Center of mass and relative motion in time dependent density functional theory

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Abstract

It is shown that the exchange-correlation part of the action functional $A_{xc}[\rho(\vec{r}, t)]$ in time-dependent density functional theory, where $\rho(\vec{r}, t)$ is the time-dependent density, is invariant under the transformation to an accelerated frame of reference $\rho(\vec{r}, t) \rightarrow \rho'(\vec{r}, t) = \rho(\vec{r} + \vec{x}(t), t)$, where $\vec{x}(t)$ is an arbitrary function of time. This invariance implies that the exchange-correlation potential in the Kohn-Sham equation transforms in the following manner: $V_{xc}[\rho'; \vec{r}, t] = V_{xc}[\rho; \vec{r} + \vec{x}(t), t]$. Some of the approximate formulas that have been proposed for $V_{xc}$ satisfy this exact transformation property, others do not. Those which transform in the correct manner automatically satisfy the “harmonic potential theorem”, i.e. the separation of the center of mass motion for a system of interacting particles in the presence of a harmonic external potential. A general method to generate functionals which possess the correct symmetry is proposed.
Time dependent density functional theory (TDFT) \([1,3]\) is a very valuable tool for the study of the dynamic behavior of correlated electronic systems under the influence of external probes which can be represented as time-dependent potentials. The range of problems to which this formalism is successfully applied is expanding \([3]\): it includes the calculation of atomic collision cross sections, the behavior of atoms under very strong electromagnetic fields, the calculation of excitation energies in atoms, molecules, and solids. Crucial to the success of the theory is the availability of simple approximations for the exchange-correlation potential \(V_{xc}[\rho; \vec{r}, t]\), which is an ordinary function of \(\vec{r}\) and \(t\), but a complicated, non-local functional of the density distribution \(\rho(\vec{r}', t')\) for times \(t'\) earlier than \(t\). Examples of approximations for \(V_{xc}\) are the “adiabatic time dependent local density approximation” (ATLDA) of Zangwill and Soven \([5]\), and the local linear response approximation, with a frequency-dependent exchange-correlation kernel, of Gross and Kohn \([2]\). In constructing such approximations, one should try to make sure that the approximate form satisfies as many of the known exact properties of the functional as possible. One example of rigorous constraints on admissible approximate functionals is provided by the scaling relations for the static density functional theory \([4]\). Another type of constraint, which is peculiar to the time-dependent theory, has been recently pointed out by Dobson \([6]\). He has observed that, according to a general “harmonic potential theorem” (HPT), a system of interacting electrons confined by an external harmonic potential \(V_0(\vec{r}) = (1/2)\vec{r} \cdot \vec{K} \cdot \vec{r}\), must possess solutions in which the dynamics of the center of mass is completely decoupled from that of the internal degrees of freedom. Assuming that the system is initially in the ground state, the center of mass wave function is a minimum uncertainty gaussian centered about the origin. When a time-dependent uniform electric field \(\vec{E}(t)\) is applied to such a system, the time dependence of the center of mass wave function is such that the gaussian is rigidly transported (to within a time-dependent phase factor), the position of its center being determined by the solution of the classical equation of motion

\[
m\frac{d^2 \vec{R}_{CM}(t)}{dt^2} = -e\vec{E}(t) - \vec{K} \cdot \vec{R}_{CM}(t) - \frac{e}{c} \frac{d\vec{R}_{CM}(t)}{dt} \times \vec{B},
\]  

(1)
where $\vec{B}$ is a uniform and constant magnetic field. The fact that the “relative” dynamics is not affected by the external force implies that the electronic density must also be rigidly transported, following the motion of the center of mass, i.e.,

$$\rho(\vec{r}, t) = \rho_0(\vec{r} - \vec{R}_{CM}(t))$$

(2)

where $\rho_0(\vec{r})$ is the static electronic density in the absence of the driving field. Of course, one would hope that approximate versions of TDFT were able to reproduce this elegant exact result. Dobson’s discovery [6] is that this is not always the case. For example, the Zangwill-Soven [5] adiabatic ATLDA does satisfy this requirement, but the Gross-Kohn [2] linearized response theory, which includes a frequency dependence (i.e., a memory) in the exchange-correlation kernel, does not. Other approximations, based on inhomogeneous hydrodynamics, also fail to satisfy the HPT [5]. The root of the difficulty was traced by Dobson to the inclusion of non-locality in time but not in space. He developed a simple modification of the TDLDA, whereby the density modulation induced by the driving field is decomposed in two parts, one corresponding to a rigid shift of the whole distribution (i.e, a motion of the center of mass), the other including the remaining internal deformations. The Gross-Kohn formalism is applied only to the latter part, while the center of mass component is still treated in the adiabatic LDA. This formalism satisfies the HPT.

