum_i \{ \hat{v}_{i\alpha}, \{ \hat{v}_{i\beta}, \delta(\vec{r} - \hat{r}_i) \} \} \right\rangle, \quad (9)$$

where $\langle \rangle$ denotes the average in the quantum state of the unprimed system at time t . Notice that the “divergence” of the tensor $\vec{\sigma}(\vec{r}, t)$ is a vector with components $[\vec{\nabla} \cdot \vec{\sigma}(\vec{r}, t)]_\alpha = \sum_\beta \partial \sigma_{\alpha\beta}(\vec{r}, t) / \partial r_\beta$. By hypothesis, the current density also obeys the equation

$$\begin{aligned} \frac{d\vec{j}(\vec{r}, t)}{dt} &= \frac{n(\vec{r}, t)}{m} \frac{\partial \vec{A}'(\vec{r}, t)}{\partial t} - \frac{\vec{j}(\vec{r}, t)}{m} \times [\vec{\nabla} \times \vec{A}'(\vec{r}, t)] + \frac{\vec{\mathcal{F}}'(\vec{r}, t)}{m} \\ &\quad + \vec{\nabla} \cdot \vec{\sigma}'(\vec{r}, t). \end{aligned} \quad (10)$$

Notice that $\vec{\sigma}'(\vec{r}, t)$ differs from $\vec{\sigma}(\vec{r}, t)$ in two ways: first, because it contains the velocity operator \hat{v}'_i instead of \hat{v}_i ; and, second, because it is computed as an average in the quantum state of the primed system at time t . On the other hand, $\vec{\mathcal{F}}'$ differs from $\vec{\mathcal{F}}$ only because it is derived from U' instead of U . Taking the difference of the two equations (7) and (10) we get

$$\frac{n(\vec{r},t)}{m} \frac{\partial \vec{\Delta A}(\vec{r},t)}{\partial t} = \frac{\vec{j}(\vec{r},t)}{m} \times [\vec{\nabla} \times \vec{\Delta A}(\vec{r},t)] + \vec{Q}(\vec{r},t) - \vec{Q}'(\vec{r},t), \quad (11)$$

where $\vec{\Delta A}(\vec{r},t) \equiv \vec{A}'(\vec{r},t) - \vec{A}(\vec{r},t)$ and

$$\vec{Q}(\vec{r},t) \equiv \frac{\vec{\mathcal{F}}(\vec{r},t)}{m} + \vec{\nabla} \cdot \vec{\sigma}(\vec{r},t), \quad (12)$$

while $\vec{Q}'(\vec{r},t)$ is the primed counterpart of $\vec{Q}(\vec{r},t)$. This equation determines, in principle, the vector potential $\vec{A}'(\vec{r},t)$ that produces the same current density as $\vec{A}(\vec{r},t)$, and the questions to which we seek an answer is whether a solution of this equation exists and whether it is unique. Unfortunately, $\vec{A}'(\vec{r},t)$ enters the equation not only explicitly, but also implicitly, via $\vec{Q}'(\vec{r},t)$: a theorem of existence and uniqueness of the solution for this type of equation is not immediately available. Lacking that, we take a different, more informal approach. Since, by hypothesis, both $\vec{A}(\vec{r},t)$ and $\vec{A}'(\vec{r},t)$ are expandable in a Taylor series of time in a neighborhood of $t=0$, it follows that their difference, $\vec{\Delta A}(\vec{r},t)$, is Taylor expandable, too. We can therefore write

$$\vec{\Delta A}(\vec{r},t) = \sum_{k=0}^{\infty} \Delta A_k(\vec{r}) t^k, \quad (13)$$

where

$$\Delta A_k(\vec{r}) \equiv \frac{1}{k!} \left. \frac{\partial^k \vec{\Delta A}(\vec{r},t)}{\partial t^k} \right|_{t=0}.$$

