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Effects of non-orthogonality and electron correlations on the time-dependent current through quantum dots

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Three issues are analyzed in the physics of time-dependent tunneling current through a quantum dot with strongly correlated electrons coupled to two external contact leads: (i) nonorthogonality of the states of electrons in the leads and in the quantum dot, (ii) non-Fermi statistics of the excitations in the quantum dot, and iii) kinematic shift of the quantum dot levels. The contributions from nonorthogonality effectively decrease the mixing interaction between the leads and the quantum dot and the width of the quantum dot level whereas the Gibbs statistics slightly changes the spectral weights of quantum dot levels, and decreases the widths, but does not introduce drastical changes to the current. The kinematic interactions are taken into account within the loop correction. For the case of block signal, the time-dependent current shows oscillations starting at the onset and termination of the bias voltage pulse.

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I. INTRODUCTION

During a course of the last two decades, the possibility of producing electronic devices on the length scale of nanometres have compelled a reassessment of our technological, experimental and theoretical views of electron transport. For example, nowadays capability in producing tunnel junctions having the effective width in the range of 1–100 nm (Refs. 1–5) is more or less routine. Connecting nanotubes to metallic droplets of a diameter $\sim 5-20$ nm, thereby constructing a single electron transistor, is a reality today.[6] The technological advances have provided physicists with tools for investigations of both weakly and strongly correlated electrons by means of open and closed quantum dots (QD's), respectively, coupled to external contact leads. There are many more applications of the state-of-the-art technology for mesoscopic systems.

Theoretically, the developments of tunnel transport through interacting regions[7–12] have been performed in the stationary regime as well as in the time-dependent case. Many major breakthroughs in the understanding of the tunnel transport have been based on the transfer Hamiltonian[13,14] which relies on a very simple, although phenomenological, concept. The idea is to split the system into subsystems,[15] each of which can be treated individually, and describe the interactions between the parts by a transfer of electrons from one into another. The motivation is that the building blocks of the system can have completely different physical properties for which it is preferable to employ different descriptions. Moreover, the approach offers a conceptually uniform way to describe any system which can be regarded in terms of subsystems coupled via transfer of electrons between the subsystems. However, the conventional transfer Hamiltonian suffers from serious problems for an acceptable quantitative account of the transport through nanostructures. The model scheme of the transfer Hamiltonian have been criticized by Svidzinskii.[16] First, the left and right states are not well defined in this scheme. Indeed, it has been shown[17,18] that the result depends on the method of introducing the left and the right states. When Prange[17] used orthogonal states, the suggested model scheme was not obtained whereas in the case with nonorthogonal states the model scheme was derived, however, an over-complete basis set and a restriction on the energies of the allowed states were used. Second, the transfer (tunneling) of an electron between two subsystems arises due to an overlap of the wave functions of the two parts. The overlap, on the other hand, is usually regarded as important only in the region of the tunnel barrier or, put in another (mathematical) way, the electron operators of the different subsystems are *assumed* to anticommute. This severe simplification leads not only to a lack of precision in computational studies, but, also to a loss of nontrivial physical implications. As discussed by Emberly and Kirczenow[19] there are existing mathematical methods to express the nonorthogonal bases which spans the subsystems but these are, however, of no help since the simple physical interpretation is lost at the same time as the nonorthogonality disappears. The proven success and the physical transparency of the transfer Hamiltonian approach makes it desirable to extend its applicability to more general situations where the overlap is large. One of the purposes of this paper is to show, by means of a generalization of the transfer Hamiltonian formalism,[20,21] that the well-known formulas for the tunnel current through interacting regions coupled to external contact leads[11,22] formally can be recovered. Furthermore, we will make a thorough analysis of the implications of taking the nonorthogonality into account. Then, we study effects from strong electron correlations for QD's in a region of parameters where Kondo contributions[9,23–28] are not relevant. We will not discuss here any kinds of assisted tunnel processes which restrict our investigations to low temperatures. Our three main tasks here are (i) to investigate the effect of the nonorthogonality between the states of the subsystems, (ii) to inspect if there is any visible manifestation of Gibbs (non-Fermi) statistics of the excitations in the QD, and (iii) to study the role played by the kinematic interactions in the QD in the formation of the current through the quantum

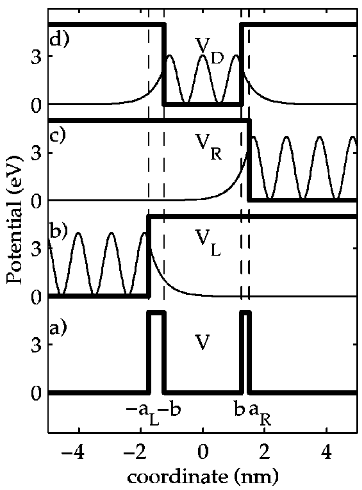

FIG. 1. The potential V in the original system (bottom) is divided into the auxiliary left V_L, right V_R, and middle V_M potentials. For the auxiliary potentials the squared modulus of examples of wave functions in each system are plotted.

device. It is worth to note that we cannot use directly the Keldysh diagram technique[29] since the operators of the electrons in the leads and the QD do *not* (anti) commute due to nonorthogonality and, therefore, the *zero* Hamiltonians of the subsystems cannot be extracted, i.e., $\exp(H_0^c+H_0^D) \neq \exp H_0^c \exp H_0^D$. For this reason we perform the calculations within the Kadanoff-Baym approach.[30]

We begin the paper with description of the system and the nonorthogonal approach used in Sec. II and continue in Sec. III by deriving the expression for the time-dependent current. We present some results in Sec. IV and summarize the paper in Sec. V. In the appendix we derive the anticommutators for the electron operators, a general expression for the QD GF and the equation of motion for the conduction electrons population numbers.

II. DESCRIPTION OF THE SYSTEM WITHIN THE NONORTHOGONAL BASIS SET

Consider a system of interacting electrons moving in an external potential V characterizing the system, see Fig. 1(a) for an example (actually, in the numerical results presented in Sec. IV, we use the model potentials given in Fig. 1). We assume that the part of the Coulomb repulsion which is included to the spectrum of carriers in the leads is sufficient for our description and we neglect collisions between the carriers in the leads. Let $\psi(x,t)$, $x=(\mathbf{r},\sigma)$, be the exact particle-field operator associated with the Hamiltonian of the system satisfying the usual anticommutation relations for Fermion operators. Suppose that H_α, $\alpha=L,D,R$ is a set of auxiliary Hamiltonians for single particles in the potentials V_α. Here the Hamiltonians correspond to the left (L) and right (R) leads and the QD (D). For instance, the left potential may be taken as $V_L(z)=V(z)\,\theta(-z-a_L)+V(-a_L)\,\theta(z+a_L)$, where z is the direction of the transport in our case and a_L is a turning point of the left subsystem, see Fig. 1(b). The two other potentials may be defined analogously, see Figs. 1(c) and 1(d). Corresponding to the Hamiltonian H_α there is an orthonormal set of eigenstates $\{\epsilon_{k\sigma},\phi_{k\sigma}\}$. Here the index k merely labels the eigenstate and does not correspond to the quasimomentum of the electron. Examples of the squared modulus of these wave functions are illustrated in Fig. 1. By the projections[31,32] $\tilde{c}_{k\sigma}(t)=\int \phi^*_{k\sigma}(\mathbf{r})\psi_\sigma(\mathbf{r},t)d\mathbf{r}$ of ψ onto the auxiliary system α, where $k\sigma\in\alpha$, an annihilation operator of a particle in the state $\phi_{k\sigma}$ with the spin projection σ is defined. A creation operator $\tilde{c}^\dagger_{k\sigma}$ is defined analogously. However, if we write the Hamiltonian in terms of these operators, it will contain not only the matrix elements on the functions $\phi_{k\sigma}(\mathbf{r})$, but, also, the overlap matrices. In order to avoid the latter we include the inverse of the overlap matrices into the definition of the annihilation and creation operators

$$c_{k\sigma}(t)=\sum_{k'} \mathcal{O}^{-1}_{kk'\sigma}\tilde{c}_{k'\sigma}(t),$$

$$c^\dagger_{k\sigma}(t)=\sum_{k'} (\mathcal{O}^{-1}_{kk'\sigma})^*\tilde{c}^\dagger_{k'\sigma}(t), \tag{1}$$

where k' runs over all states in $L\cup D\cup R$ and $\mathcal{O}_{kk'\sigma}=\langle\phi_k|\phi_{k'}\rangle=\mathcal{O}^*_{k'k\sigma}$ defines the overlap between the subsystems α and α'. Here we have used the approximation $\mathcal{O}^{-1}_{k\sigma k'\sigma'}=\delta_{\sigma\sigma'}\mathcal{O}^{-1}_{k\sigma k'\sigma}$ and introduced the short-cut notation $\mathcal{O}^{-1}_{kk'\sigma}\equiv\mathcal{O}^{-1}_{k\sigma k'\sigma}$. The definition of the electron operators as in Eq. (1) yields the anticommutator $\{c_{k\sigma},c^\dagger_{k'\sigma}\}=\mathcal{O}^{-1}_{kk\sigma}$, which is derived in detail in Appendix A. In terms of the operators given in Eq. (1) we define the field operators $\psi_{\alpha\sigma}(\mathbf{r},t)=\Sigma_{k\sigma\in\alpha}c_{k\sigma}(t)\phi_{k\sigma}(\mathbf{r})$, $\alpha=L,D,R$.