In this paper, we demonstrate that the occurrence of the HPT in TDFT is in fact the consequence of a simple symmetry of the exchange-correlation part of the action. The approximations that Dobson finds to satisfy HPT are the ones that satisfy this symmetry, and those that violate the HPT are the ones that violate this symmetry. Furthermore, the cure he proposes to make the TDLDA consistent with the HPT can be viewed as an instance of a general procedure whereby the correct symmetry of the exchange-correlation potential can be built at the outset in any approximation.

We now present our results in detail. The basic theorem of TDFT is the Runge-Gross theorem, according to which, for any time-dependent density $\rho(\vec{r}, t)$ defined within an appropriate class of functions in the interval $t_0 < t < t_1$, there exists an essentially unique time
dependent potential $V(\vec{r}, t)$, such that the solution $|\psi(t)\rangle$ of the time-dependent Schroedinger equation

$$
(i\frac{\partial}{\partial t} - \hat{H}_0 - \hat{V}(t))|\psi(t)\rangle = 0,
$$

(3)

with the condition that $\psi(t_0)$ is the Hohenberg-Kohn ground-state wave function corresponding to the density $\rho_0(\vec{r}) = \rho(\vec{r}, t_0)$, yields $\rho(\vec{r}, t)$ as the expectation value $\langle \psi(t)|\hat{\rho}(\vec{r})|\psi(t)\rangle$ of the density operator $\hat{\rho}(\vec{r}) = \sum_{i=1}^{N} \delta(\vec{r} - \vec{r}_i)$. Here

$$
\hat{H}_0 = \sum_{i=1}^{N} \frac{1}{2m}(\vec{p}_i + \frac{e}{c}\vec{A}(\vec{r}_i))^2 + \frac{e^2}{2} \sum_{i,j} \frac{1}{|\vec{r}_i - \vec{r}_j|}
$$

(4)

is the familiar Hamiltonian for $N$ interacting electrons in the presence of a uniform magnetic field $\vec{B}$ described by the vector potential $\vec{A}(\vec{r}) = \vec{B} \times \vec{r}/2$, and

$$
\hat{V}(t) = \sum_{i=1}^{N} V(\vec{r}_i, t)
$$

(5)

is the time-dependent potential. The expression “essentially unique” refers to the possibility of adding to $V(\vec{r}, t)$ an arbitrary function $f(t)$ of time, which causes the wave function to be multiplied by a phase factor $\exp[i\int f(t)dt]$ without affecting the density. The “appropriate class” of densities includes all the densities for which the potential $V(\vec{r}, t)$ exists, and is Taylor expandable, with finite convergence radius, in a neighborhood of $t_0$. Under the assumption that at time $t_0$ the system is in the ground state - an assumption that we make in the rest of this paper - the Runge-Gross theorem establishes the existence of an essentially unique mapping from time-dependent densities to time-dependent potentials.

Let us now look at the density $\rho(\vec{r}, t)$ from the point of view of an accelerated observer whose position, relative to the original reference frame, is given by the function $\vec{x}(t)$. It is assumed that the accelerated observer uses cartesian axes that remain parallel to the axes of the original reference frame, i.e., there is no rotation. The density seen by the observer, in terms of his own $\vec{r}$ coordinate is $\rho'(\vec{r}, t) = \rho(\vec{r} + \vec{x}(t), t)$. It is assumed that $\vec{x}(t_0) = d\vec{x}(t)/dt(t = t_0) = 0$ so that both the density and the wave function seen by the accelerated observer coincide with those seen by the inertial observer at time $t_0$. Our
first important result is that there exists a time-dependent potential \( V'(\vec{r}, t) \) that generates \( \rho'(\vec{r}, t) \) when the Schrödinger equation is solved. The explicit form for \( V'(\vec{r}, t) \), aside from an inessential additive function of time, is

