Time-dependent transport through quantum-impurity systems with Kondo resonance

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Abstract

We investigate the time-dependent transport properties of single and double quantum-impurity systems based on the hierarchical equations of motion (HEOM) approach. In the Kondo regime, the dynamical current oscillates with time in both cases due to the temporal coherence of electrons tunneling through the device, which shares the same mechanism as the single-level resonance without e–e interactions, but shows some different characteristics. For single quantum-impurity systems, the temperature $T$ has an inhibitory effect on the oscillations of dynamic current through its suppression of the Kondo effects. The amplitude of the current oscillations is attenuated by the e–e interaction $U$ in the Kondo regime. The frequency of the current oscillations is found almost independent of $T$ and $U$. For parallel-coupling double quantum-impurity systems, the oscillation of the current shows similar behavior to the single one, but with two-to-three times larger amplitudes. At the limit of small inter-impurity coupling the oscillation of the current exhibits enhanced characters, while it is weakened at the other limit.

1. Introduction

Quantum-impurity systems are of great interest because of their fundamental physics as well as potential applications as possible quantum-computing devices [1], such as single-molecule magnets [2, 3] and bulk Kondo insulators [4]. The investigation of transport in quantum-impurity systems is of great importance to understand the phase coherence of electrons in nanodevices. Although the spatial coherence of the electron wave functions in quantum-impurity systems has been widely studied theoretically, the temporal phase coherence has not. The reason mainly comes from the difficulty in dealing with the memory effects in the time domain, especially when electron–electron (e–e) interactions can not be treated perturbatively.

The e–e interactions in most of the studies in the literature on dynamical current in quantum-impurity systems are either totally ignored or treated on the level of mean field. For example, N S Wingreen et al investigate the time-dependent current of the mesoscopic structure coupling a double-barrier relatively early [5]. An analytical formula of the time-dependent current is presented in terms of the Keldysh Green function. They find that the distinct oscillation of the time-dependent current occurs when a rectangular bias pulse is applied to the device. This is attributed to the temporal coherence of electrons tunneling through the resonant level in response to the abrupt change of bias. A theory was then developed that the Kohn–Sham equation relies on the so called wide-band limit (WBL), which assumes that the leads’ bands have no energy dependent features. Although this approach has been widely adopted in mesoscopic physics, it fails to describe leads with a realistic finite bandwidth or with an energy-dependent density-of-state. In [6], Yu Zhu et al directly solve the Green functions in the time domain beyond the WBL approximation to investigate the dynamical current through a molecule. By applying a bias voltage on device leads, the numerical $I(t)$ is solved by the time domain
decomposition (TDD) method. In order to deal with the phase memory, upper time and cutoff are adopted in the TDD for an open system [6]. When the device weakly couples to the leads, the TDD method will encounter some serious numerical problems. To overcome those difficulties, the same group provides an exact analytical solution to the transport equations in the far from equilibrium regime for some specific voltage pulses [7]. Unfortunately, one needs to derive the new transport equations when the voltage pulses change into another shape. Obviously, it is impossible to take into account the e–e interaction for the numerical TDD method or the analytical solution.

Despite the difficulty surrounding dynamical current calculations in quantum-impurity systems, there is still some work in the literature. For example, the density-matrix renormalization group (DMRG) approach is extended to a time-dependent version (TD-DMRG) to treat time-dependent 1D problems as well as the quantum single-impurity system [8–10]. The current–voltage characteristics of the single impurity for the particle–hole symmetric point and mixed valence regime are presented in [10]. The time-dependent version of the numerical renormalization group (TD-NRG) approach is also adopted to study the nonequilibrium dynamics of quantum–impurity systems, and the time-dependent occupancy with Rabi-type oscillation is calculated in [11]. Other than these examples, perturbative studies on time-dependent transport through quantum-impurity systems are far from extensive owing to computational difficulties. Moreover, the above pioneering works still focus on single-level resonance tunneling, and another interesting issue of the time-dependent transport in the Kondo regime is not well understood.

