Time-dependent quantum transport: An exact formulation based on TDDFT

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(received 30 January 2004; accepted in final form 29 April 2004)

PACS. 05.60.Gg – Quantum transport.
PACS. 72.10.Bg – General formulation of transport theory.
PACS. 85.30.Mn – Junction breakdown and tunneling devices (including resonance tunneling devices).

Abstract. – An exact theoretical framework based on Time Dependent Density Functional Theory (TDDFT) is proposed in order to deal with the time-dependent quantum transport in fully interacting systems. We use a partition-free approach by Cini in which the whole system is in equilibrium before an external electric field is switched on. Our theory includes the interactions between the leads and between the leads and the device. It is well suited for calculating measurable transient phenomena as well as a.c. and other time-dependent responses. We show that the steady-state current results from a dephasing mechanism provided the leads are macroscopic and the device is finite. In the d.c. case, we obtain a Landauer-like formula when the effective potential of TDDFT is uniform deep inside the electrodes.

Introduction. – During the last decade, the experimental progress in the fabrication/manipulation of nano-systems like quantum wires and dots has enhanced the interest in the theory of quantum transport. The Landauer-Büttiker formalism [1,2] applies to noninteracting systems and gives the steady-state current of macroscopic electrodes connected via mesoscopic (or nanoscopic) constrictions. Techniques based on nonequilibrium Green functions [3, 4] provide a natural framework for obtaining the Landauer formula starting from a microscopic theory. The first attempt was made by Caroli et al. [5, 6] who consider the two leads as isolated subsystems with different chemical potentials in the remote past. The current will flow through the system once the contacts between the device and the leads have been established, see fig. 1(a). This approach is based on a fictitious partitioning since in a real experiment the whole system is in thermodynamic equilibrium before an external bias is applied deep inside the electrodes. Later on this partitioned scheme was adopted by Meir and Wingreen [7] to obtain the steady-state current through an interacting central device. Shortly after, Wingreen et al. [8–10] generalised the Meir-Wingreen formula to time-dependent phenomena.

Despite the important results mentioned above, the partitioned scheme has several drawbacks. First, it is difficult to include the interactions between the leads and between the leads and the device. These interactions are responsible for the establishing of dipole layers and
Fig. 1 – (a) Schematic representation of the partitioned approach by Caroli et al. On the left, the electrodes are disconnected and in thermodynamic equilibrium at two different chemical potentials. On the right, the contacts are established and electrons start to flow. (b) Schematic representation of the partition-free approach by Cini. The whole system is in thermodynamic equilibrium and it is characterised by a unique chemical potential. Then, a bias is applied deep inside the electrodes.

charge transfers which shape the potential landscape in the device region and influence the contacts. Second, there is a crucial assumption of equivalence between the long-time behaviour of 1) the initially partitioned and biased system once the coupling between the subsystems is switched on and 2) the whole partition-free system once the bias is applied. Third, there is no well-defined prescription which fixes the initial equilibrium distribution of the isolated central device; this makes the transient current difficult to interpret.

A conceptually different approach from the one by Caroli et al. has been introduced by Cini [11], see fig. 1(b). Here, the system is contacted and in thermodynamic equilibrium before an external time-dependent disturbance is switched on. Cini developed the general theory for the case of free electrons with his focus on semiconductor junction devices. In this letter we extend the Cini theory to fully interacting (electrodes and device) systems. Our exact theoretical framework is based on Time Dependent Density Functional Theory (TDDFT) and is well suited to describe the steady state as well as a.c. and other time-dependent current responses.