\[
V'(\vec{r}, t) = V(\vec{r} + \vec{x}(t), t) + m\vec{a}(t) \cdot \sum_{i=1}^{N} \vec{r}_i + (e/c)(\vec{v}(t) \times \vec{B}) \cdot \sum_{i=1}^{N} \vec{r}_i,
\]  

where \( \vec{a}(t) \) and \( \vec{v}(t) \) are the second and first derivatives of \( \vec{x}(t) \) with respect to time. The wavefunction \( \psi' \) corresponding to this transformed potential is related to the wavefunction \( \psi \) corresponding to potential \( V \) by the transformation

\[
|\psi'(t)\rangle = \Pi_{i=1}^{N} \hat{U}_i(t) |\psi(t)\rangle
\]

where the unitary transformation \( \hat{U}_i(t) \) is defined as

\[
\hat{U}_i(t) = \exp[-i\vec{r}_i \cdot (m\vec{v}(t) - \frac{e}{2c} \vec{B} \times \vec{x}(t))] \exp[i\vec{p}_i \cdot \vec{x}(t)].
\]

In writing the above formulas we have assumed that there is a uniform and constant magnetic field \( \vec{B} \) acting on the electrons. This is because we want to discuss later the generalized harmonic potential theorem in the presence of a magnetic field. The familiar situation is recovered by putting \( B = 0 \) in the above formulas. The detailed mathematical proof of the key equations (6) and (7) is provided in the appendix. However, the correctness of these equations is physically evident. Equation (6) says that the potential seen by the accelerated observer is the original potential expressed in terms of the new coordinate, plus an inertial force \(-m\vec{a}(t)\) that couples like a uniform gravitational field to the center of mass of the system, plus a uniform electric field \( \vec{v} \times \vec{B}/c \) that arises from the transformation of the uniform magnetic field. Equation (8) says that the new wavefunction is obtained from the former by translating the coordinate of each electron by \( \vec{x}(t) \) and the momentum of each electron by \( m\vec{v}(t) \). When the magnetic field is present an additional translation of the momentum by \(-e\vec{B} \times \vec{x}(t)/2c \) is required in order to restore the original gauge for the vector potential. Equations (8) and (7) enable us to determine the transformation of the “internal” action functional, defined as follows:
\[ \tilde{A}[\rho] = \int_{t_0}^{t_1} \langle \psi(t) | i \frac{\partial}{\partial t} - \hat{H}_0 | \psi(t) \rangle dt \]  
(9)

(Note the absence of the external potential in this definition). We obtain

\[ \tilde{A}[\rho'] = \tilde{A}[\rho] + N \int_{t_0}^{t_1} [m\bar{a}(t) \cdot \vec{R}_{CM}(t) + \frac{e}{c} (\vec{v}(t) \times \vec{B}) \cdot \vec{R}_{CM}(t) + \frac{mv^2(t)}{2} + \frac{e}{2c} (\vec{B} \times \vec{x}(t)) \cdot \vec{v}(t)] dt, \]

(10)

where

\[ N \vec{R}_{CM}(t) = \int \vec{r} \rho(\vec{r}, t) d\vec{r} \]  
(11)

is the coordinate of the center of mass of wave function \( \psi \). The key observation is that, because the additional forces in the accelerated frame of reference depend only on the electron coordinates, the additional terms in the transformed action can be expressed explicitly in terms of the density. Clearly, these additional terms would have had exactly the same form if we had considered the transformation of the non-interacting action functional

\[ \tilde{A}_0[\rho] = \int_{t_0}^{t_1} \langle \psi_0(t) | i \frac{\partial}{\partial t} - \hat{T} | \psi_0(t) \rangle dt \]

(12)

where \( \psi_0 \) is the wave function corresponding to the density \( \rho(\vec{r}, t) \) in a non-interacting system, and \( \hat{T} \) is the kinetic energy operator.