Consider the identity $\psi_\sigma(\mathbf{r},t)=\psi_{A\sigma}(\mathbf{r},t)+\psi_{B\sigma}(\mathbf{r},t)$, where $\psi_{A\sigma}(\mathbf{r},t)=\Sigma_\alpha\psi_{\alpha\sigma}(\mathbf{r},t)$ and $\psi_{B\sigma}(\mathbf{r},t)=\psi_\sigma(\mathbf{r},t)-\psi_{A\sigma}(\mathbf{r},t)$. The accuracy of the operator $\psi_{A\sigma}$, compared to ψ_σ, is controlled by the remainder $\psi_{B\sigma}$. By adding sufficiently many states in the expansion of $\psi_{A\sigma}$ the loss of accuracy is made small and the remainder $\psi_{B\sigma}$ can in many cases be made negligible. We assume here that this is already done and therefore the remainder can be neglected. In the given expansion, then, the total population number operator $N(t)=\Sigma_\sigma\int\psi^\dagger_\sigma(\mathbf{r},t)\psi_\sigma(\mathbf{r},t)d\mathbf{r}$ is given by

$$N(t)=N_{LL}(t)+N_{DD}(t)+N_{RR}(t)+N_{LD}(t)+N_{RD}(t)$$
$$+2\mathrm{Re}\sum_\sigma\int\psi^\dagger_{L\sigma}(\mathbf{r},t)\psi_{R\sigma}(\mathbf{r},t)d\mathbf{r}, \tag{2}$$

where the operators $N_{\alpha\alpha}(t)=\Sigma_\sigma\int\psi^\dagger_{\alpha\sigma}(\mathbf{r},t)\psi_{\alpha\sigma}(\mathbf{r},t)d\mathbf{r}$, $\alpha=L,D,R$ and $N_{\alpha D}(t)=2\mathrm{Re}\Sigma_\sigma\int\psi^\dagger_{D\sigma}(\mathbf{r},t)\psi_{\alpha\sigma}(\mathbf{r},t)d\mathbf{r}$, $\alpha,=L,R$. Since the overlap between the left and the right subsystems is exponentially small, when a mesoscopic QD is present in between, the last term in Eq. (2) can be discarded. A straightforward calculation shows that $N_{\alpha\alpha}(t)=\Sigma_{k\sigma\in\alpha}n_{k\sigma}(t)$, where $n_{k\sigma}(t)=c^\dagger_{k\sigma}(t)c_{k\sigma}(t)$, and $N_{LD}(t)=2\mathrm{Re}\Sigma_{pm\sigma}\mathcal{O}_{mp\sigma}c^\dagger_{m\sigma}(t)c_{p\sigma}(t)$ and $N_{RD}(t)=2\mathrm{Re}\Sigma_{qm\sigma}\mathcal{O}_{mq\sigma}c^\dagger_{m\sigma}(t)c_{q\sigma}(t)$, where p,q,m run over the states in the L,R,D, respectively.

III. THE TIME-DEPENDENT CURRENT THROUGH AN INTERACTING REGION

The systems we are interested in can be characterized by an interacting region, which we refer to as the QD for briefness. In order to not obscure the physical meaning and readability of the equations we use the simplest possible model which displays two of our main-target interests, namely, the nonorthogonality and strong correlations. For this reason, we choose a large Coulomb repulsion U such that the doubly occupied states do not contribute to the conduction. The levels in the QD are assumed to have a large energetic separation and, thus, a negligible influence from the attached contacts and the applied external field. The QD is coupled via tunnel (mixing) interactions $v_{k\sigma}$, to external contact leads. We are mainly interested in effects from the strong electron correlations in the QD and therefore the leads are expressed in a free electronlike approximation with the quasichemical potentials $\mu_L(t)$ and $\mu_R(t)$ for the left (L) and the right (R) leads, respectively. We assume that the bias voltage Φ_{sd} applied to the system drops entirely over the interacting region. The quasichemical potentials $\mu_\alpha(t)$ are related to the equilibrium chemical potential μ by $\mu_L(t)=\mu+\Phi_L(t)$, $\mu_R(t)=\mu+\Phi_R(t)$, where $\Phi_L(t)$ and $\Phi_R(t)$ are the time dependences of the single particle energies imposed by the applied voltage such that $\Phi_L(t)+\Phi_R(t)=\Phi_{sd}(t)$. The physical meaning of the potentials $\Phi_{L,R}(t)$ can be understood from the speculations given by Mahan (p. 788 in Ref. 33). The time-dependence of the tunneling matrix element v_{LD} is determined by the numbers of particles in the contacts and the QD,

$$\begin{aligned} v_{LD}(t)=&\exp[i(\mu_L\mathcal{H}_L+\mu_D\mathcal{H}_D+\mu_R\mathcal{H}_R)]v_{LD}\\ &\times\exp[-i(\mu_L\mathcal{H}_L+\mu_D\mathcal{H}_D+\mu_R\mathcal{H}_R)]\\ &\times\sum_k v_{k\sigma}\exp[-i(\mu_L-\Delta_{\sigma 0})tc^\dagger_{k\sigma}X^{0\sigma}], \end{aligned}$$

where $\Phi_L(t)=\mu_L-\Delta_{\sigma 0}$, see below for definitions of $c^\dagger_{k\sigma}$, $X^{0\sigma}$, and $\Delta_{\sigma 0}$. Similarly $\Phi_R(t)=\Delta_{\sigma 0}-\mu_R$ and $\Phi_L(t)+\Phi_R(t)=V$. In our case $[\mathcal{H}_L,\mathcal{H}_D]\neq 0$ and these parameters are taken phenomenologically, since we do not calculate the matrix elements of the transitions self-consistently. However, this shows that the voltage is dropping differently on different inhomogeneities and this problem requires a separate consideration. The system can be modeled by the extended Anderson Hamiltonian,[34] in which the QD is given by $\mathcal{H}_{\rm QD}=\Sigma_\sigma\varepsilon_\sigma d^\dagger_\sigma d_\sigma+Un_\uparrow n_\downarrow$, where $d^\dagger_\sigma$ (d_σ) creates (annihilates) an electron in the QD at the energy ε_σ and $n_\sigma=d^\dagger_\sigma d_\sigma$. However, since U is the largest parameter in the present situation it is convenient to express the QD in terms of many-body operators, e.g., Hubbard operators,[35] $X^{pp'}=|p\rangle\langle p'|$ describing the transition $|p'\rangle\rightarrow|p\rangle$. For a more transparent notation we introduce $Z^{pp'}$ for transitions of the kind $|\sigma\rangle\rightarrow|\bar{\sigma}\rangle$, where the number of particles is unchanged, and let h^p denote the diagonal transition $|p\rangle\rightarrow|p\rangle$. Such transitions will be referred to as Bose-like whereas Fermi-like transitions refer to $|0\rangle\rightarrow|\sigma\rangle$. Here, $\bar{\sigma}$ signifies the opposite spin state of σ. The QD Hamiltonian is diagonalized in terms of the Hubbard operators and reads $\mathcal{H}_{\rm QD}=\Sigma_p E_p h^p$, where the state label $p=0,\uparrow,\downarrow$. A conduction electron in the lead $\alpha=L,R$ with the energy $\epsilon_{k\sigma}(t)=\epsilon_{k\sigma}+\Phi_\alpha(t)$ is created (annihilated) by the operator $c^\dagger_{k\sigma}$ ($c_{k\sigma}$). Thus, the Hamiltonian for the system can be written

$$\begin{aligned} \mathcal{H}=&\sum_{k\sigma\in L,R}\epsilon_{k\sigma}(t)c^\dagger_{k\sigma}c_{k\sigma}+\sum_p E_p h^p\\ &+\sum_{k\sigma}[v_{k\sigma}(t)c^\dagger_{k\sigma}X^{0\sigma}+\text{H.c.}]. \end{aligned} \tag{3}$$

For the sake of transparency, we will only consider this simple model below although the formalism allows for considerations of much more complicated structures, see Ref. 36 for the equilibrium case. The time dependence in the mixing arises due to the time dependence in the contacts while the time dependence of the QD states can be neglected due to a large level separation and a small dipole moment induced by the electric field. Thus, the model differs from the standard Anderson Hamiltonian by the presence of two conduction bands, the time dependence of the parameters and by the anticommutation relations for electron operators ($\{c_{d\sigma},d^\dagger_\sigma\}=\mathcal{O}^{-1}_{k\sigma}$, $k\in L,R$, see Appendixes A and B).

The time-dependent current through the QD is calculated by the total charge rate of change in the system

$$\begin{aligned} J(t)=&-\frac{\partial}{\partial t}\langle N(t)\rangle=-\frac{\partial}{\partial t}\sum_{\alpha=L,D,R}\langle N_{\alpha\alpha}(t)\rangle\\ &-\frac{\partial}{\partial t}\sum_{\alpha=L,R}\langle N_{\alpha D}(t)\rangle=0, \end{aligned} \tag{4}$$

by charge conservation. As will be shown below, it is possible to divide the total current into a left and a right current term, i.e., $J(t)=J_L(t)+J_R(t)$, and we study the current through the system by investigating one of these terms, say, the left. In turn, each of terms $J_L(t)$, $J_R(t)$ can be separated into contributions from both the tunnel and the displacement currents.[22,37–39] We consider them separately.