General formulation. – To be specific, let us focus on the Coulomb interaction and on paramagnetic systems. In the case we only ask for the time-dependent density \( n(r, t) \) the original Density Functional Theory [12,13] and its finite-temperature generalisation [14] have been extended to time-dependent phenomena [15,16]. This theory applies only to those cases where the external disturbance is local in space, \( \int d^3r \ U(r, t)n(r, t) \). Runge and Gross [15] have shown that one can compute \( n(r, t) \) in a one-particle manner using an effective potential

\[
U_{\text{eff}}(r, t) = U_C(r, t) + v_{\text{xc}}(r, t).
\]

Here, \( U_C = U + V_H + V_n \) is the classical electrostatic potential and it is given by the sum of the external potential \( U \), the Hartree potential \( V_H \) and the Coulomb potential from the nuclei \( V_n \). Furthermore, \( v_{\text{xc}} \) accounts for exchange and correlations and is obtained from an exchange-correlation action functional, \( v_{\text{xc}}(r, t) = \delta A_{\text{xc}}[n]/\delta n(r, t) \) (as pointed out in ref. [17], the
causality and symmetry properties require that the action functional $A_{xc}[n]$ is defined on the Keldysh contour. Thus, the effective one-body Hamiltonian reads $\mathcal{H}_{\text{eff}}(t) = \int d\mathbf{r} \left[ \left(-\frac{\hbar^2}{2m} \right) + U_{\text{eff}}(\mathbf{r}, t) \right]$. Here and in what follows, we use boldface for operators in one-particle Hilbert space, and $n$ is 1 in our units.

It is convenient to define the projectors $P_\alpha = \int_\alpha d\mathbf{r} |\mathbf{r}\rangle \langle \mathbf{r}|$ onto the left or right leads ($\alpha = L, R$) or the central device ($\alpha = D$) and to introduce the notation $\mathcal{O}_{\alpha\beta} = P_\alpha \mathcal{O} P_\beta$, where $\mathcal{O}$ is an arbitrary operator in one-body space [18]. The one-particle scheme of Time Dependent Density Functional Theory (TDDFT) corresponds to a fictitious Green function $\mathcal{G}(t; t')$ which satisfies a one-particle equation of motion,

$$\left\{ i \frac{d}{dt} - \mathcal{E}(t) - V \right\} \mathcal{G}(t; t') = \delta(t - t'). \tag{1}$$

In eq. (1) $\mathcal{E} = \mathcal{H}_{\text{eff}}^{LL} + \mathcal{H}_{\text{eff}}^{DD} + \mathcal{H}_{\text{eff}}^{RR}$ is the uncontacted one-body Hamiltonian of TDDFT while $V = \mathcal{H}_{\text{eff}} - \mathcal{E}$ accounts for the contacting part. The fictitious $\mathcal{G}$ will not in general give correct one-particle properties. However, by definition, $\mathcal{G}^< \equiv n(\mathbf{r}, t) = -2ie\langle \mathbf{r}\rangle |\mathcal{G}^<(t; t')|\mathbf{r}\rangle$

(where the factor of 2 comes from spin). Also total currents are correctly given by TDDFT. If, for instance, $J_{\alpha}$ is the total current from a particular region $\alpha$ we have

$$J_{\alpha}(t) = -e \int_\alpha d\mathbf{r} \frac{d}{dt} n(\mathbf{r}, t), \tag{2}$$

where the space integral extends over the region $\alpha$ ($e$ is the electron charge). The TDDFT gives the exact density, and from eq. (2) we see that it also gives the exact longitudinal current density and total current from subregions.

Since $V_{LR} = V_{RL} = 0$, from eqs. (1) and (2) the current from the $\alpha = L, R$ electrode to the central region can be written as

$$J_{\alpha}(t) = 2e \Re \left[ \operatorname{tr} \left\{ \mathcal{G}^<(t; t)V_{\alpha D} \right\} \right], \quad \alpha = L, R. \tag{3}$$

Without loss of generality, we may assume that the partition-free system is in equilibrium when $t \leq 0$, i.e., $\mathcal{E}(t \leq 0) \equiv \mathcal{E}^0$. For the noninteracting system of TDDFT everything is known once we know how to propagate the one-electron orbitals in time and how they are populated before the system is perturbed. The time evolution is fully described by the retarded or advanced Green functions $\mathcal{G}^{R,A}$, and the initial population at zero time, i.e., by $\mathcal{G}^<(0, 0) = if(\mathcal{E}^0 + V)$, where $f$ is the Fermi distribution function (since $\mathcal{E}^0 + V$ is a matrix, so is $f(\mathcal{E}^0 + V)$). Then, for any $t, t' > 0$ we have [11,19,20]

