Time-dependent i-DFT exchange-correlation potentials with memory: Applications to the out-of-equilibrium Anderson model

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We have recently put forward a steady-state density functional theory (i-DFT) to calculate the transport coefficients of quantum junctions. Within i-DFT it is possible to obtain the steady density on and the steady current through an interacting junction using a fictitious noninteracting junction subject to an effective gate and bias potential. In this work we extend i-DFT to the time domain for the single-impurity Anderson model. By a reverse engineering procedure we extract the exchange-correlation (xc) potential and xc bias at temperatures above the Kondo temperature $T_K$. The derivation is based on a generalization of a recent paper by Dittmann et al. [arXiv:1706.04547]. Interestingly the time-dependent (TD) i-DFT potentials depend on the system’s history only through the first time-derivative of the density. We perform numerical simulations of the early transient current and investigate the role of the history dependence. We also empirically extend the history-dependent TD i-DFT potentials to temperatures below $T_K$. For this purpose we use a recently proposed parametrization of the i-DFT potentials which yields highly accurate results in the steady state.

I. INTRODUCTION

The enormous success of density functional theory (DFT) in describing equilibrium properties of weakly correlated systems has triggered interest towards the development of DFT approximations to deal with strong electronic correlations. The extension of DFT to non-equilibrium situations has been put forward by Runge and Gross in a milestone paper from 1984. Time-dependent DFT (TDDFT) has been successfully applied to atoms, molecules and solids and, more recently, to strongly correlated systems like, e.g., Hubbard wires or nanoclusters using approximations borrowed from static DFT. These approximations have also been extended to nanoscale systems in contact with metallic leads to investigate transient currents and more generally transport coefficients.

The single impurity Anderson model (SIAM) is the simplest model exhibiting nontrivial strong correlations effects, namely the formation of the Kondo singlet at temperatures below the Kondo temperature $T_K$ and the Coulomb blockade (CB) phenomenon at temperatures lower than the charging energy (or on-site repulsion) $U$. Both effects leave clear fingerprints on the steady-state and time-dependent transport properties of the SIAM, and until a few years ago there were no suitable DFT approximations for their description.

In 2011 we and two other groups independently proposed a DFT exchange-correlation (xc) potential able to capture the Kondo plateau in the zero-bias conductance at vanishing temperature. In Ref the xc potential $v_{xc}$ was obtained by reverse engineering the exact solution of the SIAM with the uncontacted impurity (equivalent to the single-site Hubbard model). However, it was soon realized that such a $v_{xc}$ fails dramatically at temperatures $T > T_K$ (or at finite bias) to the cause of the failure being the lack of dynamical xc effects. In fact, DFT is an equilibrium theory and it is not supposed to describe nonequilibrium properties like transport coefficients. The fortunate success in reproducing the Kondo plateau is a direct consequence of the Friedel sum rule according to which the zero-bias and zero-temperature conductance is completely determined by the ground state density of the impurity.

A consistent framework to deal with quantum transport is TDDFT where the xc potential at a certain spacet ime point depends on the density everywhere and at all previous times. This memory dependence is what we mean by dynamical xc effects. Their inclusion, however, is far from trivial since it requires the knowledge of the TD density deep inside the leads, a portion of the system which is usually integrated out by an embedding procedure. To overcome this complication we formulated a steady-state density functional theory applicable to any interacting junction to extract differential conductances as well as equilibrium spectral functions. In this framework, henceforth named i-DFT, the basic variables are the density on and the steady current through the junction, $(n, I)$, whereas the conjugated variables are the potential acting on the junction, or gate voltage $v$, and the external bias $V$. The map $(n, I) \leftrightarrow (v, V)$ is bijective in a finite (gate dependent) window around $V = 0$. 

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II. TD I-DFT FUNCTIONAL WITH MEMORY

The nonequilibrium SIAM Hamiltonian describes a single impurity level, subject to a TD gate \( v(t) \), coupled to a left \((L)\) and right \((R)\) electronic reservoirs, subject to a TD bias \( V_L(t) = V(t)/2 \) and \( V_R(t) = -V(t)/2 \). Since the bandwidth of the reservoirs is the largest energy scale, the density of states in \( L \) and \( R \) is assumed to be a frequency independent constant, i.e., we work in the wide band limit \((WBL)\). Consequently, the broadening \( \gamma = \gamma_L + \gamma_R \) of the impurity level is also frequency independent. The electrons interact with repulsion energy \( U \) only if they are located on the impurity. In Fig. 1 we show a schematic illustration of the SIAM along with the various energy scales.