A. The tunnel current

The purpose of this section is to show that in spite of the nonorthogonality of the wave functions of the subsystems, the standard expressions[11] for the tunnel current can be written in a familiar and a well-know form, however, the meaning of the parameters is altered. Therefore, we study the rate of change of the number of particles in the left lead where the total number of electrons is $\langle N_{LL}(t)\rangle=\Sigma_{p\sigma\in L}\langle n_{p\sigma}(t)\rangle$ and the $p\sigma$-dependent occupation number $\langle n_{p\sigma}(t)\rangle=\langle c^\dagger_{p\sigma}(t)c_{p\sigma}(t)\rangle$. The tunnel current, $J_{LL}(t)=-\partial\langle N_{LL}(t)\rangle/\partial t$, from the left lead into the interacting region becomes

$$\begin{aligned} J_{LL}(t)=&-2\,\text{Re}\sum_{p\sigma}[V^*_{pD\sigma}(t)F^<_{p\sigma}(t,t)-\mathcal{O}^{-1}_{k\sigma}(t)v^*_{p\sigma}(t)\\ &\times\langle(h^0+h^\sigma)(t)\rangle g^<_{p\sigma}(t,t)], \end{aligned} \tag{5}$$

where the time derivative of $\langle n_{k\sigma}(t)\rangle$ is derived in Appendix C, see Eq. (C8). Here the lesser GF $F^{<}_{k\sigma\bar{a}}(t,t) = i\langle X^{\bar{a}}(t)c_{k\sigma}(t)\rangle$ and $g^{<}_{k\sigma}(t,t)=i\langle c^{\dagger}_{k\sigma}(t)c_{k\sigma}(t)\rangle$. Due to the nontrivial anticommutation relations there appear new contributions both to the tunnel coefficient $v_{k\sigma}\rightarrow V_{kD\sigma}=v_{k\sigma}+\mathcal{O}^{-1}_{kD\sigma}\Delta_{\sigma 0}$ and to the time development of $\langle n_{k\sigma}(t)\rangle$. To the first order in $V_{kD\sigma}$, it is straight forward to see that the equation of motion for the transfer GF $F_{k\sigma}(t,t') = (-i)\langle Tc_{k\sigma}(t)X^{\sigma 0}(t')\rangle$ is contour integrated[30] to

$$F_{k\sigma}(t,t')=\mathcal{O}^{-1}_{k\sigma}P_{\sigma}(t)g_{k\sigma}(t,t') + \int_{t_0}^{t_0-i\beta} g_{k\sigma}(t,t'')V_{kD\sigma}(t'')G_{\sigma}(t'',t')dt'', \tag{6}$$

where $G_{\sigma}(t,t')=(-i)\langle TX^{0\sigma}(t)X^{\sigma 0}(t')\rangle_U$ and $P_{\sigma}(t) =\langle T\{X^{0\sigma}(t)X^{\sigma 0}(t)\}\rangle_U$ are defined in Appendix C. By analytical continuation[40,41] of $F_{k\sigma}$, the lesser GF $F^{<}_{k\sigma}$ is given by

$$F^{<}_{k\sigma}(t,t')=\mathcal{O}^{-1}_{k\sigma}P_{\sigma}(t)g^{<}_{k\sigma}(t,t') + \int_{-\infty}^{\infty} V_{kD\sigma}(t'')[g^{<}_{k\sigma}(t,t'')G^{a}_{\sigma}(t'',t') + g^{r}_{k\sigma}(t,t'')G^{<}_{\sigma}(t'',t')]dt''. \tag{7}$$

Substituting this expression into Eq. (5) and observing that

$$\begin{aligned}\mathrm{Re}([V^{*}_{kD\sigma}-v^{*}_{k\sigma}]\mathcal{O}^{-1}_{kD\sigma}\langle(h^0+h^{\sigma})(t)\rangle g^{<}_{k\sigma}(t,t)) &= \mathrm{Re}(\{|\mathcal{O}^{-1}_{kD\sigma}|^2\Delta_{\sigma}(t)+[v^{*}_{k\sigma}-v^{*}_{k\sigma}]\mathcal{O}^{-1}_{kD\sigma}\}\\ &\quad\times\langle(h^0+h^{\sigma})(t)\rangle g^{<}_{k\sigma}(t,t))=0\end{aligned}$$

the tunnel current becomes

$$J_{LL}(t)=2\mathrm{Re}\sum_{p\sigma} V_{pD\sigma}(t)\int_{-\infty}^{\infty} V^{*}_{p\sigma}(t')[G^{<}_{\sigma}(t,t')g^{a}_{p\sigma}(t',t) + G^{r}_{\sigma}(t,t')g^{<}_{p\sigma}(t',t)]dt'. \tag{8}$$

Since scattering between the conduction electrons in the leads are not taken into account, the lesser, retarded and advanced counterparts of the GF $g_{k\sigma}(t,t') =(-i)\langle Tc_{k\sigma}(t)c^{\dagger}_{k\sigma}(t')\rangle$ are given by

$$\begin{aligned} g^{<}_{k\sigma}(t,t')&=if_L(\epsilon_{k\sigma})e^{-i\epsilon_{k\sigma}(t-t')-i\int_{t'}^{t}V_L(t'')dt''},\\ g^{r,a}_{k\sigma}(t,t')&=\mp i\theta(\pm t\mp t')e^{-i\epsilon_{k\sigma}(t-t')-i\int_{t'}^{t}V_L(t'')dt''},\end{aligned} \tag{9}$$

where $f_L(\epsilon_{p\sigma})=f(\epsilon_{p\sigma}-\mu_L)$ is the Fermi-Dirac distribution function. The p summation in Eq. (8) is replaced by an integration over the density of states of the lead $\rho_{\sigma}(\epsilon)$ and the coupling between the lead and the interacting region is defined by

$$\Gamma^{L}_{\sigma}(t,t',\varepsilon)=2\pi V_{LD\sigma}(t)V^{*}_{LD\sigma}(t')\rho_{\sigma}(\varepsilon)e^{i\int_{t'}^{t}\Phi_L(t'')dt''}. \tag{10}$$

In terms of these quantities the general expression for the time-dependent tunnel current through an interacting region can be written in the familiar[11] form as

$$J_{LL}(t)=-\frac{1}{\pi}\mathrm{Im}\sum_{\sigma}\int_{-\infty}^{t}\int \Gamma^{L}_{\sigma}(t,t',\varepsilon)[G^{<}_{\sigma}(t,t') + f_L(\varepsilon)G^{r}_{\sigma}(t,t')]e^{i\varepsilon(t-t')}d\varepsilon dt'. \tag{11}$$

A similar derivation of the current through the right barrier into the interacting region leads to an analogous equation for $J_{RR}(t)$. The conclusion, then, is that although we are working within the nonorthogonal representation, we have shown that the formula for the tunnel current through a noninteracting or interacting region is formally equal to the result derived in Ref. 11. We stress that the formula given in Eq. (11) generalizes expressions for the tunnel current based on the orthodox transfer Hamiltonian, with respect to the couplings $\Gamma^{L,R}_{\sigma}$ between the leads and the interacting region. Indeed, as the overlap $\mathcal{O}^{-1}_{kD\sigma}\rightarrow 0$, illustrating the case of the orthodox transfer Hamiltonian, Eq. (11) identically equals the result derived in Ref. 11. In this respect, the current is expressed in terms of the local properties of the interacting region, such as the density of electron states (DOS) and the density of electrons, proportional to $\mathrm{Im}G^{r}_{\sigma}$ and $\mathrm{Im}G^{<}_{\sigma}$, respectively.

B. The displacement currents

As is seen from the expansion of the total population number operator in terms of the operators of the subsystems, not only the contributions from $N_{LL}(t)$ and $N_{RR}(t)$ have to be considered for full description of the transport. Also, the operators $N_{DD}(t)$ and $N_{LD}(t)$, $N_{RD}(t)$ give significant contributions. First we consider the time derivative of the QD population, i.e.,

$$\begin{aligned} J_{DD}(t)&=-\frac{\partial}{\partial t}\langle N_{DD}(t)\rangle=-\frac{\partial}{\partial t}\sum_{\sigma}\langle N_{\sigma}(t)\rangle\\ &=-\mathrm{Im}\frac{\partial}{\partial t}\sum_{\sigma} G^{<}_{\sigma}(t,t),\end{aligned} \tag{12}$$

since $\langle N_{\sigma}(t)\rangle=\mathrm{Im}G^{<}_{\sigma}(t,t)$. This contribution can be partitioned into a left and a right term, i.e., $J_{DD}(t)=J^{L}_{DD}(t) +J^{R}_{DD}(t)$ since the lesser QD GF $G^{<}_{\sigma}(t,t')=G^{<}_{L\sigma}(t,t') +G^{<}_{R\sigma}(t,t')$, see Appendix C. Thus, the *left* part of the QD displacement current is given by

$$J^{L}_{DD}(t)=-\mathrm{Im}\frac{\partial}{\partial t}\sum_{\sigma} G^{<}_{L\sigma}(t,t). \tag{13}$$

Next, we look at the part of the displacement current which comes from the population number $\langle N_{LD}(t)\rangle$, i.e.,

$$J_{LD}(t)=-\frac{\partial}{\partial t}\langle N_{LD}(t)\rangle$$
$$=-2\mathrm{Re}\frac{\partial}{\partial t}\sum_{\sigma}\sum_{p\in L}\mathcal{O}_{p\sigma}\langle X^{\sigma 0}(t)c_{p\sigma}(t)\rangle$$
$$=-2\mathrm{Im}\frac{\partial}{\partial t}\sum_{p\sigma}\mathcal{O}_{p\sigma}F^{<}_{p\sigma}(t,t). \tag{14}$$

Using Eq. (7), replacing the sum over p by an integration over the density of states $\rho^L_\sigma(\varepsilon)$ and defining

$$\gamma^L_\sigma(t,t',\varepsilon)=2\pi\mathcal{O}^*_{LD\sigma}V_{LD\sigma}(t')\rho^L_\sigma(\varepsilon)e^{i\int_{t'}^{t}\Phi_L(s)ds}, \tag{15}$$

the current $J_{LD}(t)$ is found as

$$J_{LD}(t)=-\frac{1}{\pi}\mathrm{Re}\frac{\partial}{\partial t}\sum_{\sigma}\int\Big\{\mathcal{O}_{DL\sigma}\mathcal{O}^{-1}_{LD\sigma}\rho^L_\sigma(\varepsilon)P_\sigma(t)f_L(\varepsilon)$$
$$-\int_{-\infty}^{t}\gamma^L_\sigma(t,t')[G^<_\sigma(t,t')$$
$$+f_L(\varepsilon)G^r_\sigma(t,t')]e^{i\varepsilon(t-t')}dt'\Big\}d\varepsilon. \tag{16}$$

By means of the expressions in Eqs. (11), (13), and (16) the left net current can now be written as

$$J_L(t)=J_{LL}(t)+J^L_{DD}(t)+J_{LD}(t). \tag{17}$$

This formula is the main result of the paper and is the starting point for a discussion of the effects of the overlap, the statistics of the QD states and the many-body interactions in the QD. We stress that in the orthodox theory, where the anticommutators $\{c_{k\sigma},d_\sigma\}=\mathcal{O}^{-1}_{kD\sigma}$ and $\int\psi^*_\alpha(x,t)\psi_D(x,t)dx$ are neglected, the last contribution in Eq. (17) is absent. Furthermore, the first two terms also include additional contributions in the tunnel coefficients $V_{kD\sigma}=v_{k\sigma}+\mathcal{O}^{-1}_{kD\sigma}\Delta^0_{\sigma0}$. In Sec. IV we will analyze the effect of the overlap $\mathcal{O}^{-1}_{k\sigma}$ on the current.