$$\mathcal{G}^<(t, t') = \mathcal{G}^R(t, 0)\mathcal{G}^<(0, 0)\mathcal{G}^A(0, t') = i \mathcal{G}^R(t, 0)f(\mathcal{E}^0 + V)\mathcal{G}^A(0, t'), \tag{4}$$

and the total time-dependent current can be rewritten as

$$J_{\alpha}(t) = -2e \Im \left[ \operatorname{tr} \left\{ \mathcal{G}^R(t, 0)f(\mathcal{E}^0 + V)\mathcal{G}^A(0, t)V_{\alpha D} \right\} \right]. \tag{5}$$

The above equation is an exact result. For noninteracting electrons, eq. (4) agrees with the formula obtained by Cini [11] in the partition-free scheme. Indeed, the derivation by Cini does not depend on the details of the noninteracting system and therefore it is also correct for the Kohn-Sham system, which however has the extra merit of reproducing the exact density.
The advantage of this approach is that the interaction in the leads and in the conductor are treated on the same footing via self-consistent calculations on the current-carrying system. It also allows for detailed studies of how the contacts influence the conductance properties. We note in passing that eq. (4) is also gauge invariant since it does not change under an overall time-dependent shift of the external potential which is constant in space. Neither is it modified by a simultaneous shift of the classical electrostatic potential and $\mu$ for $t < 0$.

**Asymptotic current.** Once the effective potential of TDDFT is known, the problem is reduced to a fictitious one-particle problem. For any such one-particle problem we now show that the partitioned scheme by Caroli et al. and the partition-free scheme are equivalent in the long-time limit. To this end, we consider the Dyson equation that relates a noninteracting system contacted all the time (Green function $G$) to the corresponding uncontacted one (Green function $g$). Both systems are exposed to the same, possibly time-dependent, potential for $t > 0$. As is well known, the noninteracting Green function $g$ can be expressed in terms of the one-body evolution operator $S(t)$ which fulfills $iS'(t) = E(t)S(t)$ and $S(0) = 1$. The retarded and advanced components are $g^R_A(t; t' = \pm t') = \pm i\Theta(\pm t \mp t')S(t)S^\dagger(t')$. Since also the uncontacted system is initially in equilibrium, we have $g^\gamma(t; t') = ig^R(0; t)G^\gamma(0; t')$ (cf. eq. (3)).

The two schemes are equivalent if

$$\lim_{t \to \infty} \Sigma^R_\alpha(t; t') = \lim_{t \to \infty} \Sigma^A_\alpha(t' ; t) = 0$$

for any nonsingular $V$. Indeed, from the equation of motion (1) and eq. (5) one can verify that the projected Green functions satisfy

$$\lim_{t \to \infty} G^R_{DD}(t; t') = \lim_{t \to \infty} G^A_{DD}(t' ; t)V_{\alpha\delta} = 0.$$  

Making use of the above relations, one finds [20] that the asymptotic ($t \to \infty$) time-dependent current of eq. (4) becomes

$$J_\alpha(t) = -2e \Im \left[ \text{tr} \left\{ G^R(t, 0) F(0, t) G^A(0, t) V_{\alpha\delta} \right\} \right].$$

Thus, the long-time limit washes out the initial effect induced by the conducting term $V$. Moreover, due to eq. (6), the asymptotic current is independent of the initial equilibrium distribution of the central device. Expressing $G^R_{D\beta}$ and $G^A_{\beta\alpha}$ in terms of $G^R_{DD}$ and $G^A_{DD}$, respectively, eq. (7) can be rewritten in a more familiar form,

$$J_\alpha(t) = 2e \int d\bar{t} \Re \left[ \text{tr} \left\{ G^R_{DD}(t, \bar{t}) \Sigma^R_\alpha(\bar{t}, t) + G^A_{DD}(\bar{t}, t) \Sigma^A_\alpha(\bar{t}, t) \right\} \right],$$