Now, according to Runge and Gross the interacting and non-interacting action functionals are related as

\[ \tilde{A}[\rho] = \tilde{A}_0[\rho] + A_H[\rho] + A_{xc}[\rho] \]  
(13)

which constitutes a definition of the “exchange-correlation” part of the action functional. Since the Hartree part of the functional

\[ A_H[\rho] = -\frac{e^2}{2} \int_{t_0}^{t_1} dt \int d\vec{r} \int d\vec{r}' \frac{\rho(\vec{r}, t) \rho(\vec{r}', t)}{|\vec{r} - \vec{r}'|} \]  
(14)

is manifestly invariant under the transformation \( \rho \rightarrow \rho' \), we conclude, comparing the transformation equations for \( \tilde{A} \) and \( \tilde{A}_0 \) that \( A_{xc} \) is invariant under this transformation:
This is the most important result in this paper. The transformation law for the exchange correlation potential is derived in the following way. We consider the difference between the \( A_{xc} \) action calculated for two neighboring densities \( \rho \) and \( \rho + \delta \rho \):

\[
A_{xc}[\rho + \delta \rho] - A_{xc}[\rho] = \int_{t_0}^{t_1} dt' \int d\vec{r}' V_{xc}[\rho; \vec{r}', t'] \delta \rho(\vec{r}', t')
\]  

which follows from the definition of \( V_{xc} \) as a first functional derivative of \( A_{xc} \) with respect to the density. We can write the same relation for the transformed densities \( \rho' \) and \( \rho' + \delta \rho' \):

\[
A_{xc}[\rho' + \delta \rho'] - A_{xc}[\rho'] = \int_{t_0}^{t_1} dt' \int d\vec{r}' V_{xc}[\rho'; \vec{r}', t'] \delta \rho'(\vec{r}', t')
\]

Now, according to eq. (15) the left hand sides of these two equations must be equal. It follows then that the right hand sides are also equal. By doing a change of variable in one of the two integrals and using the fact that \( \delta \rho \) is arbitrary, we easily establish the transformation property

\[
V_{xc}[\rho'; \vec{r}, t] = V_{xc}[\rho; \vec{r} + \vec{x}(t), t]
\]

We now show that an exchange-correlation potential that correctly transforms according to equation (18) automatically satisfies the “harmonic potential theorem”. We suppose that for \( t \leq t_0 \) the density of the interacting electron system is described by the usual Kohn-Sham equation with a \textit{time-independent} external \textit{harmonic} potential \( V_0(\vec{r}) \), and a static Hartree potential \( V_H(\rho_0; \vec{r}) \) and exchange correlation potential \( V_{xc}[\rho_0; \vec{r}] \). \( \rho_0(\vec{r}) \) is the unperturbed ground-state density, given by the sum of the squares of the \( N \) lowest lying eigenfunctions of the Kohn-Sham equation

\[
[\hat{T} + V_0(\vec{r}) + V_H[\rho_0; \vec{r}] + V_{xc}[\rho_0; \vec{r}]]\phi_i(\vec{r}) = \epsilon_i \phi_i(\vec{r}).
\]

The time dependence of these orbitals is given by \( \phi_i(\vec{r}, t) = \phi_i(\vec{r}) \exp[-i \epsilon_i t] \), and they satisfy the time-dependent equation
\[ i \frac{\partial}{\partial t} - \hat{T} - V_0(\vec{r}) - V_H[\rho_0; \vec{r}] - V_{xc}[\rho_0; \vec{r}] \phi_i(\vec{r}, t) = 0. \]  
\hspace{1cm} (20)

The system is now perturbed by a uniform time-dependent electric field \( \vec{E}(t) \): the center of mass moves according to eq. (1) and the harmonic potential theorem says that the density must evolve according to eq. (2). Our task is to show that in fact \( \rho(\vec{r}, t) = \rho_0(\vec{r} - \vec{R}_{CM}(t)) \) is a self-consistent solution of the time-dependent Kohn-Sham equation in the presence of the driving electric field:

\[ i \frac{\partial}{\partial t} - \hat{T} - V_0(\vec{r}) - V_H[\rho; \vec{r}; t] - V_{xc}[\rho; \vec{r}; t] - e\vec{E}(t) \cdot \vec{r} \phi_i^E(\vec{r}, t) = 0 \]  
\hspace{1cm} (21)