C. Stationary regime

In the stationary regime, the couplings $\Gamma^L_\sigma(t,t',\varepsilon)=\Gamma^L_\sigma(\varepsilon)$ and $\gamma^L_\sigma(t,t',\varepsilon)=\gamma^L_\sigma(\varepsilon)$ become time independent and the time integral in Eq. (17) is simply the Fourier transform of the lesser and retarded GF. We thus note that N_{LD}, N_{RD} and N_{DD} are time independent, hence the contributions from $\partial/\partial t\langle N_{LD}(t)\rangle$, $\partial/\partial t\langle N_{RD}(t)\rangle$, and $\partial/\partial t\langle N_{DD}(t)\rangle$ vanish. Therefore, $J_{LL}=-J_{RR}$ and if we use that $J_{\mathrm{net}}=(J_{LL}-J_{RR})/2$, we obtain

$$J_{\mathrm{net}}=\frac{i}{4\pi}\sum_\sigma\int\{[\Gamma^L_\sigma(\varepsilon)-\Gamma^R_\sigma(\varepsilon)]G^<_\sigma(\varepsilon)+[f_L(\varepsilon)\Gamma^L_\sigma(\varepsilon)$$
$$-f_R(\varepsilon)\Gamma^R_\sigma(\varepsilon)][G^r_\sigma(\varepsilon)-G^a_\sigma(\varepsilon)]\}d\varepsilon. \tag{18}$$

Further simplifications are achieved when restricting the analysis to the case when $\Gamma^L_\sigma(\varepsilon)\propto\Gamma^R_\sigma(\varepsilon)$, commonly referred to as proportionate coupling. Then, it is easily shown that the tunnel current through the interacting region can be written as

$$J_{\mathrm{net}}=-\frac{1}{2\pi}\mathrm{Im}\sum_\sigma\int\Gamma_\sigma(\varepsilon)[f_L(\varepsilon)-f_R(\varepsilon)]G^r_\sigma(\varepsilon)d\varepsilon, \tag{19}$$

where $\Gamma_\sigma(\varepsilon)=\Gamma^L_\sigma(\varepsilon)\Gamma^R_\sigma(\varepsilon)/[\Gamma^L_\sigma(\varepsilon)+\Gamma^R_\sigma(\varepsilon)]$ is the total coupling for each spin projection between the leads and the interacting region. The expressions given in Eqs. (18) and (19) were previously reported in Refs. 9–11, however, in the present formulation all couplings $\Gamma^\alpha_\sigma(\varepsilon)$ contain explicit contributions from the overlap matrix and the single-electron transitions between the many-electron states of the QD via the new definition of the mixing matrix elements $v_{k\sigma}\to v_{k\sigma}+\mathcal{O}^{-1}_{kD\sigma}\Delta_{\sigma0}$.

IV. RESULTS

For a discussion of the three main tasks of this paper, stated in the introduction, we need to express the QD GF. We will do that in three different schemes to enable an analysis of the different aspects. In Appendix C a general expression for the QD GF is derived from which we first pick out the Hubbard I approximation (HIA), obtained by neglecting all functional derivatives in Eq. (C2), i.e.,

$$\int_{t_0}^{t_0-i\beta}\Bigg(\Bigg[i\frac{\partial}{\partial t}-\Delta^0_{\sigma0}-\sum_{k\in L,R}\mathcal{O}^{-1}_{Dk\sigma}v^*_{k\sigma}(t)\Bigg]\delta(t-t_1)$$
$$-P_\sigma(t^+)V_\sigma(t,t_1)\Bigg)G^{\mathrm{HIA}}_\sigma(t_1,t')dt_1$$
$$=[\delta(t-t')+v_\sigma(t,t')P_\sigma(t')]P_\sigma(t). \tag{20}$$

Here we have introduced the interactions

$$v_\sigma(t,t')=\Sigma_{k\in L,R}V_{Dk\sigma}(t)g_{k\sigma}(t,t')\mathcal{O}^{-1}_{kD\sigma}$$

and

$$V_\sigma(t,t')=\Sigma_{k\in L,R}V_{Dk\sigma}(t)g_{k\sigma}(t,t')V_{kD\sigma}(t'),$$

where

$$V_{Dk\sigma}(t)=v^*_{k\sigma}+\mathcal{O}^{-1}_{Dk\sigma}\varepsilon_{k\sigma}.$$

For a time-independent external field Eq. (20) can be Fourier transformed to

$$G^{\mathrm{HIA}}_\sigma(i\omega)=\frac{1+v_\sigma(i\omega)P_\sigma}{i\omega-\Delta^0_{\sigma0}-\sum_{k\in L,R}\mathcal{O}^{-1}_{Dk\sigma}v^*_{k\sigma}-P_\sigma V_\sigma(i\omega)}P_\sigma. \tag{21}$$

Already in this approximation there appears a level shift induced by the overlap, i.e., $\Delta^0_{\sigma0}\to\Delta^0_{\sigma0}+\Sigma_{k\in L,R}\mathcal{O}^{-1}_{Dk\sigma}v^*_{k\sigma}$. In order to analyze the effects of the overlap we put $\mathcal{O}^{-1}_{kD\sigma}\to\lambda\mathcal{O}^{-1}_{kD\sigma}$, $\lambda\in[0,1]$. The overlap $\mathcal{O}^{-1}_{pD\sigma}\equiv\langle\phi_p|\phi_D\rangle$ is, apart from normalizing constants, given by

$$\langle \phi_p | \phi_D \rangle \sim \left(2\,\mathrm{Re}\frac{a}{\kappa_{D\sigma} - ip_\sigma} e^{-\kappa_{D\sigma}(a_L - b)} + \frac{e^{-\kappa_{L\sigma}(a_L-b)} - e^{-\kappa_{D\sigma}(a_L-b)}}{\kappa_{D\sigma} - \kappa_{L\sigma}} + \frac{e^{-\kappa_{L\sigma}(a_L-b)}}{\kappa_{L\sigma} + \kappa_{D\sigma}} \right) \cos(k_{D\sigma} b) + \frac{2}{k_{D\sigma}^2} \frac{k_{D\sigma}\cosh(\kappa_{L\sigma} b)\sin(k_{D\sigma} b) + \kappa_{L\sigma}\sinh(\kappa_{L\sigma} b)\cos(k_{D\sigma} b)}{1 + (\kappa_{L\sigma}/k_{D\sigma})^2} e^{-\kappa_{L\sigma} a_L},$$

where $a = (k_{L\sigma} + i\kappa_{L\sigma})/(2k_{L\sigma})$, $p_\sigma = \sqrt{2\varepsilon_{p\sigma}}$, $\kappa_{L\sigma} = \sqrt{2(V_0 - \varepsilon_{p\sigma})}$, $k_{D\sigma} = \sqrt{2\Delta_{\sigma 0}^0}$, and $\kappa_{D\sigma} = \sqrt{2(V_0 - \Delta_{\sigma 0}^0)}$. The barrier height V_0 is measured from the equilibrium chemical potential μ and a_L, b are defined in Fig. 1. The overlap $\mathcal{O}_{qD\sigma}^{-1}$ is calculated similarly. There are also contributions from the overlap in the level width $P_\sigma V_\sigma$ and the spectral weight $(1 + v_\sigma P_\sigma) P_\sigma$. In Fig. 2(a) the dashed line shows the J-V characteristics for the case when the overlap is neglected. The picture is reduced to the single-electron case by letting the cumulant $P_\sigma \to 1$ [dotted line in Fig. 2(a)]. The difference between the two curves is small which, thus, supports that the many-body population numbers in the QD give a small effect on the current. This is expected since, for example, the cumulant $P_\uparrow = N_0 + N_1/2 = N_0 + N_\uparrow \approx 1$, $N_\uparrow = N_\downarrow = N_1/2$. However, the population numbers differ significantly in the two cases, shown in Fig. 2(b) (N_0) and (N_1) as a function of the bias voltage, see Appendix C for details of the QD population numbers. Thus, in the paramagnetic case the changes in the population numbers N_0 and N_1 compensate each other and the current remains nonaltered. However, they are manifested in some situations, e.g., spin transport.[42] As the overlap is turned on, the level width is decreased since $v_{k\sigma} = \langle \phi_k | H | \phi_D \rangle = \mathcal{O}_{kD\sigma}\varepsilon_{k\sigma} - V_0 \int_{-b}^{\infty} \phi_k^* \phi_D dx$ and, roughly, $\mathcal{O}_{kD\sigma}^{-1} \sim -\mathcal{O}_{kD\sigma}/(1 - \Sigma_k |\mathcal{O}_{kD\sigma}|^2)$ giving $V_{kD\sigma} \sim \mathcal{O}_{kD\sigma}[\varepsilon_{k\sigma} - \Delta_{\sigma 0}^0/(1 - \Sigma_k |\mathcal{O}_{kD\sigma}|^2)] - V_0 \int_{-b}^{\infty} \phi_k^* \phi_D dx$ and similarly for $V_{Dk\sigma} = v_{k\sigma}^* + \mathcal{O}_{Dk\sigma}^{-1}\varepsilon_{k\sigma}$. This readily shows that the magnitude $|V_{kD\sigma}| < |v_{k\sigma}|$ which, in turn, furnishes the level with a longer lifetime. The decreased width implies a faster onset of the current at a higher bias voltage given by the level shift. However, the level shift in this case is many orders of magnitudes smaller than the bare level position with respect to μ, thus causing a negligible renormalization. The many-body population numbers are seen to have faster shifts while the deviations from their corresponding equilibrium values are smaller, than in the case without the overlap.