In this paper, we propose a general approach based on a hierarchical equations of motion (HEOM) formalism [5, 12–16] to characterize the time-dependent current of quantum-impurity systems. We will deal with the issue of the oscillation of the dynamical current in the Kondo regime. The effects of finite impurity e–e interactions (U), temperature (T), and the bandwidth (W) of the leads will be investigated in detail. These are of relevance to experiments on quantum dots and quantum wires.

The paper is organized as follows. In section 2 we briefly review the HEOM approach, and give the common formalism for time-dependent quantum transport in quantum-impurity systems and present the results for electron current in quantum-impurity systems driven by an external bias. Then, we compare the single-level resonance tunneling results obtained from our HEOM approach to those from the analytical formula in terms of the Keldysh Green function [5], nonequilibrium Green functions (NEGF) [6], TD-DMRG [8], and TD-NRG [11]. In section 3, with the e–e interaction (U) being considered, we investigate the time-dependent current in single-impurity quantum systems in and out of the Kondo regime at different conditions, followed by the transport current in parallel-coupling double quantum-impurity systems. In section 4 we give a summary of our work.

2. General formalism of HEOM in quantum-impurity systems

The hierarchical equations of motion approach (HEOM) is potentially useful for addressing quantum-impurity systems. The outstanding issue of characterizing both equilibrium and nonequilibrium properties achieved in our previous work is referred to [16–18]. The HEOM approach has been employed to study dynamic properties, for instance, the dynamic Coulomb blockade and dynamic Kondo memory phenomena in quantum dots [14, 15]. It is essential to adopt an appropriate truncated level to close the coupled equations. The numerical results are considered to be quantitatively accurate with increasing truncated level.

In the present paper, we solve the time-dependent quantum transport problem and focus on the nonequilibrium dynamics of quantum-impurity systems based on the HEOM. The localized impurities constituting the open system are of primary interest, and the surrounding reservoirs of itinerant electrons are treated as the environment. The total Hamiltonian for the quantum-impurity systems

\[ H_T = H_S + H_B + H_{SB} \]  \hspace{1cm} (1)

where the interacting impurities

\[ H_S = \sum_{\sigma} \epsilon_{\sigma} \hat{a}_{\sigma \sigma} \hat{a}^\dagger_{\sigma \sigma} + \frac{U}{2} \sum_{\sigma} n_{\sigma \sigma} n_{\bar{\sigma} \bar{\sigma}} + \gamma \sum_{\sigma \neq \bar{\sigma}} \left( \hat{a}_{\sigma \sigma} \hat{a}_{\bar{\sigma} \bar{\sigma}} + H.c. \right). \]  \hspace{1cm} (2)

Here \( \epsilon_{\sigma} \) denotes the on-site energy of the electron with spin \( \sigma \) (\( \sigma = \uparrow, \downarrow \)) in impurity \( i \), \( \hat{a}_{\sigma \sigma} \) and \( \hat{a}^\dagger_{\sigma \sigma} \) correspond to the creation and annihilation operators for an electron with spin \( \sigma \). \( n_{\sigma \sigma} = \hat{a}^\dagger_{\sigma \sigma} \hat{a}_{\sigma \sigma} \) is the operator for the electron number of impurity \( i \), and \( U \) is the Coulomb interaction between electrons with spin \( \sigma \) and \( \bar{\sigma} \) (opposite spin of \( \sigma \)) within one impurity. \( \gamma \) is the inter-impurity coupling between the impurities \( i \) and \( j \), determined by their overlapping integral. \( H.c. \) stands for the Hermitian conjugate.