We work in the regime \( \gamma \ll T, U \). Then, in accordance with Ref.\([15]\) we can write a set of coupled equations for the probabilities \( P_0, P_1 \) and \( P_2 \) that the impurity is occupied by one, one of (spin up or down) and two electrons respectively:

\[
\frac{1}{\gamma} \frac{dP_0}{dt} = -P_0 \sum_{\alpha} f_{\alpha}(v) + \frac{P_1}{2} \sum_{\alpha} f_{\alpha}(v),
\]

\[
\frac{1}{\gamma} \frac{dP_1}{dt} = -P_0 \sum_{\alpha} [f_{\alpha}(v + U) + f_{\alpha}(v)] + P_0 \sum_{\alpha} f_{\alpha}(v) + P_2 \sum_{\alpha} f_{\alpha}(v + U),
\]

\[
\frac{1}{\gamma} \frac{dP_2}{dt} = -P_0 \sum_{\alpha} f_{\alpha}(v + U) + \frac{P_1}{2} \sum_{\alpha} f_{\alpha}(v + U).
\]

These are known as rate equations \((RE)\). The sum runs over \( \alpha = L, R \) and

\[
f_{\alpha}(\epsilon) = \frac{1}{e^{(\epsilon - V_{\alpha})/T} + 1}
\]

is the Fermi function of lead \( \alpha \) at inverse temperature \( \beta = 1/T \) and (without loss of generality) vanishing chemical potential. The function \( f_{\alpha}(\epsilon) \equiv 1 - f_{\alpha}(\epsilon) \). The three \( RE \) are not linearly independent; it is easy to verify that

\[
P_0 + P_1 + P_2 = 1,
\]

as it should be. From the probabilities the electronic occupation \( N \) of the impurity and the current \( I_0 \) at the
The steady-state solution at finite (constant) bias is obtained by setting \(dP_3/dt = 0\). Using the first and third RE together with the probability normalization Eq. (5) one finds

\[
P_0 = \frac{1}{R(0)} P_1, \quad P_2 = R(U) P_1/2,
\]

with

\[
P_1 = \frac{1}{1 + \frac{1}{2R(0)} + \frac{R(U)}{2}}
\]

and the ratio

\[
R(\epsilon) = \frac{\sum_\alpha f_\alpha(v + \epsilon)}{\sum_\alpha f_\alpha(v)}
\]

Substituting these results into Eq. (7) one finds \(I_L + I_R = 0\), as it should be. Interestingly, for \(V = 0\) one recovers the thermal equilibrium distribution of the isolated impurity, i.e., \(P_0 = 1/Z, P_1 = 2e^{-V}/Z \) and \(P_2 = e^{-(2e+U)} / Z\), with \(Z = 1 + 2e^{-V} + e^{-(2\epsilon+U)}\) the partition function.

We next consider the (more general) time-dependent case and find an explicit solution for \(N(t)\) and \(I_s(t)\). We write the probability vector \(\vec{P} = (P_0, P_1, P_2)^T\) as proposed in Ref[23]

\[
\vec{P} = \left( \begin{array}{c} 1 - N \\ N \\ 0 \end{array} \right) + p \left( \begin{array}{c} -2 \\ 1 \\ 1 \end{array} \right).
\]

This parametrization satisfies Eqs. (5) and (6) by construction. Using Eq. (11) to rewrite the RE one finds

\[
\frac{1}{\gamma} \frac{d}{dt} \vec{P} = \left( \begin{array}{c} (N - 1)F(v) + NF(v)/2 \\ (1 - N)F(v) - NF(v + U)/2 \\ NF(v + U)/2 \end{array} \right),
\]

where

\[
F(\epsilon) = \sum_\alpha f_\alpha(\epsilon), \quad F(\epsilon) = \sum_\alpha f_\alpha(\epsilon).
\]

Notice that, as in the case of the single reservoir considered in Ref[23], the right hand side is independent of \(p\).