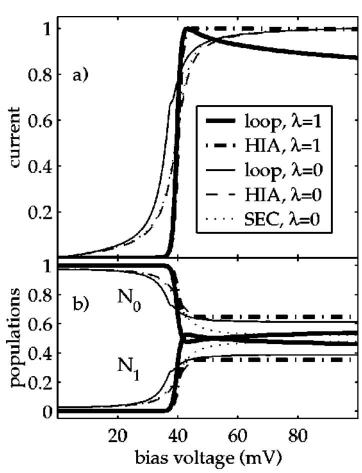

FIG. 2. Characteristic features of the current (a) and the population numbers (b), for a 4 nm wide QD connected via 0.5 nm thick and 1 eV high tunnel barriers, as functions of the bias voltage. The bare level $\Delta_{\sigma 0}^0 = 20$ meV and the conduction electron DOS $\rho_\sigma^\alpha = 1/(2W)$, where $W = 1$ eV is the conduction band width. The plots are made for the single-electron case (dotted lines), within the HIA with (dash-dotted lines), and without (dashed lines) the overlap and with the loop correction with (bold solid lines) and without (solid lines) the overlap.

The third approximation scheme we employ is obtained by evaluating the first functional derivative in Eq. (C2) giving the loop corrected[42] equation for the QD GF

$$\int_{t_0}^{t_0 - i\beta} \left(\left[i\frac{\partial}{\partial t} - \Delta_{\sigma 0}(t) - \sum_{k \in L,R} \mathcal{O}_{Dk\sigma}^{-1} v_{k\sigma}^*(t) \right] \delta(t - t_1) - P_\sigma(t^+) V_\sigma(t, t_1) \right) G_\sigma^{\mathrm{loop}}(t_1, t') dt_1 = [\delta(t - t') + v_\sigma(t, t') P_\sigma(t')] P_\sigma(t), \quad (22)$$

where the dressed many-body level $\Delta_{\sigma 0}(t)$ is found from the self-consistent equation

$$\Delta_{\sigma 0}(t) - \Delta_{\sigma 0}^0 = i \int_{t_0}^{t_0 - i\beta} V_{\bar{\sigma}}(t, t_1) D_{\bar{\sigma}}(t_1, t^+) dt_1. \quad (23)$$

The loop correction arises due to kinematic interactions between the states in the QD, which here is induced by the interactions with the conduction bands. Mathematically this is caused by the nontrivial anticommutation relations between the Hubbard operators. It is worth to note that the level $\Delta_{\sigma 0}$ depends on the characteristics of the level and conduction sub-bands of the opposite spin $\bar{\sigma}$, a property that can be used in connection with spin-dependent transport.[42] In the time-independent regime the QD GF is Fourier transformed to the same expression as in the HIA, that is, Eq. (21), however, now with the dressed level $\Delta_{\sigma 0}$ given by

$$\Delta_{\sigma 0} - \Delta_{\sigma 0}^0 = \sum_{k \in L,R} V_{Dk\bar{\sigma}} V_{kD\bar{\sigma}} \frac{f(\varepsilon_{k\bar{\sigma}}) - f(\Delta_{\bar{\sigma} 0})}{\varepsilon_{k\bar{\sigma}} - \Delta_{\bar{\sigma} 0}}. \quad (24)$$

The resulting J-V characteristics and population numbers are shown in Fig. 2 with (bold solid) and without (solid) the overlap, respectively. One main difference between the curves is the rapid onset of the current as the level becomes resonant (lies between the left and right quasichemical potentials), when the overlap is not neglected. Another peculiar feature which is only observed in the case when the overlap is not neglected is that, the population numbers N_0 and N_1 are not monotonic functions of the bias voltage. Combined with the smaller effective interaction $V_{kD\sigma}$, this gives a nonmonotonic behavior of the current and a small negative differential conductance as the voltage is increased when the level has become resonant.

Time-dependent current in the wide-band limit approximation. One of the simplest ways to illustrate time-dependent phenomena in the current is by employing a wide-band-limit- (WBL-) like approximation. Then, (i) the level shifts from $\Sigma_k \mathcal{O}^{-1}_{Dk\sigma} v^*_{k\sigma}$ and $\mathrm{Re}V_\sigma(t,t')P_\sigma(t)$ are neglected since they are small compared to $\Delta_{\sigma 0}$, (ii) the energy dependence of the linewidths $\Gamma^D_\sigma(t,t',\varepsilon) \equiv \mathrm{Im}V_\sigma(t,t')P_\sigma(t) = \Gamma^D_\sigma(t,t')$ can be disregarded because of their slow variation in the voltage regime considered here, and, (iii) allowing only $\Phi_L(t)=\Phi_R(t)$ for the energies in the leads. In this limit one rather easily can obtain analytical results for the QD GF which then are inserted into the current formula. Furthermore, since transport is often dominated by states close to the quasichemical potentials and the level shift and width are generally slowly varying functions of the energy, the WBL for this case is fair approximation. The approximation also allows for asymmetric barriers ($\Gamma^L_\sigma \neq \Gamma^R_\sigma$).

The retarded effective interactions V^r_σ and v^r_σ are thus given by

$$V^r_\sigma(t,t') = -\frac{i}{2\pi}\theta(t-t')\sum_\alpha \Gamma^{D\alpha}_\sigma(t,t')\int e^{i\varepsilon(t-t')}d\varepsilon = -i\delta(t-t')\Gamma^D_\sigma(t), \tag{25}$$

$$v^r_\sigma(t,t') = -\frac{i}{2\pi}\theta(t-t')\sum_\alpha \gamma^{D\alpha}_\sigma(t,t')\int e^{i\varepsilon(t-t')}d\varepsilon = -i\delta(t-t')\gamma^D_\sigma(t). \tag{26}$$

Here we have introduced the notations $\Gamma^D_\sigma(t) = \Gamma^{DL}_\sigma(t) + \Gamma^{DR}_\sigma(t)$, where $\Gamma^{D\alpha}_\sigma(t) = \Gamma^{D\alpha}_\sigma(t,t)$ and $\Gamma^{D\alpha}_\sigma(t,t') \equiv 2\pi V_{D\alpha\sigma}(t)V_{\alpha D\sigma}(t')\rho^\alpha_\sigma \exp[i\int_t^{t'}\Phi_\alpha(s)ds]$, and $\gamma^D_\sigma(t) = \gamma^{DL}_\sigma(t)+\gamma^{DR}_\sigma(t)$, where $\gamma^{D\alpha}_\sigma(t) = \gamma^{D\alpha}_\sigma(t,t)$ and $\gamma^{D\alpha}_\sigma(t,t') \equiv 2\pi V_{D\alpha\sigma}(t)\mathcal{O}^{-1}_{\alpha D\sigma}\rho^\alpha_\sigma \exp[i\int_t^{t'}\Phi_\alpha(s)ds]$. With these effective interactions the retarded (advanced) QD GF becomes

$$G^{r,a}_\sigma(t,t') = \mp i\theta(\pm t \mp t')[1 \mp i\gamma^D_\sigma(t)P_\sigma(t)] \times P_\sigma(t)e^{-i\int_{t'}^{t}[\tilde{\Delta}_{\sigma 0}(s) \mp i\Gamma^D_\sigma(s)P_\sigma(s)]ds}, \tag{27}$$

where $\tilde{\Delta}_{\sigma 0}(t)$ equals $\Delta^0_{\sigma 0}$ in the HIA and $\Delta_{\sigma 0}(t)$ within the loop correction. This expression can now be used to calculate the lesser QD GF and the time-dependent current through the system. Up to now, all formulas have contained a time-dependence both in the conduction electron energy $\epsilon_{k\sigma}(t)$ and in the mixing $v_{k\sigma}(t)$, providing a time dependence of the couplings $\Gamma^{L/R}_\sigma(t)$, the level width $\Gamma^D_\sigma(t)$ and the cumulant $P_\sigma(t)$. For numerical simplicity, though, we neglect the time dependence of the mixing $v_{k\sigma}$ in the following discussion which gives constant couplings $\Gamma^{L/R}_\sigma$, the level width Γ^D_σ and the cumulant P_σ. Then for a block signal (steplike bias voltage pulse) $\Phi_{sd}(t) = \Phi_0 + \Phi_1(t)$, where Φ_0 is a constant and $\Phi_1(t) = \Phi_1[\theta(t-t_0)-\theta(t-t_1)]$, the function $A^\alpha_\sigma(\omega,t) = \int_{-\infty}^{\infty} G^r_\sigma(t,t')\exp[i\omega(t-t') + i\int_{t'}^{t}\Phi_\alpha(s)ds]dt'$, where $\Phi_L(t)+\Phi_R(t) = \Phi_1(t)$, becomes for $t<t_1$