Substituting this expansion into Eq. (11) and equating the l th term of the Taylor expansion on each side of it, we easily arrive at

$$\sum_{k=0}^l \frac{n_{l-k}(\vec{r})}{m} \left[\frac{\partial \vec{\Delta A}(\vec{r},t)}{\partial t} \right]_k = \sum_{k=0}^l \left\{ \frac{\vec{j}_{l-k}(\vec{r})}{m} \times [\vec{\nabla} \times \vec{\Delta A}_k(\vec{r})] \right\} + [\vec{Q}(\vec{r},t)]_l - [\vec{Q}'(\vec{r},t)]_l, \quad (14)$$

where $n_k(\vec{r})$ and $\vec{j}_k(\vec{r})$ denote the k th coefficients in the Taylor expansions of $n(\vec{r})$ and $\vec{j}(\vec{r})$ about $t=0$, and, more generally $[f(\vec{r},t)]_l$ denotes the l th coefficient (a function of \vec{r} alone) in the expansion of a function $f(\vec{r},t)$ in powers of t about $t=0$. The fact that all the quantities appearing in the above equation admit such an expansion is a consequence of the analyticity of the vector potential and of the time-dependent Schrödinger equation

$$i\hbar \frac{\partial |\psi(t)\rangle}{\partial t} = \hat{H}(t) |\psi(t)\rangle. \quad (15)$$

Since

$$\left[\frac{\partial \vec{\Delta A}(\vec{r},t)}{\partial t} \right]_k = (k+1) \Delta \vec{A}_{k+1}(\vec{r}), \quad (16)$$

we can rewrite Eq. (14) in the following form:

$$n_0(\vec{r})(l+1) \Delta \vec{A}_{l+1}(\vec{r}) = - \sum_{k=0}^{l-1} n_{l-k}(\vec{r})(k+1) \Delta \vec{A}_{k+1}(\vec{r}) + \sum_{k=0}^l \{ \vec{j}_{l-k}(\vec{r}) \times [\vec{\nabla} \times \vec{\Delta A}_k(\vec{r})] \} + m \{ [\vec{Q}(\vec{r},t)]_l - [\vec{Q}'(\vec{r},t)]_l \}, \quad (17)$$

where we have isolated on the left-hand side the $k=l$ term of the sum which originally appeared on the left-hand side of Eq. (14).

We now show that Eq. (17) is effectively a recursion relation for the coefficients of the Taylor expansion of $\vec{\Delta A}(\vec{r},t)$, i.e., a relation that expresses $\Delta \vec{A}_{l+1}(\vec{r})$ in terms of $\Delta \vec{A}_k(\vec{r})$, with $k \leq l$. To this end, we must show that the right-hand side of Eq. (17) depends only on coefficient $\Delta \vec{A}_k(\vec{r})$, with $k \leq l$. This is obviously true for the terms in which $\Delta \vec{A}_k$ appears explicitly. There are also *implicit* $\Delta \vec{A}_k$ s, which are hidden in the coefficients of the expansion of $\vec{Q}'(\vec{r},t)$. However, the structure of the time-dependent Schrödinger equation (15), which is of first order in time, guarantees that the l th coefficient in the Taylor expansion of the quantum states $|\psi(t)\rangle$ and $|\psi'(t)\rangle$ is entirely determined by coefficients of order $k < l$ in the Taylor expansion of \vec{A} and \vec{A}' : hence all the quantities on the right-hand side of Eq. (17) are completely determined by the coefficients $\Delta \vec{A}_k(\vec{r})$, with $k \leq l$. (In this argument \vec{A} is considered a known quantity, and $\vec{A}' = \vec{A} + \vec{\Delta A}$ is the quantity we are trying to determine.)

At this point, in order to make the recursion relation (17) work we only need to determine the initial value of $\Delta \vec{A}$, namely $\Delta \vec{A}_0(\vec{r}) = \vec{A}'(\vec{r},0) - \vec{A}(\vec{r},0)$. This is easily done, since from the equality of the densities and current densities of the primed and unprimed systems it follows that

$$n(\vec{r},0) \Delta \vec{A}_0(\vec{r}) = \langle \psi'(0) | \hat{j}_p(\vec{r}) | \psi'(0) \rangle - \langle \psi(0) | \hat{j}_p(\vec{r}) | \psi(0) \rangle, \quad (18)$$

where $\hat{j}_p(\vec{r}) \equiv (1/2m) \sum_i \{ \hat{p}_i, \delta(\vec{r} - \hat{r}_i) \}$ is the “paramagnetic” current density operator that has the same form in the primed and unprimed system. Thus, the recursion relation (17), together with the initial condition (18), completely determines the Taylor expansion of the potential $\vec{A}'(\vec{r},t)$ that yields, in the primed system, the same current density that $\vec{A}(\vec{r},t)$ yields in the unprimed one. According to our hypotheses, a knowledge of the coefficients of the Taylor expansion of $\vec{A}'(\vec{r},t)$ is equivalent to a knowledge of the function $\vec{A}'(\vec{r},t)$ itself, provided the series itself converges within a nonvanishing convergence radius $t_c > 0$. If this is the case then $\vec{A}'(\vec{r},t)$ is uniquely determined, for under this assumption the solution for $\vec{A}'(\vec{r},t)$ can be computed up to t_c , then the process can be iterated taking t_c as the initial time.