To obtain the impurity occupation we take the inner product of Eq. (12) with the vector \((0, 1, 2)\), see Eq. (6), and find

\[
\frac{\dot{N}}{\gamma} = -N + \left( 1 - \frac{N}{2} \right) F(v) + \frac{N}{2} F(v + U).
\]

Equation (14) gives the correct steady-state occupation for \(N = 0\). For the current we consider the combination

\[
I = \frac{1}{2} (I_L - I_R).
\]

From knowledge of \(\dot{N}\) and \(I\) one can always extract \(I_L\) and \(I_R\) using the continuity equation \(I_L + I_R = \dot{N}\). Taking into account Eq. (7) and the parametrization of Eq. (11), it is straightforward to find

\[
I = \left( 1 - \frac{N}{2} \right) \Delta f(v) + \frac{N}{2} \Delta f(v + U),
\]

with

\[
\Delta f(\epsilon) = f_L(\epsilon) - f_R(\epsilon).
\]

With the occupation and current as functions of gate and bias we can invert the map for finite \(U\) and for vanishing \(U\). Denoting by \(v, V\) the interacting (finite \(U\) ) inverse map and by \((v_s, V_s)\) the noninteracting \((U = 0)\) inverse map, the TD i-DFT potentials are given by

\[
v_{\text{Hxc}}[n, I] \equiv v[n, I] - v[n, I], \quad V_{\text{xc}}[n, I] \equiv V[n, I] - V[n, I].
\]

The key observables to simplify the inversion problem is that Eqs. (14, 16) can be written as

\[
\frac{\dot{N}}{\gamma} + N = \int [f(\omega - V/2) + f(\omega + V/2)] A_U(\omega - v) \, d\omega, \quad I = \frac{\gamma}{2} \int [f(\omega - V/2) - f(\omega + V/2)] A_U(\omega - v),
\]

with the spectral function

\[
A_U(\omega) = 2\pi \left[ \frac{N}{2} (\omega - U) + (1 - \frac{N}{2}) (\omega) \right].
\]

Therefore, in terms of the variables \(w_{\pm} = v \pm V/2\) the problem is separable since Eqs. (19) read

\[
N + (N + 2I)/\gamma = 2 \int f(\omega) A_U(\omega - w_\pm) \equiv n_U(w_\pm),
\]

which can be solved, e.g., by the bisection method. For \(N = 0\), Eq. (21) is the same equation used in Ref[23] to obtain the steady-state xc potentials of i-DFT. In that work we also took into account that the spectral peaks are broadened due to the coupling to the leads and replaced the delta functions in Eq. (20) with normalized Lorentzians of width \(\gamma\). It was then shown that an accurate parametrization for the difference of the noninteracting and interacting inverse maps is

\[
v_{\text{Hxc}} \pm \frac{V_{\text{xc}}}{2} = n_{U=0}(N \mp 2I/\gamma) - n_{U=0}^{-1}(N \mp 2I/\gamma) \approx \frac{U}{2} + \frac{U}{\pi} \arctan \left( \frac{N \mp I/\gamma - 1}{W_\pm} \right),
\]

where...
with $W = 0.16\gamma/U$. Writing down the (H)xc potentials explicitly, we have
\[ v_{\text{Hxc}}^{\text{ad}}[N, I] = \frac{U}{2} \]
\[ + \frac{U}{2} \sum_{s=\pm} \frac{1}{\pi} \arctan \left( \frac{N + sI/\gamma - 1}{\lambda W} \right) \]  
\[ (23a) \]
\[ V_{\text{xc}}^{\text{mem1}}[N, I] = -U \sum_{s=\pm} \frac{s}{\pi} \arctan \left( \frac{N + sI/\gamma - 1}{\lambda W} \right) \]  
\[ (23b) \]

where the superscript “ad” indicates that the functional will be used in an adiabatic sense and we also have introduced, for later use, the parameter $\lambda$ which here is set to unity, $\lambda = 1$.

As the mathematical structure of $n_U$ does not change for $N \neq 0$, we can obtain a parametrization for the TD i-DFT potentials with memory by simply replacing $I \to I \neq N/2$
\[ v_{\text{Hxc}}^{\text{mem1}}[N, I] = \frac{U}{2} \]
\[ + \frac{U}{2} \sum_{s=\pm} \frac{1}{\pi} \arctan \left( \frac{N + (N/2) + sI/\gamma - 1}{\lambda W} \right) \]  
\[ (24a) \]
\[ V_{\text{xc}}^{\text{mem1}}[N, I] = -U \sum_{s=\pm} \frac{s}{\pi} \arctan \left( \frac{N + (N/2) + sI/\gamma - 1}{\lambda W} \right) . \]  
\[ (24b) \]