In what follows, we use the symbol \( \mu \) to denote the electron orbital (including spin, space, etc.) in the system for brevity, i.e., \( \mu = \{ \sigma, i \ldots \} \). The Hamiltonian of the device leads, treated as noninteracting electron reservoirs,
can be written as
\[ H_B = \sum_{k_{\mu \nu} = L,R} \epsilon_{k_{\mu \nu}} a_{k_{\mu \nu}}^\dagger a_{k_{\mu \nu}} \]  
(3)

with \( \epsilon_{k_{\mu \nu}} \) being the energy of an electron with wave vector \( k \) in the \( \alpha \) lead, and \( a_{k_{\mu \nu}}^\dagger \) (\( a_{k_{\mu \nu}} \)) corresponding to the creation (annihilation) operator for an electron with the \( \alpha \)-reservoir state \( |k\rangle \) of energy \( \epsilon_{k_{\mu \nu}} \). In the bath interaction picture, the Hamiltonian of coupling between the two leads and the impurity is
\[ H_{SB} = \sum_{\mu} \left[ f_{\mu} (t) a_{\mu} + a_{\mu}^\dagger f_{\mu} (t) \right]. \]  
(4)

Here, \( f_{\mu} = e^{iH_{SB} t} \left( \sum_{k_{\nu \mu}} t_{\kappa_{\mu \nu}} a_{k_{\mu \nu}}^\dagger \right) e^{-iH_{SB} t} \) is the stochastic interactional operator and satisfies the Gauss statistics with \( t_{\kappa_{\mu \nu}} \) denoting the transfer coupling matrix element. The influence of electron reservoirs on the impurities is taken into account through the hybridization functions, which are assumed to be of Lorentzian form, \( \Delta_{\omega} (\alpha) \equiv \pi \sum_{k_{\nu \mu}} t_{\kappa_{\mu \nu}} \delta (\omega - \epsilon_{k_{\mu \nu}}) = \Delta W^2 / [2 (\omega - \mu^\alpha)^2 + W^2] \), where \( \Delta \) is the effective impurity-lead coupling strength, \( W \) is the band width, and \( \mu^\alpha \) is the chemical potential of the \( \alpha \) lead [17, 19].

The HEOM that governs the dynamics of the open system assumes the form of [16, 17]:
\[ \rho_{\mu \nu}^{(n)} (t) = - i [ L + \sum_{r=1}^{n} A_j \rho_{\mu \nu}^{(n-j)} - \sum_{r=1}^{n} (-)^{n-r} C_k \rho_{\mu \nu}^{(n-r)} - \sum_{r=1}^{n} a_{\mu}^\dagger a_{\nu} \rho_{\nu \mu}^{(n-r)}] \]  
(5)

The \( n \)-th order auxiliary density operator \( \rho_{\mu \nu}^{(n)} \) can be defined via the auxiliary influence functional \( F_{\{n\}} \) as
\[ \rho_{\mu \nu}^{(n)} (t) \equiv U_{\{n\}} (t, t_0) \rho (t_0) \]  
(6)

with the reduced Liouville-space propagator,
\[ U_{\{n\}} (\psi, t; \psi_0, t_0) \equiv \int_{\psi_0 (t_0)}^{\psi (t)} D\psi e^{iS[\psi]} F_{\{n\}} (\psi) e^{-iS[\psi]} \]  
(7)

\( S[\psi] \) is the classical action functional of the reduced system. The definition of the auxiliary influence functional \( F_{\{n\}} \) together with its equations is referred to in [16].

We denote \( j = [j_1 \cdots j_n] \) and \( j' = [j_1' \cdots j_{n+1}'] \), the action of superoperators respectively is
\[ A_j \rho_{\mu \nu}^{(n+1)} = a_{\mu}^\dagger \rho_{\alpha \mu}^{(n+1)} + (-)^{n+1} a_{\nu} \rho_{\mu \nu}^{(n+1)} + \sum_{v} \left( C_{\mu \alpha v} a_{\nu} \rho_{\nu \alpha}^{(n+1)} - (-)^{n+1} C_{\nu \alpha v} \rho_{\mu \nu}^{(n+1)} a_{\mu}^\dagger \right) \]  
(8)

\[ C_{\mu \alpha v} \rho_{\nu \alpha}^{(n+1)} = \sum_{v} \left( C_{\mu \alpha v} a_{\nu} \rho_{\nu \alpha}^{(n+1)} - (-)^{n+1} C_{\nu \alpha v} \rho_{\mu \nu}^{(n+1)} a_{\mu}^\dagger \right) \]  
(9)