where the asymptotic relation $(t, t' \to \infty)$ $G^R_{DD}(t; t') = \int d\bar{t} d\bar{t}' G^R_{DD}(t, \bar{t})G^R_{DD}(\bar{t}, \bar{t}')G^R_{DD}(\bar{t}', t')$ has been used. Equation (8) is valid for interacting devices connected to interacting electrodes. It provides a useful framework for studying the transport in interacting systems from first principles. Our results can be applied both to the case of a constant (d.c.) bias as well as to the case of a time-dependent (e.g., a.c.) one.
To summarise, if the retarded/advanced self-energy satisfies eq. (5), the exact formula in eq. (4) reduces to eq. (8) in the long-time limit. For noninteracting electrons the Green function $\mathbf{G}$ of TDDFT coincides with the Green function of the real system and eq. (8) agrees with the formula by Wingreen et al. [8,9].

**Steady state.** Next, we wish to investigate the steady state, i.e., $\lim_{t \to -\infty} \mathbf{E}(t) = \mathbf{E}^\infty = \text{const}$. In this case, it must exist a unitary operator $\mathbf{S}$ such that $\lim_{t \to -\infty} \mathbf{S}(t) = e^{-i\mathbf{E}^\infty t} \mathbf{S}$. Then, in terms of diagonalising one-body states $|\phi_{m\alpha}^\infty\rangle$ of $\mathbf{E}_{\alpha\alpha}$ with eigenvalues $\epsilon_{m\alpha}^\infty$ we have

$$
\Sigma^\infty_\alpha(t; t') = i \sum_{m, m'} e^{-i(\epsilon_{m\alpha}^\infty - \epsilon_{m'\alpha}^\infty) t'} \mathbf{V}_{D\alpha} |\phi_{m\alpha}^\infty\rangle \langle \phi_{m\alpha}^\infty | f(\mathbf{E}) |\phi_{m'\alpha}^\infty\rangle \langle \phi_{m'\alpha}^\infty | \mathbf{V}_{A\alpha},
$$

where $\mathbf{E}^0 = \mathbf{S} \mathbf{E}_0^0 \mathbf{S}^\dagger$. For $t, t' \to \infty$, the left and right contraction with a nonsingular $\mathbf{V}$ causes a perfect destructive interference for states with $|\epsilon_{m\alpha}^\infty - \epsilon_{m'\alpha}^\infty| \gtrsim 1/(t + t')$ and hence the restoration of translational invariance in time

$$
\Sigma^\infty_\alpha(t; t') = i \sum_m f_{m\alpha} \Gamma_{m\alpha} e^{-i\epsilon_{m\alpha}^\infty (t - t')} ,
$$

where $f_{m\alpha} = \langle \phi_{m\alpha}^\infty | f(\mathbf{E}) |\phi_{m\alpha}^\infty\rangle$ while $\Gamma_{m\alpha} = \mathbf{V}_{D\alpha} |\phi_{m\alpha}^\infty\rangle \langle \phi_{m\alpha}^\infty | \mathbf{V}_{A\alpha}$ [21]. The above *dephasing mechanism* is the key ingredient in the developing of a steady state. Substituting eq. (9) into eq. (8), we get the steady-state current

$$
J_\alpha = -2e \sum_{m\beta} f_{m\beta} \delta_{\alpha\beta} \text{tr} \left\{ \Gamma_{m\alpha} \Im \left[ \mathbf{G}^R_{DD}(\epsilon_{m\alpha}^\infty) \right] \right\} +
$$

\begin{equation}
+ \text{tr} \left\{ \mathbf{G}^R_{DD}(\epsilon_{m\beta}^\infty) \Gamma_{m\beta} \mathbf{G}^A_{DD}(\epsilon_{m\beta}^\infty) \Im \left[ \Sigma^A_\alpha(\epsilon_{m\beta}^\infty) \right] \right\}
\end{equation}