To prove this fact, we observe that the Kohn-Sham equation, in the presence of the driving field, eq. (21), can be generated starting from the Kohn-Sham equation without the driving field, eq. (20), simply by applying to the latter a transformation to an accelerated frame of reference with \( \vec{x}(t) = -\vec{R}_{CM}(t) \) where \( \vec{R}_{CM}(t) \) is the solution of the equation of motion (1). In fact, using eq. (35) of the Appendix, it is easy to prove that the transformed wave functions \( \phi'_i(\vec{r}, t) = \hat{U}\phi_i(\vec{r}, t) \) satisfy the equation

\[ i \frac{\partial}{\partial t} - \hat{T} - V_0(\vec{r} - \vec{R}_{CM}(t)) - V_H[\rho_0; \vec{r} - \vec{R}_{CM}(t)] - V_{xc}[\rho_0; \vec{r} - \vec{R}_{CM}(t)] \\
+ m\vec{a}_{CM}(t) \cdot \vec{r} + \frac{e}{c} (\vec{v}_{CM}(t) \times \vec{B}) \cdot \vec{r} + \frac{mv_{CM}^2(t)}{2} + \frac{e}{2c}(\vec{B} \times \vec{R}_{CM}(t)) \cdot \vec{v}_{CM}(t) ] \phi'_i(\vec{r}, t) = 0 \]  
\hspace{1cm} (22)

Now, we substitute the harmonic potential form for

\[ V_0(\vec{r} - \vec{R}_{CM}) = V_0(\vec{r}) - \vec{R}_{CM} \cdot \vec{K} \cdot \vec{r} + \frac{1}{2} \vec{R}_{CM} \cdot \vec{K} \cdot \vec{R}_{CM}, \]  
\hspace{1cm} (23)

and we use the transformation of the Hartree and exchange-correlation potentials \( V_{xc}[\rho_0; \vec{r} - \vec{R}_{CM}] = V_{xc}[\rho; \vec{r}] \). Using the equation of motion essentially equivalent to the Kohn-Sham equation (21) in the presence of the driving field. The only difference is a time dependent additive term in the potential which can be eliminated by further multiplying each wavefunction by the phase factor \( exp[iS(t)] \) where

\[ S(t) = \int_{t_0}^{t_1} \left[ \frac{m}{2} v_{CM}^2(t) - \frac{1}{2} \vec{R}_{CM}(t) \cdot \vec{K} \cdot \vec{R}_{CM}(t) + \frac{e}{c} \vec{A}(\vec{R}_{CM}(t)) \cdot \vec{v}_{CM}(t) \right] dt \]  
\hspace{1cm} (24)
is the classical action for the motion of the center of mass. Since the new orbitals \( \phi'_i \) (with the additional phase factor incorporated) yield the density \( \rho_0(\vec{r} - \vec{R}_{CM}(t)) \) and satisfy the time-dependent Kohn-Sham equation, in the presence of the driving field, with Hartree and exchange-correlation potentials evaluated at that same density, we conclude that they are the self-consistent solution of the driven Kohn Sham equation. Any approximation for \( V_{xc} \) that satisfies eq. (18) will automatically satisfy the HPT.

Consider the adiabatic local density approximation [5]. The action functional in this approximation has the form

\[
A_{xc}[\rho(\vec{r},t)] = -\int_{t_0}^{t_1} dt \int d\vec{r} \epsilon_{xc}(\rho(\vec{r}),t) \tag{25}
\]

where \( \epsilon_{xc}(\rho) \) is the exchange-correlation energy density of the uniform electron gas of density \( \rho \). This expression is manifestly invariant under the transformation \( \rho \rightarrow \rho' \) since the latter amounts to a simple change of variable in the space part of the integral. Therefore, eq.