In this formalism, \( a_{\mu}^\dagger (a_{\mu}) \) corresponds to the creation (annihilation) operator for an electron with the \( \mu \) electron orbital (including spin, space, etc.). The reduced system density operator \( \rho_{\mu \nu}^{(n)} (t) \equiv \operatorname{tr}_{\text{res}} \rho_{\text{total}} (t) \) and auxiliary density operators \( \rho_{\mu \nu}^{(n)} (t) \) are the basic variables, here \( L \) denotes the terminal or truncated tier level. The Liouvillian of impurities, \( \mathcal{L} \equiv \frac{d}{dt} [H_{\text{sys}} \cdot] \), may contain both e–e interactions and time-dependent external fields. The index \( j \equiv (\text{qumt}) \) corresponds to the transfer of an electron to/from (\( o = + / - \)) the impurity state \( |\sigma\rangle \), associated with the characteristic memory time \( t_m \). The correlation function
\[ C_{\mu \alpha v} (t - t') = \langle f_{\mu} (t) f_{\alpha v}^\dagger (t') \rangle \]  
immediately follows the time-reversal symmetry and detailed balance relations.

In our calculations, if the errors of the numerical results of each element of the density matrix or the matrix of spectral function between the truncation \( L = N \) and \( L = N + 1 \) are less than 5%, we regard the results as converging. This will output sufficiently accurate current, for example, when the bias voltage applied on the system is \( V_i = -V_g = 2 \) mV, the steady-state currents for different truncation level are \( I = 21.6368 \) nA (\( L = 2 \), \( I = 20.7969 \) nA (\( L = 3 \), \( I = 20.8235 \) nA (\( L = 4 \)) and \( I = 20.8279 \) nA (\( L = 5 \)) and the error of current between \( L = 4 \) and \( L = 5 \) is about 0.021139%. Therefore, we adopt \( L = 4 \) in the following calculations.

We prepare the initial total system at equilibrium, where \( \mu^\alpha = \mu^{eq} = 0 \). When applying a voltage to the left (L) and the right (R) leads, the system goes out of equilibrium, and the time-dependent current flowing into the \( \alpha \)-lead \( L_\alpha (t) \) can be presented [19]
\[ I_\alpha (t) = i \sum_{\mu} \text{tr}_{\text{res}} \left[ \rho_{\mu \mu}^\dagger (t) \dot{a}_\mu - a_\mu^\dagger \rho_{\mu \mu} (t) \right] \]  
(10)

Here, \( \rho_{\mu \mu}^\dagger = (\rho_{\mu \mu})^\dagger \) is the first-tier auxiliary density operator which is acquired via solving Equation(5). A closed EOM formalism can be achieved via the extended Meier–Tannor parametrization method and multiple-
Before proceeding further, let us make some comments on the advantages and disadvantages of the HEOM approach applied to the dynamical processes of a Kondo system. The main advantages are as follows: 1) the HEOM approach adopts a general form of the system Hamiltonian. It is applicable to a wide range of system parameters without additional derivation and programming efforts. The different transport processes can be handled in a unified manner and the transient dynamics can be studied readily; 2) the HEOM method is nonperturbative. It treats quantum impurity systems from the perspective of open dissipative dynamics. In principle, the HEOM formalism is formally exact for noninteracting electron reservoirs. It also resolves nonperturbatively the combined effects of e–e interactions; 3) the HEOM theory is established based on the Feynman–Vernon path–integral formalism, in which all the system–bath correlations are taken into consideration. It is capable of characterizing both static and transient electronic properties of strongly correlated systems; and 4) the HEOM is a high-accuracy numerical approach. It has the ability to achieve the same level of accuracy as the latest high-level NRG method [17]. On the other hand, the HEOM method only studies the case of finite temperatures, and cannot deal with the zero temperature case at present. The computational cost increases dramatically as the system temperature decreases. For a lower temperature, a higher truncation level is necessary to ensure numerical convergence, leading to a rapid growth of the required computational resources. It is, however, possible to design more efficient reservoir memory decomposition schemes to dramatically reduce the computational resource requirements [12, 13, 20].