with $\mathbf{G}^R_{DD}(\epsilon) = [\epsilon - \mathbf{E}^\infty_{DD} - \Sigma^R_{DD}(\epsilon)]^{-1}$. Using the equalities $\Im \left[ \mathbf{G}^R_{DD} \right] = [\mathbf{G}_{DD}^R - \mathbf{G}_{DD}^A]/2i$ and $\mathbf{G}_{DD}^A - \mathbf{G}_{DD}^R = [\mathbf{G}_{DD}^R - \mathbf{G}_{DD}^A]$ together with

$$
[\mathbf{G}^R_{DD}(\epsilon) - \mathbf{G}^A_{DD}(\epsilon)] = -2\pi i \sum_{m\alpha} \delta(\epsilon - \epsilon_{m\alpha}^\infty) \mathbf{G}^R_{DD}(\epsilon_{m\alpha}^\infty) \Gamma_{m\alpha} \mathbf{G}^A_{DD}(\epsilon_{m\alpha}^\infty)
$$

and $\Im \left[ \Sigma^A_\alpha(\epsilon) \right] = \pi \sum_m \delta(\epsilon - \epsilon_{m\alpha}^\infty) \Gamma_{m\alpha}$, the steady-state current in eq. (10) can be rewritten in a Landauer-like form

$$
J_R = -e \sum_m [f_{mL} T_{mL} - f_{mR} T_{mR}] = -J_L.
$$

In the above formula, $T_{mR} = \sum_n T_{mL}^{nR}$ and $T_{mL} = \sum_n T_{mL}^{nR}$ are the TDDFT transmission coefficients expressed in terms of the quantities

$$
T_{m\alpha}^{n\beta} = 2\pi \delta(\epsilon_{m\alpha}^\infty - \epsilon_{n\beta}^\infty) \text{tr} \left\{ \mathbf{G}^R_{DD}(\epsilon_{m\alpha}^\infty) \Gamma_{m\alpha} \mathbf{G}^A_{DD}(\epsilon_{n\beta}^\infty) \Gamma_{n\beta} \right\} = T_{m\beta}^{n\alpha} .
$$

Despite the formal analogy with the Landauer formula, eq. (11) contains an important conceptual difference since $f_{m\alpha}$ is not simply given by the Fermi distribution function. For example, if the induced change in effective potential varies widely in space deep inside the electrodes, the band structure $\mathbf{E}^0_{\alpha\alpha}$ may be completely different from that of $\mathbf{E}_{\alpha\alpha}^\infty$. However, if we asymptotically have equilibrium far away from the central region, as we would expect for leads with a macroscopic cross-section, the change in effective potential must be uniform. To leading order in $1/N$ we then have

$$
\mathbf{E}_{\alpha\alpha}(t) = \mathbf{E}_{\alpha\alpha}^0 + \Delta U_{\alpha\alpha}^\text{eff}(t),
$$

where $\Delta U_{\alpha\alpha}^\text{eff}(t)$ is the effective change in the potential due to dephasing.
and $E_{\alpha \alpha}^{\infty} = E_{\alpha \alpha}^0 + \Delta U_{\alpha \alpha}^{\text{eff}}$. Hence, except for corrections which are of lower order with respect to the system size, $E_{\alpha \alpha}^0 = E_{\alpha \alpha}^{\infty}$ and

$$f_{\alpha \sigma} = f\left(e_{\alpha \sigma}^{\infty} - \Delta U_{\alpha \alpha}^{\text{eff}}\right).$$

We emphasise that the steady-state current in eq. (11) comes out from a pure dephasing mechanism in the fictitious noninteracting problem. The damping effects from scatterings is described by $A_{\sigma \sigma}$ and $v_{\alpha \sigma}$. Furthermore, if eq. (12) holds, the current depends only on the asymptotic value of the effective potential, $U_{\alpha \alpha}^{\text{eff}}(r, t \to \infty)$. However, $U_{\alpha \alpha}^{\text{eff}}(r, t \to \infty)$ may depend on the history of the external bias $U$. Thus, the steady-state current of fully interacting systems may be history dependent. In the case of Time Dependent Local Density Approximation, the exchange-correlation potential $v_{\alpha \sigma}$ depends only locally on the instantaneous density and has no memory at all. If the density tends to a constant, so does the effective potential $U_{\alpha \alpha}^{\text{eff}}$, which again implies that the density tends to a constant. Owing to the nonlinearity of the problem, there might still be more than one steady-state solution or none at all.