On the other hand, consider the linear response theory of Gross and Kohn [2] for \( V_{xc} \). It has the form

\[
V_{xc}[\rho;\vec{r},t] = V_{xc}^{LDA}[\rho_0(\vec{r});\vec{r}] + \int_{t_0}^{t_1} f_{xc}[\rho_0(\vec{r});t-t'] \delta \rho(\vec{r},t') dt' \tag{26}
\]

where it is assumed that the density \( \rho(\vec{r},t) = \rho_0(\vec{r}) + \delta \rho(\vec{r},t) \) deviates only slightly from the static equilibrium density. \( V_{xc}^{LDA}[\rho_0(\vec{r});\vec{r}] \) is the usual local density approximation for the static density \( \rho_0 \). Notice that the kernel \( f_{xc} \) is a function of a time difference, but only one position (i.e. we have locality in space but not in time). In the case of harmonically confined electrons we know from eq. (2) that \( \delta \rho(\vec{r},t) = -\vec{R}_{CM}(t) \cdot \vec{\nabla} \rho_0(\vec{r}) \) if \( \vec{R}_{CM}(t) \) is small. On the other hand, from eq. (18), we know that \( V_{xc}[\rho;\vec{r},t] = V_{xc}[\rho_0,\vec{r} - \vec{R}_{CM}(t)] \sim V_{xc}[\rho_0,\vec{r}] - \vec{R}_{CM}(t) \cdot \vec{\nabla} V_{xc}[\rho_0,\vec{r}], \) and \( V_{xc}[\rho_0,\vec{r}] = V_{xc}^{LDA}[\rho_0,\vec{r}] \). Substituting this in eq. (26) we see that the integral on the right hand side must equal \( \vec{\nabla} V_{xc}^{LDA}[\rho_0,\vec{r}] \cdot \vec{R}_{CM}(t) \). Because this must be true for an arbitrary (small) driven motion of \( \vec{R}_{CM}(t) \) we see that the only admissible time dependence of \( f_{xc}(t-t') \) is proportional to a \( \delta \) function of \( t-t' \), i.e. the only admissible approximation in this class must be local in time as well as in space. Since
the Gross-Kohn potential is non-local in time, it violates eq. (18) and therefore also the harmonic potential theorem.

How can one make sure that approximate forms of the exchange-correlation potential satisfy eq. (18)? A general way is to start from an action that depends only on the “relative density” defined as follows. For a given density \( \rho \) we construct the position of the center of mass, and then we refer \( \rho \) to an accelerated frame in which the center of mass is at rest. The so defined density

\[
\rho_{\text{rel}}(\vec{r}, t) = \rho(\vec{r} + \vec{R}_{\text{CM}}(t), t)
\]  

(27)
is what we call the relative density. By construction, it is invariant with respect to transformation to an arbitrary accelerated frame of reference. Therefore, if the action functional is written as a functional of the relative density \( A_{\text{xc}}[\rho(\vec{r}, t)] = \tilde{A}_{\text{xc}}[\rho_{\text{rel}}(\vec{r}, t)] \) it will automatically satisfy the symmetry embodied by eq. (15). The exchange-correlation potential will then be given by

\[
V_{\text{xc}}[\rho; \vec{r}, t] = \frac{\delta \tilde{A}_{\text{xc}}[\rho_{\text{rel}}]}{\delta \rho_{\text{rel}}}(\vec{r} - \vec{R}_{\text{CM}}(t), t).
\]  

(28)

An example of application of this method is the procedure proposed by Dobson [6] to go beyond the adiabatic linearized LDA without violating the HPT. The idea is to divide the density variation into two parts: one corresponding to a rigid shift of the center of mass, the other including the remaining internal deformations. The Gross-Kohn frequency dependent kernel is applied only to the relative density variation, while the center of mass variation is still treated in the ordinary ATLDA.

In the language of this paper, this idea corresponds to the following procedure. Write the relative density as \( \rho_{\text{rel}}(\vec{r}, t) = \rho_0(\vec{r}) + \delta \rho_{\text{rel}}(\vec{r}, t) \), where \( \rho_0(\vec{r}) \) coincides with the absolute initial density, because the center of mass is initially at the origin of the absolute coordinates. Of course, the correction \( \delta \rho_{\text{rel}} \) vanishes in the case of uniformly driven harmonically confined system, but it need not vanish in more general cases (for example, in a non-uniformly driven harmonic system). Approximate the action functional as
\[ \bar{A}_{xc}[\rho_{\text{rel}}(\vec{r}, t)] = -\int_{t_0}^{t_1} dt \int d\vec{r} \epsilon_{xc}(\rho_0(\vec{r})) + \frac{1}{2} \int_{t_0}^{t_1} dt \int_{t_0}^{t_1} dt' \int d\vec{r} f_{xc}[\rho_0(\vec{r}); t - t'] \delta \rho_{\text{rel}}(\vec{r}, t) \delta \rho_{\text{rel}}(\vec{r}, t'), \]  