As a test, we compare our HEOM results of the single-level resonance tunneling with those obtained by the analytical method and other numerical approaches in the literature [5, 6, 8, 11], and summarize the results in figures 1(a)–(d). Figure 1(a) reproduces the time-dependent current \( I(t) \) through a symmetric double-barrier tunneling structure in response to a rectangular bias pulse, as obtained by the analytical formula in [5]; figure 1(b) reproduces the \( I(t) \) for a single energy level model in response to rectangular bias voltage pulses as obtained by the NEGF method in [6]; figure 1(c) reproduces the \( I(t) \) for a spinless quantum dot system, as obtained with the TD-DMRG method in [8]; and figure 1(d) reproduces the time-dependent occupancy \( n_{\sigma}(t) \) at different temperatures in response to a sudden change in the energy of the quantum dot, as obtained by the TD-NRG approach in [11]. In the HEOM calculations, the parameters are chosen as close as possible to those in other numerical approaches corresponding to [6, 8, 11], while figure 1(a) just shows one numerical example to compare with the analytical formula in [5]. The temperature \( T \) is chosen much lower than \( \Delta \), under which condition the current is proved to be almost independent of \( T \); thus the value of \( T \) is not shown in figures 1(a)–(c).

By referring to figures 1(a)–(c) and corresponding references [5, 6, 8], one can see that our HEOM approach can achieve consistent results of the oscillation of \( I(t) \) through single-level resonance tunneling. Let us make some comments on its mechanism. The time-dependent current flowing in the systems will include capacitive contributions from the accumulation and depletion layers on either side of the tunneling leads. The temporal coherence of electrons tunneling through the resonant level leads to the oscillations, which means the charge in the accumulation layers does not have sufficient time to follow the external bias. The period of the current oscillation is about \( \Delta T_{LR} = \frac{2\pi \hbar}{\left| eV_{LR} - \epsilon_k \right|} \), where \( V_{LR} \) is the bias voltage of the left(right) lead and the \( \epsilon_k \) is the energy of the resonance level of the quantum dot [5]. The oscillations of the current reflect the movement of density of states of the sidebands through the left and right Fermi energies, and the form of the oscillations depends strongly on the size of the applied bias [6, 8].

### 3. Current driven by voltage pulse in quantum-impurity systems

Now we consider the oscillation of dynamical current in the Kondo regime, which is more interesting than above single-level resonance tunneling. There is no energy level near the Fermi energy or within the transport window in this case, thus neither large current nor current oscillation can be observed without the Kondo effect. As we know, the Kondo resonance at low temperature will induce large current. In this case, a new kind of current oscillating behavior different from that in figure 1 is expected. We will study the oscillation of dynamical current for two such cases: 1) a single quantum-impurity system; and 2) a parallel-coupling double quantum-impurity system. For the former case, we will investigate in detail the dependence of the current oscillation on various factors, such as the form of the bias voltage, temperature and band width of the leads.
3.1. Single quantum-impurity systems

We first consider the single quantum-impurity systems. The Hamiltonian of the impurity can be written as

\[ H_{\text{single}} = \sum_{\sigma} \epsilon_{\sigma} \hat{a}_{\sigma}^{\dagger} \hat{a}_{\sigma} + \frac{U}{2} \sum_{\sigma} n_{\sigma} n_{\sigma}, \]  

(11)

which is exactly the single impurity version of equation (2), thus the meanings of each symbol in equation (11) are the same as those in equation (2).

