of which the system is constituted.[10]

That such a description is possible is guaranteed by the very same theorems that lie at the foundation of TDDFT and TDCDFT.[11,12] Indeed, consider a system of particles of mass m described by the time-dependent hamiltonian

$$\hat{H}(t) = \hat{H}_0 + \int d\mathbf{r}\,\hat{n}(\mathbf{r})V_1(\mathbf{r}, t) \tag{1}$$

where

$$\hat{H}_0 = \hat{T} + \hat{W} + \hat{V}_0 \tag{2}$$

is the sum of kinetic energy ($\hat{T}$), interaction potential energy ($\hat{W}$), and the energy associated with an external *static* potential $V_0(\mathbf{r})$,

$$\hat{V}_0 = \int d\mathbf{r}\,V_0(\mathbf{r})\hat{n}(\mathbf{r}), \tag{3}$$

where $\hat{n}(\mathbf{r})$ is the particle density operator. $V_1(\mathbf{r}, t)$ is an external time-dependent potential.

The exact Heisenberg equations of motion for the density and the current density operators, averaged over the quantum state, lead to equations of motion for the average particle density $n(\mathbf{r}, t)$ and the average particle current density $\mathbf{j}(\mathbf{r}, t)$:

$$\partial_t n(\mathbf{r}, t) = -\partial_\mu j_\mu(\mathbf{r}, t) \tag{4}$$

and

$$m\partial_t j_\mu(\mathbf{r}, t) = -\ n(\mathbf{r}, t)\partial_\mu[V_0(\mathbf{r}) + V_1(\mathbf{r}, t)]$$
$$-\ \partial_\nu P_{\mu\nu}(\mathbf{r}, t), \tag{5}$$

where ∂_t denotes the partial derivative with respect to time and ∂_ν is a short-hand for the derivative with respect to the cartesian component ν of the position vector $\mathbf{r}$. Here and in the following we adopt the convention that repeated indices are summed over. These equations simply express the local conservation of particle number (Eq. (4)) and momentum (Eq. (5)). The key quantity on the right hand side of Eq. (5) is the *stress tensor $P_{\mu\nu}(\mathbf{r}, t)$* – a symmetric tensor which will be defined in the next section as the expectation value of a hermitian operator, and whose divergence with respect to one of the indices yields the *force density* arising from internal quantum-kinetic and interaction effects.

Now the Runge-Gross theorem of TDDFT guarantees that the stress tensor, like every other observable of the system, is a functional of the current density and of the initial quantum state. Thus, Eq. (5) is in principle a closed equation of motion for $\mathbf{j}$ – the only missing piece of information being the *explicit* expression for $P_{\mu\nu}$ in terms of the current density.

In recent years much effort has been devoted to constructing an approximate QCM[13–21] and several applications have appeared in the literature (see Ref. 22 for some representative examples). All approximation schemes so far have been based on the local density approximation

and generalizations thereof. The objective of this paper is to derive and discuss an approximate expression for $P_{\mu\nu}(\mathbf{r}, t)$, and, more importantly, for the associated force density $-\partial_\nu P_{\mu\nu}(\mathbf{r}, t)$, as functionals of the current density and the initial state. We will do this in the *linear response regime*, i.e. for systems that start from the ground-state of the static hamiltonian $\hat{H}_0$ and perform small-amplitude oscillations about it. The external potential $V_1(\mathbf{r}, t)$ will be treated as a small perturbation. In this regime the equations of motion (4) and (5) are conveniently expressed in terms of the displacement field $\mathbf{u}(\mathbf{r}, t)$, defined by the relation

$$\mathbf{j}(\mathbf{r}, t) = n_0(\mathbf{r})\partial_t \mathbf{u}(\mathbf{r}, t), \tag{6}$$

where $n_0(\mathbf{r})$ is the ground-state density. It is also convenient to write the density and the stress tensor as sums of a large ground-state component and a small time-dependent part, in the following manner

$$n(\mathbf{r}, t) = n_0(\mathbf{r}) + n_1(\mathbf{r}, t),$$
$$P_{\mu\nu}(\mathbf{r}, t) = P_{\mu\nu,0}(\mathbf{r}) + P_{\mu\nu,1}(\mathbf{r}, t), \tag{7}$$

where the equilibrium components, marked by the subscript 0, satisfy the equilibrium condition

$$n_0(\mathbf{r})\partial_\mu V_0(\mathbf{r}) + \partial_\nu P_{\mu\nu,0}(\mathbf{r}) = 0. \tag{8}$$

Then the two equations (4) and (5) take the form

$$n_1(\mathbf{r}, t) = -\partial_\mu[n_0(\mathbf{r})u_\mu(\mathbf{r}, t)], \tag{9}$$

and

$$mn_0(\mathbf{r})\partial_t^2 u_\mu(\mathbf{r}, t) = -n_0(\mathbf{r})\partial_\mu V_1(\mathbf{r}, t)$$
$$-n_1(\mathbf{r}, t)\partial_\mu V_0(\mathbf{r}) - \partial_\nu P_{\mu\nu,1}(\mathbf{r}, t). \tag{10}$$

Our task is to find an expression for the force density $\partial_\nu P_{\mu\nu,1}(\mathbf{r}, t)$ as a linear functional of $\mathbf{u}(\mathbf{r}, t)$. If this can be achieved, then the excitation energies of the system will be obtained from the frequencies of the time-periodic solutions of Eq. (10) in the absence of external field (i.e., with $V_1 = 0$).

It is easy to see that the spatial dependence of these solutions will be proportional to the matrix element of the current density operator between the ground-state and the excited state in question. This is because, in a many-body system with stationary states $|\psi_0\rangle, |\psi_1\rangle, ..., |\psi_n\rangle, ...$ ($|\psi_0\rangle$ is the ground-state), and corresponding energies $E_0, E_1, ..., E_n...$, the n-th linear excitation is described by the time-dependent state

$$|\psi_0\rangle e^{-iE_0 t} + \varepsilon|\psi_n\rangle e^{-iE_n t}, \tag{11}$$

where ε is an arbitrarily small "mixing parameter". The expectation value of the current density operator in this state is

$$\mathbf{j}(\mathbf{r}, t) = \varepsilon\langle\psi_0|\hat{\mathbf{j}}(\mathbf{r})|\psi_n\rangle e^{-i(E_n - E_0)t} + c.c. \tag{12}$$