Notice that, as anticipated, the dependence on history occurs through the first time-derivative of the impurity occupation. We further observe that along the “physical” solutions the continuity equation implies that $I_L = I + N/2$ and $I_R = -I + N/2$. Therefore, along the physical solutions we can rewrite the TD i-DFT potential as
\[ v_{\text{Hxc}}^{\text{mem1}}[N, I] = \frac{U}{2} \lim_{t \to -\infty} \left[ \frac{N + I_L/\gamma - 1}{\lambda W} \right] \]  
\[ + \frac{U}{2\pi} \lim_{t \to -\infty} \left[ \frac{N + I_R/\gamma - 1}{\lambda W} \right] \]  
\[ (25a) \]
\[ V_{\text{xc}}^{\text{mem1}}[N, I] = U \lim_{t \to -\infty} \left[ \frac{N + I_L/\gamma - 1}{\lambda W} \right] \]  
\[ - \frac{U}{\pi} \lim_{t \to -\infty} \left[ \frac{N + I_R/\gamma - 1}{\lambda W} \right] . \]  
\[ (25b) \]

This is the form used for the time-dependent simulations of the next Section.

III. RESULTS

We have performed time-dependent transport simulations for the Anderson model using a modified version of the algorithm of Ref[99] which allows to take into account not only an Hxc gate potential on the dot but also a (time-dependent) xc contribution to the bias both at zero and at finite temperatures. In our TD simulations we use one-dimensional tight binding leads which means that our leads have a semi-circular density of states of finite bandwidth while the functionals described in the previous section were derived for the WBL case. However, by proper choice of parameters one can ensure that the WBL is (approximately) achieved: at equilibrium, the leads are taken to be at half-filling, the coupling between the impurity and the leads is taken sufficiently small, and all relevant energies (on-site gate potential, electron-electron interaction) are well within the bandwidth of the lead bands. We are interested in the effects of the memory term (i.e. $N$) in the functionals. We study two distinct situations, a bias quench and a quench of the gate potential.

In Fig. 2 we show the TD current $I_L$ after a bias quench, i.e. after switching on a bias of the form $V(t) = V\theta(t)$ where $\theta(t)$ is the Heaviside step function. For times $t < 0$ the system is in equilibrium. The bias is applied symmetrically in left and right leads, $V_L(t) = -V_R(t) = V(\theta(t)/2$. The different panels of Fig. 2 show the currents obtained from the functional without and with memory, Eqs. (23) and (25), respectively, for different values of the (static) gate potential $v$ at fixed temperature $T/\gamma = 1.0$. We also show the steady state currents (dashed lines) obtained from the functional of Eq. (23) in the WBL. As it should be, in the long-time limit both functionals lead to the same steady currents which agree well with those of the WBL, confirming that we have chosen our parameters properly.

As for the TD currents, we see that at the particle-hole symmetric point $v = -U/2$ (upper left panel), both functionals by symmetry give exactly the same TD current. This is easily understood by the fact that in this particular case the density is constant, $N = 1$, at all times and thus $\dot{N} = 0$ and the two functionals become completely equivalent. For other values of the gate, both functionals lead to slightly different TD currents where the transient current oscillations in $I_L$ tend to be more pronounced for the functional without memory.

Both the functionals of Eqs. (23) and (25) are derived from the rate equations and thus contain Coulomb blockade but no Kondo physics. In Ref[99] we have designed a steady-state functional which also incorporates Kondo physics. At zero temperature this functional can be written as
\[ v_{\text{Hxc}}^{\text{ad2}}[N, I] = (1 - a[I]) v_{\text{Hxc}}^{\text{ad1}}[N, I] + a[I] v_{\text{Hxc}}^{(0)}[N, I] \]  
\[ (26a) \]
\[ V_{\text{xc}}^{\text{ad2}}[N, I] = (1 - a[I]) V_{\text{xc}}^{\text{ad1}}[N, I] \]  
\[ (26b) \]

where $a[I]$ is defined as
\[ a[I] = 1 - \left[ \frac{2}{\pi} \arctan \left( \frac{I}{\gamma W} \right) \right]^2 \]  
\[ (27) \]
and $v_{\text{Hxc}}^{(0)}[N, I]$ is the accurate parametrization of the SIAM Hxc potential at zero temperature given in Ref[99]. Furthermore, in both $v_{\text{Hxc}}^{\text{ad1}}$ and $V_{\text{xc}}^{\text{ad1}}$, the value of the parameter $\lambda$ is set to $\lambda = 2$. The above functional (and its extension to finite temperature) has been used in Ref[99] to
FIG. 2. Time-dependent currents from left lead to the Anderson impurity after a bias quench at time \( t = 0 \). Results are shown both for the adiabatic (ad1) and memory functionals (mem1) of Eqs. (23) and (25), respectively. Different panels correspond to different values of the gate potential. Steady currents in the wide band limit (WBL) are also shown for comparison. Parameters: \( U/\gamma = 3 \) for the interaction and \( T/\gamma = 1.0 \) for the temperature.