Figure 2 depicts the current \( I(t) \) characteristics of a single quantum-impurity system which possesses electron–hole symmetry \( (\epsilon_{\uparrow} = -\epsilon_{\downarrow}) \) subject to various forms of the time-dependent step voltage.

\[ V(t) = \begin{cases} \ 0 & (t < 0) \\ V_0 & (t \geq 0) \end{cases} \]  

(12)

\( V_0 \) is the step voltage values, \( V_0 = 0.10 \text{ mV}, 0.15 \text{ mV}, 0.20 \text{ mV}, 0.30 \text{ mV} \) respectively. As shown in figure 1, when the voltage pulse is applied to the leads, the current flowing through the device engenders. After the current rapidly increases to a maximal value, regular oscillations emerge, which result from the temporal coherence of electrons tunneling through the quantum impurity in response to the abrupt change of bias voltage. We find that the form of the oscillations depends strongly on the size of the applied step voltage.

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To check the details of the influence of the voltage on the behavior of current \( I(t) \), we alter the step-increasing voltages into linear-increasing ones. As shown in figure 3(a), the voltages linearly increase to \( V_0(t) = 0.25 \text{ mV} \), \( V_1(t) = -0.5 \text{ mV} \), \( V_2(t) = 0.5 \text{ mV} \), \( V_3(t) = -0.1 \text{ mV} \), \( V_4(t) = 0.1 \text{ mV} \), respectively. As shown in figure 3(b), when the voltage pulse is applied to the leads, the current flowing through the device engenders. After the current rapidly increases to a maximal value, regular oscillations emerge, which result from the temporal coherence of electrons tunneling through the quantum impurity in response to the abrupt change of bias voltage. We find that the form of the oscillations depends strongly on the size of the applied step voltage. With the increase of the voltage, the time-dependent current becomes stronger and the amplitude of oscillations intensifies. For example, the maximal amplitude of current \( I(t) \) is only 7000 pA at the voltage \( V_0 = 0.10 \text{ mV} \), while it reaches 13000 pA when \( V_0 = 0.30 \text{ mV} \); meanwhile the frequency of the oscillations increases. On the other hand, all of the current values will arrive at different stable values at \( t > 30 \text{ ps} \), independent of the form of the voltage pulse. Those current values obviously correspond to the steady-state current.

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current $I(t)$ for the above linear-increasing voltages under the same temperature $T$ and band width $W$. The other parameters are $K_B T = 0.015 \text{ meV}, \Delta = 0.2 \text{ meV}, W = 2 \text{ meV}, U = 2 \text{ meV}$ and $\epsilon_1 = \epsilon_1 = -1 \text{ meV}$. It is interesting to see that the currents under the linear-increasing voltages remain oscillating, which decreases with the increase of time and then vanish after a sufficient amount of time. The maximal amplitudes of the current reduce with the increase of $t_c$, for example, the maximal value of the current gets up to 9000 pA for $t_c = 10 \text{ ps}$, while it only reaches 5000 pA for $t_c = 80 \text{ ps}$.

It has been demonstrated that the oscillations of the current mainly result from the temporal coherence of electrons tunneling through the device, which can be manipulated by way of the applied voltage as shown in figure 3. For $t_c = 10 \text{ ps}$, the oscillation of $I(t)$ is fast (with a short period) and dramatic (with a large amplitude), since the carriers have insufficient time to redistribute and catch up the variation of voltage [19]. In contrast, when $t_c$ increases to 80 ps, the oscillation of $I(t)$ becomes very slow and insignificant due to the longer relaxation time of the carriers.