The Landauer formulæ in eq. (11) correspond closely to the result obtained by Lang and coworkers [22, 23]. In their approach, the continuum is split into left- and right-going parts which are populated according to two different chemical potentials. The density is then calculated self-consistently. In our language this corresponds to writing the uncontacted $g^<(\varepsilon)$ as

$$g^<(\varepsilon) = 2\pi i \sum_{\alpha \sigma} f_{\alpha}(e_{\alpha \sigma}^{\infty}) \delta(\varepsilon - e_{\alpha \sigma}^{\infty}) |\phi_{\alpha \sigma}^{\infty}\rangle \langle \phi_{\alpha \sigma}^{\infty}|$$

in terms of Fermi functions $f_{\alpha}$ with chemical potential $\mu_{\alpha} = \mu + \Delta U_{\alpha \alpha}^{\text{eff}}$. The chemical potentials for the two leads differ, and the final result is independent of the chosen chemical potential for the device due to eq. (5). When we apply $1 + g^R V = g^R[g^R]^{-1}$ to an unperturbed state $|\phi_{\alpha \sigma}^{\infty}\rangle$, it is transformed to an interacting, i.e., contacted eigenstate $|\psi_{\alpha \sigma}^{\infty}\rangle$. Above the conductance threshold, states originating from the left lead become right-going scattering states, and states from the right lead become left-going scattering states. In addition, fully reflected waves and discrete states may arise which contribute to the density but not to the current. Thus,

$$g^<(\varepsilon) = [1 + g^R(\varepsilon)V] g^<(\varepsilon)[1 + V g^A(\varepsilon)] = 2\pi i \sum_{\alpha \sigma} f_{\alpha}(e_{\alpha \sigma}^{\infty}) \delta(\varepsilon - e_{\alpha \sigma}^{\infty}) |\psi_{\alpha \sigma}^{\infty}\rangle \langle \psi_{\alpha \sigma}^{\infty}|.$$

Lang et al. further approximate exchange and correlation by the LDA and the leads by homogeneous jellia, but apart from these approximations it is clear that their method implements TDDFT, as described above, in the steady state. It is also clear that the correctness of Lang’s approach relies on eq. (5) and eq. (12), as we have seen before. The equivalence between the scattering state approach by Lang et al. and the partitioned nonequilibrium approach used by Taylor et al. [24, 25] has also been shown by Brandbyge et al. [26].

Conclusions. – In conclusion, we have proposed a partition-free scheme based on TDDFT in order to treat the time-dependent current response of fully interacting systems. Our formally exact theory is more akin to the way the experiments are carried out and allows us to calculate the physical (i.e., measurable) dynamical current responses. Among the advantages we stress the possibility to include the interactions between the leads and between the leads and the device in a very natural way. We have shown that the steady state develops due to a dephasing mechanism without any reference to many-body damping and interactions. The damping mechanism (due to the electron-electron scatterings) of the real problem is described by $v_{\alpha \sigma}$. The steady-state current depends on the history only through the asymptotic shape of the effective TDDFT potential $U_{\alpha \alpha}^{\text{eff}}$, provided the bias-induced change $\Delta U_{\alpha \alpha}^{\text{eff}}$ is uniform.
deep inside the electrodes. (This is the anticipated behaviour for macroscopic electrodes.) In such systems, we have shown that the nonlinear steady-state current can be expressed in a Landauer-like formula in terms of fictitious transmission coefficients and one-particle energy eigenvalues. Our scheme is equally applicable to time-dependent responses. Clearly, its usefulness depends on the quality of the approximate TDDFT functionals being used. We are presently investigating how different approximations influence the current response in model systems.

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We would like to acknowledge useful discussions with U. von Barth, P. Bokes, M. Cini, R. Godby, A.-P. Jauho, B. I. Lundqvist, P. Hyldgaard, and B. Tobyszewsk. This work was supported by the RTN program of the European Union NANOPHASE (contract HPRN-CT-2000-00167).

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