(29)

where \( f_{xc}[\rho_0, t - t'] \) is the Gross-Kohn exchange-correlation kernel. The exchange-correlation potential is then constructed by taking the functional derivative of \( \bar{a}_{xc} \) with respect to \( \rho_{\text{rel}}(\vec{r}, t) \), and translating the position vector from \( \vec{r} \) to \( \vec{r} - \vec{R}_{CM}(t) \), as indicated by eq. (28). \( \vec{R}_{CM}(t) \) itself must be determined self-consistently from the knowledge of the full density, according to eq.

We note, in closing, that all our result could be easily generalized to the case of a uniform time-dependent magnetic field. The HPT generalizes to this case. The only difference is the appearance of the additional electric field \( (e/2c) d\vec{B}(t)/dt \times \vec{x}(t) \) in eq. (8).

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**Appendix - Proof of eqs. (6) and (7)**

We start from the Schroedinger equation eq. (3) for \( \psi \) and apply to it the unitary transformation \( \hat{U}(t) \) defined in eq. in the following manner

\[ \hat{U}(t) \left( i \frac{\partial}{\partial t} - \hat{H}_0 - \hat{V}(t) \right) \hat{U}^{-1}(t) \hat{U}(t) |\psi(t)\rangle = 0 \]  

(30)

We then observe that

\[ \hat{U}(t) i \frac{\partial}{\partial t} \hat{U}^{-1}(t) = i \frac{\partial}{\partial t} - [m \vec{a}(t) + \frac{e}{2c} (\vec{v}(t) \times \vec{B})] \cdot \sum_{i=1}^{N} \vec{r}_i \]

\[ + \sum_{i=1}^{N} \vec{p}_i \cdot \vec{v}(t) + Nmv^2(t) - \frac{e}{2c} (\vec{v}(t) \times \vec{B}) \cdot \vec{x}(t), \]  

(31)

and

\[ \hat{U}(t) \vec{r}_i \hat{U}^{-1}(t) = \vec{r}_i + \vec{x}(t) \]

(32)

\[ \hat{U}(t) \vec{p}_i \hat{U}^{-1}(t) = \vec{p}_i + \vec{m} \vec{v}(t) - \frac{e}{2c} \vec{B} \times \vec{x}(t) \]  

(33)
The density associated with the wavefunction \( \psi' = \hat{U}(t)\psi \) clearly is \( \rho' \). Furthermore

\[
\hat{U}(t)\hat{H}_0 + \hat{V}\hat{U}^{-1}(t) = \hat{H}_0 + \sum_{i=1}^{N} V(\vec{r}_i + \vec{x}(t), t) + N\frac{mv^2(t)}{2} + \sum_{i=1}^{N} \vec{p}_i \cdot \vec{v}(t) + \frac{e}{2c} \sum_{i=1}^{N} \vec{r}_i \cdot (\vec{v}(t) \times \vec{B})
\]

Therefore, the transformed Schroedinger equation has the form

\[
\left[ i\frac{\partial}{\partial t} - \hat{H}_0 - \sum_{i=1}^{N} V(\vec{r}_i + \vec{x}(t), t) - m\vec{a}(t) \cdot \sum_{i=1}^{N} \vec{r}_i \\
- \frac{e}{c} \sum_{i=1}^{N} \vec{r}_i \cdot (\vec{v}(t) \times \vec{B}) + N\frac{mv^2}{2} + \frac{e}{2c} (\vec{B} \times \vec{x}(t)) \cdot \vec{v}(t) \right] |\psi'(t)\rangle = 0
\]

This can be seen as the time evolution of the wavefunction in the presence of a transformed time-dependent potential given by eq. (6) apart from an additive time dependent constant. This completes the proof of eqs. (6) and (7).
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