To further understand those effects of the transport current, we then vary the temperature $T$, the band width $W$ and the $e-e$ interaction $U$, and summarize the results in figures 4 to 6. In figure 4, we show the various $I(t)$--$t$ curves changing with the temperature in the Kondo regime ($T < T_K$). As shown in the figure, the oscillation of $I(t)$ is distinct with a large amplitude at very low temperature such as $K_B T = 0.015 \text{ meV}$. With the increase of $T$, the oscillation will be suppressed gradually, for example, it changes to a little wobble around the steady current at $K_B T = 0.045 \text{ meV}$. At $K_B T = 0.060 \text{ meV}$, the oscillation almost dies away and $I(t)$ reaches its stable value very quickly. In the insert of figure 4, we show the spectral functions of the system without the bias voltage around $\omega = 0$ corresponding to the above four temperatures. As shown in the figure, the height of the Kondo peak is
reduced with the increase of temperature, indicating the suppression of the Kondo effects. Once the bias voltages apply to the leads of the device, each of the Kondo resonance peaks at $\omega = 0$ is split into two peaks at $\omega = \pm eV$ ($V$ is the stable value of the voltage applied to the leads). The temperature plays a restraining role in the dynamic transport of the quantum-impurity systems. Summarizing figure 4 and its inset figure, one can conclude that the temperature suppresses the oscillation of dynamic current through its suppression of the Kondo effects. The temperature-dependent current oscillation shown in figure 4 is totally different from temperature-independent case shown in figure 1.

We then elucidate the influence of the finite band width $W$ on the current oscillation, which is hard to treat by the NEGF approach within the WBL approximation. The characteristics of dynamic $I(t)$ corresponding to different band widths are shown in figure 5. It can be seen that the larger band width $W$ principally leads to larger amplitude of current oscillation as well as a larger value of steady-state current. This effect mainly results from the $W$-enhancement of the capacitive contributions from the accumulation and depletion of electrons layering on either side of the device leads. On the other hand, as shown in figure 5, the frequency of the oscillation is almost independent of the band width $W$.

In the end of this subsection, we investigate the effect of e–e interaction $U$ on the current oscillation. In our calculations, electron–hole symmetry is kept, i.e. the on-site energy of each dot is chosen as $\epsilon_i = \epsilon_i = -U/2$. Figure 6 shows the results for both cases of $T < T_K$ (figure 6(a)) and $T > T_K$ (figure 6(b)). Generally speaking, the on-site e–e interaction will induce localization of the carriers, which causes the steady current to decrease with the increase of $U$, as shown both in figures 6(a) and (b). In the Kondo regime, the amplitude of the current oscillation decreases with the increase of $U$, but the frequency remains almost unchanged. The mechanism can be understood as follows: according to the analytical expression for Kondo temperature.
$T_K = \sqrt{\frac{\Delta}{2}} e^{-\Delta/\hbar + \pi \Delta/2U}$ [21] ($\Delta$ as two leads in our system), $T_K$ decreases with the increase of $U$. Since the temperature is fixed (at $K_B T = 0.015$ meV), a larger $U$ will induce a smaller distance between $T$ and $T_K$. As a consequence, the current oscillation will take place more dramatically for smaller $U$. For example, the maximal amplitude of the oscillation increases from 4600 pA at $U = 2.4$ meV to 11000 pA at $U = 2.0$ meV.

In order to verify whether the increase of current oscillation with the decrease of $T$ is a direct result of Kondo resonance or the simple temperature effect, we calculate $I(t)$ curves in the limit of non-interacting ($U = 0$) and large voltage $V = 0.6$ meV at different $T$ for $k_B T < \Delta$ (c) and $k_B T > \Delta$ (d).