FIG. 3. Same as Fig. 2 but now at \( T/\gamma = 0 \) and using the functionals of Eqs. (26) and (28) valid in the Kondo regime. Other parameters as before.

FIG. 4. Comparison of TD currents (left) and TD densities (right) for the SIAM with \( U/\gamma = 3 \) obtained with the functionals of Eqs. (23) and (25) after a sudden quench (at time \( t = 0 \) ) of the gate potential. For times \( t < 0 \), the gate is fixed at the ph symmetric point \( v = -U/2 \), at \( t = 0 \) it is suddenly switched to \( v = 0 \). For the biased case \( (V/\gamma = 2.0) \), the bias was switched on at some time (negative) \( t_0 \) and the system was then propagated until a steady state was reached before, at \( t = 0 \), the gate potential was quenched. The calculations are done for two different temperatures: \( T/\gamma = 0.0 \) (upper panels) and \( T/\gamma = 1.0 \) (lower panels).

study the influence of an AC bias on the DC conductance of the SIAM. Since Eqs. (26) derive from a steady-state functional, they do not contain any memory. In order to include memory, we propose the analogous expression for the time evolution of the currents, exactly for the same reason as before: in this case \( N = 1 \) and thus \( N = 0 \) at all times, rendering the two functionals equivalent. Away from ph symmetry, the TD currents for both functionals are qualitatively quite similar, the memory functional leading to slightly less pronounced transient oscillations in \( I_L \) as also was the case for the functionals of Eqs. (23) and (25).

In Fig. 4 we show the time evolution of the current and density on the dot after a quench of the gate potential at time \( t = 0 \) using the functionals of Eqs. (23) and (25) for two different temperatures. For times \( t < 0 \), the gate potential is kept constant at the ph symmetric point, \( v = -U/2 \). In the unbiased case \( (V/\gamma = 0) \), the time evolution starts from equilibrium when, at \( t = 0 \), the gate potential is suddenly quenched to \( v = 0 \) (and afterwards kept constant). For the biased case \( (V/\gamma = 2) \), we also start from equilibrium, but at some distant (negative) time \( t_0 \) we suddenly switch on a bias and evolve the system towards its steady state. Thus, when the gate is quenched at \( t = 0 \), the propagation starts from this non-equilibrium state. Strictly speaking, the functionals (23) and (25) are valid only for temperatures \( T \geq \gamma \). However, we have still performed some calculations for \( T = 0 \) (upper panels) in order to show that the transients at low temperature are much more pronounced than at finite temperature \( (T/\gamma = 1.0) \), lower panels). As in the previous cases and for both temperatures, the functional with memory leads to smaller transient oscillations both in the current and the density.
IV. CONCLUSIONS

The central ingredients for an i-DFT description of steady-state transport through a nanoscale region connected to two leads are the Hxc gate and xc bias potentials which are functionals both of the density in that region as well as the steady current through it\(^{13}\)\(^{13}\)\(^{14}\) For the SIAM, the first suggested i-DFT functional\(^{13}\) is valid in the CB regime. However, later a functional has been proposed\(^{15}\) which yields accurate results for a wide range of parameters not only in the CB but also in the Kondo regime.

These i-DFT steady-state functionals have been generalized in an adiabatic sense to explicitly time-dependent transport\(^{15}\)\(^{15}\) In the present work we generalize a recently proposed idea\(^{15}\) to include memory effects in the xc gate potential to the two-lead transport setup, i.e., both Hxc gate and xc bias include memory. The inclusion of memory is achieved via reverse engineering of the time-dependent rate equations\(^{15}\) and thus at first only valid in the CB regime. Since the i-DFT functional for the CB regime serves as an essential ingredient in the construction of the accurate SIAM functional for both Kondo and CB regime, the memory term can also be included in this functional. We have shown with explicit examples of TD transport simulations for the SIAM, that the adiabatic and memory functional lead to different transient evolutions in density and current but, by construction, give the same steady state.

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