$$A^\alpha_\sigma(\omega,t) = \frac{1-i\gamma^D_\sigma P_\sigma}{\omega - \tilde{\Delta}_{\sigma 0} + i\Gamma^D_\sigma P_\sigma} P_\sigma\left(1 - \Phi_\alpha \frac{1-e^{i(\omega+\Phi_\alpha-\tilde{\Delta}_{\sigma 0}+i\Gamma^D_\sigma P_\sigma)(t-t_0)}}{\omega+\Phi_\alpha-\tilde{\Delta}_{\sigma 0}+i\Gamma^D_\sigma P_\sigma}\theta(t-t_0)\right), \tag{28}$$

where $\omega = \varepsilon + \mu_\alpha$, μ_α is the constant shift of the quasichemical potential in the lead α, and Φ_α is the amplitude of $\Phi_\alpha(t)$. Here, $\tilde{\Delta}_{\sigma 0} = \Delta^0_{\sigma 0}$ in the single-electron case and the HIA whereas $\tilde{\Delta}_{\sigma 0} = \Delta_{\sigma 0}$ within the loop correction. Letting $t\to\infty$ in Eq. (28) the limit expression is $A^\alpha_\sigma(\omega, t\to\infty) = (1-i\gamma^D_\sigma P_\sigma)P_\sigma/(\omega+\Phi_\alpha-\tilde{\Delta}_{\sigma 0}+i\Gamma^D_\sigma P_\sigma)$, that is, the system settles at its new steady state value as all the transients decay. For $t>t_1$ the expression in Eq. (28) is replaced by

$$A^\alpha_\sigma(\omega,t) = \frac{1-i\gamma^D_\sigma P_\sigma}{\omega - \tilde{\Delta}_{\sigma 0} + i\Gamma^D_\sigma P_\sigma} P_\sigma \times\left(1 + \Phi_\alpha \frac{1-e^{i(\omega+\Phi_\alpha-\tilde{\Delta}_{\sigma 0}+i\Gamma^D_\sigma P_\sigma)(t_1-t_0)}}{\omega+\Phi_\alpha-\tilde{\Delta}_{\sigma 0}+i\Gamma^D_\sigma P_\sigma} \times e^{i(\omega-\tilde{\Delta}_{\sigma 0}+i\Gamma^D_\sigma P_\sigma)(t-t_1)}\right). \tag{29}$$

Similarly, the limit $t\to\infty$ gives $A^\alpha_\sigma(\omega,t\to\infty) = (1-i\gamma^D_\sigma P_\sigma)P_\sigma/(\omega-\tilde{\Delta}_{\sigma 0}+i\Gamma^D_\sigma P_\sigma)$, as expected.

The resulting time-dependent currents for the bias voltage step with and without the nonorthogonality taken into account are presented in Figs. 3(a) and 3(b), respectively. In the former the behavior of the currents is seen to differ for the the HIA (solid) and the loop correction (full) around the onset of the voltage step. In the HIA the current grows exponentially to its saturation value whereas with the loop correction the current first goes to a peak value and thereafter decays to its new steady state value. Thus, the transient behavior of the current is affected when many-body interactions in the QD are considered. As the pulse terminates both the HIA and the loop correction provides an oscillating decay of the current, as expected from Eq. (29). Figure 4(b) shows the currents provided in the single-particle picture (dashed), the HIA (solid), and with the loop correction (full) when the nonorthogonality is neglected. The three schemes display similar qualitative behavior with rapidly decaying ringing at the onset and termination of the bias voltage pulse. As seen, the single-particle picture and the HIA gives essentially the same net currents whereas within the loop correction the current has a slightly larger amplitude before and after the volt-

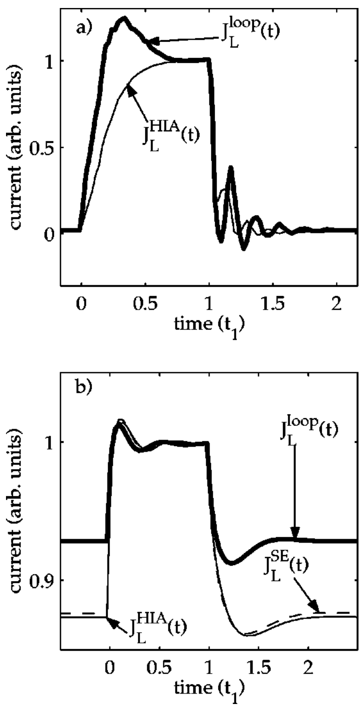

FIG. 3. The time-dependent current for the bias voltage step $\Phi_{sd}(t)=45+5[\theta(t-t_0)-\theta(t-t_1)]$ mV in the with (a) and without (b) the overlap. In (a) the currents are provided within the HIA (solid line) and with the loop correction (full line), taking the nonorthogonality into account. The time scale $t_1=600$ ps. In (b) the currents are given within single electron theory (dashed line), within the HIA (solid line), and with the loop correction (full line), without the nonorthogonality. The time scale $t_1=1$ ps.

age pulse, as expected from the stationary case (see Fig. 2). One of largest differences between the currents shown in Figs. 4(a) and 4(b) are the different time scales. As previously discussed, the nonorthogonality decreases the couplings $\Gamma_\sigma^{L,R}$ and the level width Γ_σ^D and therefore the relax-

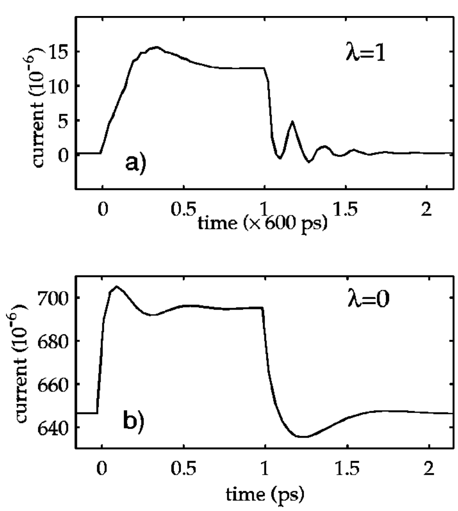

FIG. 4. The time-dependent currents within the HIA with the loop correction with (a) ($\lambda=1$) and without (b) ($\lambda=0$) the nonorthogonality taken into account. Note the very different scales of the times and the amplitudes of the current.

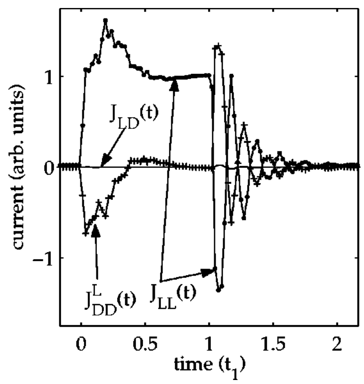

FIG. 5. The different contributions to the net current shown in Fig. 4(a). The plot shows the tunnel current $J_{LL}(t)$ (solid-dotted line) and the displacement currents $J_{DD}^L(t)$ (solid line with pluses) and $J_{LD}(t)$ (solid line).

ation time τ becomes longer, since $\tau\sim 1/(\Gamma_\sigma^D P_\sigma)$. As a result, the time scale of the tunneling process is longer within the nonorthogonal picture than in the orthodox. A comparison of the net currents with and without the nonorthogonality within the loop correction is shown in Figs. 3(a) and 3(b), respectively, from which the different time scales are directly seen. In this connection we also stress that the magnitudes of the two curves are actually very different, where the nonorthogonal picture results in a current which is approximately one to two orders of magnitudes less than that of the orthodox. Thus, the interpretation of experimental results require very different theoretical values of the couplings and the level width, and hence the barrier widths and heights, within the two pictures. In Fig. 5 the different contributions to the net current in Fig. 4(a) are shown and it is readily seen that the tunnel current gives the main contribution to the current while the displacement currents tend to retard the tunnel current. However, the displacement current do not cancel out the ringing of the tunnel current completely and therefore there remains a rapidly decaying ringing in the net current. The contribution from $J_{LD}(t)$ is seen to be small in this example but when the amplitude of $\Phi_1(t)$ is increased we have observed that this contribution plays an important role of the complete picture.

V. CONCLUSIONS

In summary, we have shown how the transfer Hamiltonian formalism can be generalized by including the nonorthogonality between the subsystems. It is formally shown that the tunnel current flowing through the left/right barrier into an interacting region, e.g., QD, can be expressed in a well-known formulation [Eq. (11)], however, with an interpretation of the tunneling coefficient that differs from orthodox theories $[v_{k\sigma}(t)\rightarrow V_{kD\sigma}(t)=v_{k\sigma}(t)+\mathcal{O}_{kD\sigma}^{-1}\Delta_{\sigma0}^*(t)]$. Moreover, we derived expressions for the displacement currents [Eqs. (13), (16)] and showed that the total current can be partitioned into two contributions, one for the flow through the left barrier and for the right. The QD was described in terms of Hubbard operator GF describing many-body interactions within the QD. The QD GF was given within the HIA

[Eq. (20)] and with the loop correction [Eq. (22)], thus giving us the opportunity to analyze the significance of non-Fermi the statistics of the population numbers compared to Fermi statistics on the resulting current. The conclusion is that, although the behavior of the population numbers of the QD level differ considerably, the behavior of the current is only slightly affected. A comparison of the two approximate schemes for the QD GF gives that, the many-body effects given by the loop correction from kinematic interactions alters the output current. Consequently, many-body effects in the QD should be considered for an adequate description of the current. However, the main differences in the current, in the non-spin-polarized case, is shown to be given by taking the nonorthogonality into account. Actually, a comparison of the amplitudes of the currents with and without the overlap shows a difference in the order of one to two magnitudes, where the nonorthogonal representation provides the smaller. This difference can be understood by that the coupling between, say, the left contact and the QD is not given by just the matrix element $v_{LD\sigma}$, as within the orthodox transfer Hamiltonian approach, but by $V_{LD\sigma}=v_{LD\sigma}+\mathcal{O}^{-1}_{LD\sigma}\Delta_{\sigma 0}$, where $\mathcal{O}^{-1}_{LD\sigma}\approx-\mathcal{O}_{LD\sigma}/(1-|\mathcal{O}_{LD\sigma}|^2-|\mathcal{O}_{RD\sigma}|^2)$ has the opposite sign of $v_{LD\sigma}$ and, therefore, *decreases* the coupling strength. The comparison of the J-V characteristics for orthogonal and nonorthogonal cases, given in Fig. 1 of Ref. 21, shows that the current starts to grow at much smaller voltage in orthogonal case than in nonorthogonal, whereas for the solution on quasiclassical wave functions[43] the discrepancy even more drastical. Thus we conclude that, when interpreting experimental results in terms of theoretical predictions given within the nonorthogonal representation the effective widths and/or heights of the tunnel barriers are thinner and/or lower than without the nonorthogonality.