We must now examine the possibility that the convergence radius might be zero, in which case a solution for $\vec{A}'(\vec{r},t)$ would not exist. It is here that our “reasonable as-

sumptions” come in. Physically, the possibility of a vanishing convergence radius seems very remote since, in order for t_c to vanish, the k th time derivative of $\vec{A}'(\vec{r}, t)$ at $t=0$ should grow more rapidly than $k!a^k$, where a is an arbitrary positive constant. The smooth dynamics of the Schrödinger equation does not appear to offer any mechanism for such a dramatic explosion in the values of the initial derivatives. It is for this reason that we think that the possibility of a zero convergence radius can be safely discounted. If this step is granted, then the chain of reasoning presented above guarantees that the solution for $\vec{A}'(\vec{r}, t)$ is indeed unique (up to a gauge transformation).

A nice feature of the present proof of uniqueness of the vector potential is that, at variance with the proof of van Leeuwen’ theorem, it does not require the imposition of the subsidiary condition that the current density vanish at infinity.^{10,11} The reason for this difference is that our recursion relation (17) determines directly the coefficients of the Taylor expansion of $\vec{A}'(\vec{r}, t)$, leaving no room for alternative solutions. The corresponding equation of van Leeuwen does not directly determine the coefficients of the Taylor expansion of the scalar potential $V'(\vec{r}, t)$ in the primed system, but rather the coefficients of the expansion of $\vec{\nabla} \cdot [n(\vec{r}, t)\vec{\nabla}V'(\vec{r}, t)]$: this leaves open a degree of freedom in $V'(\vec{r}, t)$, which must be eliminated by the subsidiary boundary condition on the current. The ability to describe situations in which the current does not vanish at infinity is of course a major asset in the application of TDCDFT to transport theory.

III. DISCUSSION

Two special cases of the theorem presented in Sec. II deserve a special discussion.

(1) The primed system coincides with the unprimed system, i.e., $U=U'$ and $|\psi(0)\rangle=|\psi'(0)\rangle$. In this case Eq. (18) above implies that $\Delta A_0(\vec{r})=0$, and then it follows from Eq. (17) that $\Delta A_k(\vec{r})=0$ for all k , i.e., $\vec{A}'(\vec{r}, t)=\vec{A}(\vec{r}, t)$ at all times. This important result is just a statement of the Runge-Gross

theorem for TDCDFT: it asserts that two vector potentials that produce the same current density starting from the same initial state of a many-particle system must necessarily coincide, up to a gauge transformation: the map from vector potentials to current densities is invertible. As noted in the Introduction, this theorem was proved by Ghosh and Dhara⁹ by a different method, similar in spirit to the original proof of the Runge-Gross theorem. The present proof provides a simpler route to the same conclusion.

(2) The primed system is noninteracting, i.e., $U'=0$. In this case our theorem provides a resolution of what could be called the noninteracting \vec{A} -representability problem. In other words, the theorem shows that the current density produced by a vector potential \vec{A} in an interacting many-particle system can also be obtained in a noninteracting system, under the action of a suitable vector potential \vec{A}' . This is certainly possible if $|\psi'(0)\rangle=|\psi(0)\rangle$ [in which case we must have $\vec{A}'(\vec{r}, 0)=\vec{A}(\vec{r}, 0)$], but it may be more generally possible if one chooses for $|\psi'(0)\rangle$ a single Slater determinant that yields the correct initial density and current density. Thus, the theorem provides a solid basis for the use of the time-dependent Kohn-Sham equation, which indeed attempts to reproduce the correct current density in a system of noninteracting particles. As pointed out in the Introduction, this important result lays the foundation for the application of TDCDFT to molecular transport problems. Notice, however, that the theorem does not say anything about the possibility of producing an *arbitrary* time-dependent current density by means of a suitable vector potential.

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²An additional hypothesis of the Runge-Gross theorem is that the quantity $n(\vec{r}, t)|\vec{\nabla}V^2(\vec{r}, t)|$ vanishes at infinity more rapidly than $1/r^2$ in three dimensions, or satisfies periodic boundary conditions at infinity.

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