ACKNOWLEDGMENTS

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APPENDIX A: THE COMMUTATORS OF THE ELECTRON OPERATORS

By the definition of the electron operators in Eq. (1) the nonvanishing anticommutator of two electron operators is given by

$$\begin{aligned}\{c_{k\sigma},c^{\dagger}_{k'\sigma'}\}&=\sum_{k_1k_2,s_1s_2}\mathcal{O}^{-1}_{k\sigma k_1s_1}\mathcal{O}^{-1}_{k_2s_2k'\sigma'}\int\phi^{*}_{k_1}(x_1)\phi_{k_2}(x_2)\\&\quad\times\{\psi(x_1),\psi^{\dagger}(x_2)\}dx_1dx_2\\&=\sum_{k_1k_2,s_1s_2}\mathcal{O}^{-1}_{k\sigma k_1s_1}\mathcal{O}^{-1}_{k_2s_2k'\sigma'}\delta_{s_1s_2}\mathcal{O}_{k_1s_1k_2s_2}\\&=\mathcal{O}^{-1}_{k\sigma k'\sigma'},\end{aligned}\tag{A1}$$

since

$$\{\psi(x),\psi^{\dagger}(x')\}=\delta_{\sigma'\sigma}\delta(\mathbf{r}-\mathbf{r}')$$

and

$$\sum_{k_1s_1}\mathcal{O}^{-1}_{k\sigma k_1s_1}\mathcal{O}_{k_1s_1k_2s_2}=\delta_{kk_2}\delta_{\sigma s_2}.$$

APPENDIX B: THE COMMUTATORS OF THE FERMION AND HUBBARD OPERATORS

When the overlap between the leads and the interacting region is taken into account the general anticommutation relation of a conduction and a localized electron is, in general, given by[36]

$$\{c_{k\sigma},X^{\bar{a}}\}=\mathcal{O}^{-1}_{k\sigma\mu}(d_{\mu})^{b}\varepsilon^{b\bar{a}}_{\xi}Z^{\xi},\tag{B1}$$

where ξ is a Bose-like transition, a and b are Fermi-like transitions, $\bar{a}=[qp]$ is the reverse transition of $a=[pq]$ and $(d_{\mu})^{a}\equiv\langle p|d_{\mu}|q\rangle$. It should be understood that summation is taken over the Fermi-like and Bose-like transition indices occurring twice. In the case when the dot effectively contains only a single-orbital level and in the limit of infinite Coulomb repulsion, each single electron operator in the interacting region becomes $d_{\sigma}=X^{0\sigma}$, where $\sigma=\uparrow,\downarrow$. Then, the Eq. (B1) can, with $X^{\bar{a}}=X^{\sigma'0}$ be written explicitly as

$$\begin{aligned}\{c_{k\sigma},X^{\sigma'0}\}&=\mathcal{O}^{-1}_{k\sigma\sigma}\langle 0|d_{\sigma}|\sigma\rangle\{X^{0\sigma},X^{\sigma'0}\}\\&=\mathcal{O}^{-1}_{k\sigma\sigma}(\delta_{\sigma'\sigma}h^{0}+Z^{\sigma'\sigma}),\end{aligned}\tag{B2}$$

under the assumption that opposite spin projections are orthogonal. With $a=[0\sigma']$ we have

$$\{c_{k\sigma},X^{0\sigma'}\}=0.\tag{B3}$$

The commutator

$$[c_{k\sigma},h^{p}]=\mathcal{O}^{-1}_{k\sigma\mu}(d_{\mu})^{b}\varepsilon^{bp}_{a}X^{a},\tag{B4}$$

where a is a Fermi-like transition, is also nonzero, in general. In particular, for any diagonal transition $p\equiv[pp]\in\{[\sigma\sigma],[22]\}$ the commutator in Eq. (B4) is given explicitly by

$$\begin{aligned}[c_{k\sigma},h^{p}]&=\mathcal{O}^{-1}_{k\sigma\mu}\langle 0|d_{\mu}|\mu\rangle\varepsilon^{[0\mu]p}_{a}X^{a}\\&=\mathcal{O}^{-1}_{k\sigma\sigma}\langle 0|d_{\sigma}|\sigma\rangle[X^{0\sigma},h^{p}]\\&=\delta_{\sigma p}\mathcal{O}^{-1}_{k\sigma\sigma}X^{0}\sigma,\end{aligned}\tag{B5}$$

whereas for the transition $[pp]=[00]$ the commutator $[c_{k\sigma},h^{0}]=-\mathcal{O}^{-1}_{k\sigma\sigma}X^{0\sigma}$.

APPENDIX C: THE QUANTUM DOT GREEN FUNCTION

In this appendix we will show that the lesser QD GF can be partitioned into a left and a right term, i.e., $G^{<}_{\sigma}(t,t')=G^{<}_{L\sigma}(t,t')+G^{<}_{R\sigma}(t,t')$. The QD GF is defined by

$$G_{\sigma\sigma'}(t,t')\equiv(-i)\langle TX^{0\sigma}(t)X^{\sigma'0}(t')\rangle_U$$
$$=(-i)\frac{\langle TSX^{0\sigma}(t)X^{\sigma'0}(t')\rangle}{\langle TS\rangle} \quad \text{(C1)}$$

with the action $S=\exp[i\int_{t_0}^{t_0-i\beta}\mathcal{H}'(t)dt]$ which contains the source fields $\mathcal{H}'(t)=\{U_{00}(t)h^0+\Sigma_\sigma[U_{\sigma\sigma}(t)h^\sigma+U_{\bar{\sigma}\sigma}(t)Z^{\bar{\sigma}\sigma}]\}$. The source fields $U_\xi(t)$ are used for constructing a perturbation expansion[36] for the QD GF by means of the functional derivatives $R_{\sigma\sigma'}(t)=i[\delta_{\sigma\sigma'}\delta/\delta U_{00}(t)+\delta/\delta U_{\sigma'\sigma}(t)]$. All information about the physics contained in the QD GF is obtained by letting the source fields $U_\xi(t)\to 0$, in which limit all expectation values that do not conserve the longitudinal part of the spin projection [e.g., $P_{\sigma\bar{\sigma}}(t)$, $G_{\sigma\bar{\sigma}}(t,t')$] vanish. We are looking for an expression for the QD GF on the form $G_{\sigma\sigma'}(t,t')=D_{\sigma\sigma''}(t,t')P_{\sigma''\sigma'}(t')$, where $D_{\sigma\sigma'}(t,t')$ is the locator of the QD GF. For briefness we put $G_\sigma(t,t')=G_{\sigma\sigma}(t,t')$. The QD GF is thus given by[36,42]

$$G_\sigma(t,t')=\int_{t_0}^{t_0-i\beta}d_\sigma(t,t_1)\{[\delta(t_1-t')+v_\sigma(t_1,t')P_\sigma(t')]P_\sigma(t_1)+\delta P_\sigma(t_1,t')\}dt_1+\int_{t_0}^{t_0-i\beta}d_\sigma(t,t_1)\Sigma_\sigma(t_1,t_2)G_\sigma(t_2,t')dt_1dt_2, \quad \text{(C2)}$$

where $d_\sigma(t,t')$ is the bare QD locator satisfying $(i\,\partial/\partial t-\Delta^0_{\sigma 0})d_\sigma(t,t')=\delta(t-t')$,

$$\delta P_\sigma(t_1,t')=\sum_{s=\sigma,\bar{\sigma}}\left(v_s(t_1,t')+\int_{t_0}^{t_0-i\beta}V_s(t_1,t_2)D_s(t_2,t')dt_2\right)\times R_{\sigma s}(t^+)P_{s\sigma}(t') \quad \text{(C3)}$$

is a correction to the cumulant $P_\sigma(t)$ whereas the self-energy

$$\Sigma_\sigma(t_1,t_2)=\sum_{k\in L,R}\mathcal{O}^{-1}_{Dk\sigma}v^*_{k\sigma}(t_1)+P_\sigma(t_1^+)V_\sigma(t_1,t_2)-\sum_{s=\sigma,\bar{\sigma}}\int_{t_0}^{t_0-i\beta}V_s(t_1,t_3)D_s(t_3,t_4)\times R_{\sigma s}(t^+)D^{-1}_{s\sigma}(t_4,t_2)dt_3dt_4. \quad \text{(C4)}$$

Here, we have introduced the effective interactions $v_\sigma(t,t')=\Sigma_{k\in L,R}V_{Dk\sigma}(t)g_{k\sigma}(t,t')\mathcal{O}^{-1}_{kD\sigma}$ and $V_\sigma(t,t')=\Sigma_{k\in L,R}V_{Dk\sigma}(t)g_{k\sigma}(t,t')V_{kD\sigma}(t')$, where $V_{Dk\sigma}(t)=v^*_{k\sigma}+\mathcal{O}^{-1}_{Dk\sigma}\varepsilon_{k\sigma}$. The cumulant $P_{\sigma\sigma'}(t)\equiv\langle T\{X^{0\sigma},X^{\sigma'0}\}(t)\rangle_U=\delta_{\sigma\sigma'}N_0(t)+N_{\sigma'\sigma}(t)$ is the sum of time-dependent population numbers. For time-dependent source fields the QD population numbers are not well defined since the off-diagonal expectation values are nonzero as well. Nevertheless, for briefness we will refer to $N_0(t)\equiv\langle h^0(t)\rangle$ and $N_{\sigma'\sigma}(t)\equiv\langle Z^{\sigma'\sigma}(t)\rangle$ as the population numbers of the transitions $[00]$ and $[\sigma'\sigma]$, respectively. We have also put $P_\sigma(t)=P_{\sigma\sigma}(t)$.

The lesser counterpart of the QD GF is easiest found by studying the algebraic structure of Eq. (C2) $G_\sigma=d_\sigma([1+v_\sigma P_\sigma]P_\sigma+\delta P_\sigma)+d_\sigma\Sigma_\sigma G_\sigma$, remembering that d_σ, v_σ, δP_σ, Σ_σ, and G_σ are functions of two time variables, whereas P_σ is a function of one time variable. Applying the rules for analytical continuation[40,41] yields the lesser QD GF, after tidying up the formulas

$$d^r_\sigma[(d^r_\sigma)^{-1}-\Sigma^r_\sigma]G^<_\sigma=d^<_\sigma([1+v^a_\sigma P_\sigma]P_\sigma+\delta P^a_\sigma+\Sigma^a_\sigma G^a_\sigma)+d^r_\sigma(v^<_\sigma P_\sigma P_\sigma+\delta P^<_\sigma+\Sigma^<_\sigma G^a_\sigma). \quad \text{(C5)}$$

Multiplying from the left by $D^r_\sigma(d^r_\sigma)^{-1}$, where $D^r_\sigma=[(d^r_\sigma)^{-1}-\Sigma^r_\sigma]^{-1}$, and noting that $(d^r_\sigma)^{-1}d^<_\sigma=0$ identically, we arrive at

$$G^<_\sigma(t,t')=\int_{-\infty}^{\infty}D^r_\sigma(t,t_1)\left([v^<_\sigma(t_1,t')\times P_\sigma(t')P_\sigma(t_1)+\delta P^<_\sigma(t_1,t')]+\int_{-\infty}^{\infty}\Sigma^<_\sigma(t_1,t_2)G^a_\sigma(t_2,t')dt_2\right)dt_1. \quad \text{(C6)}$$

The effective interactions v_σ and V_σ are actually sums over the left and the right conduction bands, i.e. $v_\sigma(t,t')=v_{L\sigma}(t,t')+v_{R\sigma}(t,t')$ and $V_\sigma(t,t')=V_{L\sigma}(t,t')+V_{R\sigma}(t,t')$, where

$$v_{L\sigma}(t,t')=\Sigma_{p\in L}V_{Dp\sigma}(t)g_{p\sigma}(t,t')\mathcal{O}^{-1}_{pD\sigma}$$

and

$$V_{L\sigma}(t,t')=\Sigma_{p\in L}V_{Dp\sigma}(t)g_{p\sigma}(t,t')V_{pD\sigma}(t'),$$

and analogously for the right terms. Therefore, the right hand side of Eq. (C6) can be partitioned into a left and a right term according to $G^<_\sigma(t,t')=G^<_{L\sigma}(t,t')+G^<_{R\sigma}(t,t')$, where, for example, $G^<_{\alpha\sigma}(t,t')$ is given the replacements $v^<_\sigma(t,t')\to v^<_{\alpha\sigma}(t,t')$, $\Sigma^<_\sigma(t,t')\to\Sigma^<_{\alpha\sigma}(t,t')$ and $\delta P^<_\sigma(t,t')\to\delta P^<_{\alpha\sigma}(t,t')$ in Eq. (C6).

The quantum dot population numbers N_0 and $N_1=N_\uparrow+N_\downarrow$ are calculated by using the fact that $N_\sigma(t)=\text{Im}G^<_\sigma(t,t)$ and the condition $N_0(t)+N_1(t)=1$. Actually, the sum of population numbers is only approximately equal to 1 because of the nonorthogonal representation. However, the deviation is in the order of $|\mathcal{O}^{-1}_{kD\sigma}|^4$ and can therefore be neglected. The bias voltage $\Phi_{sd}(t)$ is accounted for since the lesser QD GF can be partitioned into a left and right term, each of which depends on the quasichemical potential in the corresponding lead. To be specific, in $G^<_{L\sigma}(t,t')$ appear the lesser effective interactions $v^<_{L\sigma}(t,t')$ and $V^<_{L\sigma}(t,t')$, both of which containing the lesser GF $g^<_{L\sigma}(t,t')=if_L(\varepsilon)\exp(-i\int_{t'}^{t}[\varepsilon+\Phi_L(s)]ds)$, where $f_L(\varepsilon)$ depends on the quasichemical potential $\mu_L(t)=\mu+\Phi_L(t)$.

The conduction electron population numbers. In the derivation of the current in Sec. III we used some properties of the population number $\langle n_{k\sigma}(t)\rangle \equiv \langle c^{\dagger}_{k\sigma}(t)c_{k\sigma}(t)\rangle$. The dynamics of the Fermion operator $c_{k\sigma}(t)$ is given by the Heisenberg equation of motion

$$\left(i\frac{\partial}{\partial t}-\epsilon_{k\sigma}\right)c_{k\sigma}=V_{kD\sigma}(t)X^{0\sigma}+[\mathcal{O}^{-1}_{kD\sigma}v^{*}_{k\sigma}(t)(h^{\sigma}+h^{0})c_{k\sigma}+\mathcal{O}^{-1}_{kD\bar{\sigma}}v^{*}_{k\bar{\sigma}}(t)Z^{\bar{\sigma}\sigma}c_{k\bar{\sigma}}], \tag{C7}$$

where we have used the anticommutation relations derived in Appendix B and we have put $V_{kD\sigma}(t)=\mathcal{O}^{-1}_{kD\sigma}(t)\Delta^{0}_{\sigma 0}(t)+v_{k\sigma}(t)$, where $\Delta^{0}_{\sigma 0}(t)=E_{\sigma}(t)-E_{0}(t)$ is the bare QD many-body transition (analogue of the single-electron level). From Eq. (C7) we obtain the time derivative of $\partial/\partial t\langle n_{k\sigma}(t)\rangle=-i[c^{\dagger}_{k\sigma}c_{k\sigma},\mathcal{H}]=2\,\mathrm{Im}c^{\dagger}_{k\sigma}[c_{k\sigma},\mathcal{H}]$, thus

$$\frac{\partial}{\partial t}\langle n_{k\sigma}(t)\rangle=-2\,\mathrm{Im}\{V^{*}_{kD\sigma}(t)\langle TX^{\sigma 0}(t)c^{\dagger}_{k\sigma}(t)\rangle_{U}-[\mathcal{O}^{-1}_{kD\sigma}v^{*}_{k\sigma}(t)\langle T(h^{\sigma}+h^{0})(t)n_{k\sigma}(t)\rangle_{U}+\mathcal{O}^{-1}_{kD\bar{\sigma}}v^{*}_{k\bar{\sigma}}\langle Tc^{\dagger}_{k\sigma}(t)Z^{\bar{\sigma}\sigma}(t)c_{k\bar{\sigma}}(t)\rangle_{U}]\},$$

since $[c_{k\sigma},h^{\sigma}]=-[c_{k\sigma},h^{0}]$. The last two terms to the right in this equation, can be rewritten in terms of P_{ξ} and R_{ξ}, i.e.,

$$\langle T(h^{\sigma}+h^{0})(t)n_{k\sigma}(t)\rangle_{U}=[P_{\sigma}(t^{+})+R_{\sigma}(t^{+})]\langle n_{k\sigma}(t)\rangle,$$

$$\langle Tc^{\dagger}_{k\sigma}(t)Z^{\bar{\sigma}\sigma}(t)c_{k\bar{\sigma}}(t)\rangle_{U}=\lim_{t_1\to t^{-}}\lim_{t_2\to t_1^{-}}[P_{\sigma\bar{\sigma}}(t_1)+R_{\sigma\bar{\sigma}}(t_1)]\langle c^{\dagger}_{k\sigma}(t)c_{k\bar{\sigma}}(t_2)\rangle.$$

In this paper we restrict the investigations to the self-consistent field approximation where the functional derivatives of $\langle n_{k\sigma}(t)\rangle$ and $\langle c^{\dagger}_{k\sigma}(t)c_{k\bar{\sigma}}(t)\rangle$ can be neglected, i.e., $R_{\sigma}(t^{+})\langle n_{k\sigma}(t)\rangle=0$ and $R_{\sigma\bar{\sigma}}(t_1)\langle c^{\dagger}_{k\sigma}(t)c_{k\bar{\sigma}}(t_2)\rangle=0$. This is not a severe restriction, since the interactions between the localized states are taken into account in the Hubbard operators. Moreover, the product $P_{\sigma\bar{\sigma}}(t_1)\langle Tc^{\dagger}_{k\sigma}(t)c_{k\bar{\sigma}}(t_2)\rangle_{U}=0$, since we neglect all spin-flip processes for the conduction electrons. Therefore, the time development of $\langle n_{k\sigma}(t)\rangle$ will be given by the equation

$$\frac{\partial}{\partial t}\langle n_{k\sigma}(t)\rangle=-2\,\mathrm{Im}[(V^{*}_{kD\sigma}(t)\langle TX^{\sigma 0}(t)c^{\dagger}_{k\sigma}(t)\rangle_{U}-\mathcal{O}^{-1}_{kD\sigma}v^{*}_{k\sigma}(t)P_{\sigma}t^{+})\langle n_{k\sigma}(t)\rangle]. \tag{C8}$$

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