Figure 6. The $I(t)$ curves of the symmetric quantum-impurity system with different $e-e$ interactions $U$. (a) In the Kondo regime ($T < T_K$), the parameters adopted are $V_L = V_R = 0.20$ mV, $W = 2$ meV, $k_B T = 0.015$ meV, $\Delta = 0.2$ meV, and $\epsilon_1 = \epsilon_2 = -U/2$. (b) Out of the Kondo regime ($T > T_K$), the parameters adopted are $V_L = V_R = 0.20$ mV, $W = 2$ meV, $k_B T = 0.32$ meV, $\Delta = 0.2$ meV, and $\epsilon_1 = \epsilon_2 = -U/2$. The $I(t)$ curves of the symmetric quantum-impurity system in the limit of non-interacting $U = 0$ and large voltage $V_{SD} = 0.6$ meV at different $T$ for $k_B T < \Delta$ (c) and $k_B T > \Delta$ (d).

Let us make some comments on the dependence of the steady current on $U$ in the limit of small bias $V_{SD} \ll k_B T_K$. At the temperature $T = 0$, the Fermi liquid behavior of the Kondo resonance makes the spectrum function at $\omega = 0$ independent of $U$ [22], which will cause the current also become independent of $U$ for $V_{SD} \ll k_B T_K$ [23]. At finite temperature, the spectrum function at $\omega = 0$ will drop with the increase of $U$ [17], so $I(t)$ shows weak dependence on $U$ at low but finite $T$, even at small biases $V_{SD} \ll k_B T_K$, as verified in our HEOM calculations.

Summarizing figures 2–6, one can conclude that the frequency of the current oscillation is strongly dependent on the bias voltage $V(t)$ but almost independent of $T$, $W$ and $U$ as well.

3.2. Double quantum-impurity systems

Double quantum-impurity systems, also considered as artificial molecules, are very important for the study of many novel phenomena such as the two-impurity Kondo effect and non-Fermi liquid behavior. Moreover, those structures are convenient for realizing the solid state quantum bits as reported in the literature [24–26]. Here, we just focus on the oscillation of the dynamical current in the parallel-coupling double quantum-
impurity systems, with each of the impurities keeping a single occupation. The Hamiltonian for such sub-systems can be written as,

$$H_{\text{double}} = \sum_{\sigma=1,2} \left[ \epsilon_{i\sigma} \hat{a}_{i\sigma}^\dagger \hat{a}_{i\sigma} + U_i n_{i\sigma} n_{i\sigma} \right] + \gamma \sum_{\sigma} \left( \hat{a}_{1\sigma}^\dagger \hat{a}_{2\sigma} + \text{H. c.} \right)$$

which is exactly the double impurity version of equation (2), thus the meanings of each symbol in equation (13) are the same as those in equation (2), too.

Recently, R Hartle et al studied electron transport through an interacting double quantum dot system by using a modified version of our HEOM approach [27]. The interplay between interference effects and electron–electron interactions in electron transport was discussed in their paper. Decoherence due to electron–electron interactions is found to give rise to pronounced negative differential resistance [27]. We comment that their steady current at room temperature is different from the dynamical current in the Kondo regime we investigate here.

Figure 7 depicts the dynamical current $I(t)$ of a parallel-coupling double quantum-impurity system subject to a step voltage in the Kondo regime. In our calculations, each of the impurities holds the electron–hole symmetry, with the same parameters as the single quantum-impurity system as shown in figure 2. For comparison, the constant values of the step voltage are also chosen to be the same as those in figure 2, i.e. $V_0 = 0.10 \text{ mV}, 0.15 \text{ mV}, 0.20 \text{ mV}$ and $0.30 \text{ mV}$. In figure 7, we take the tunneling coupling between the two impurities as a weak one $\gamma = 0.1 \text{ meV}$. As reported in our previous work [17], this weak coupling maintains the Kondo singlet of each impurity, which will double the transport channels. That point has been clearly elucidated in figure 8, where the parameters are chosen as $K_0 T = 0.015 \text{ meV}, \Delta = 0.2 \text{ meV}, W = 2 \text{ meV}, V_L = -V_R = 0.3 \text{ mV}, U_1 = U_2 = 2 \text{ meV}, \epsilon_{11} = \epsilon_{12} = -1 \text{ meV}, \epsilon_{21} = -1 \text{ meV}$. Together with the time-dependent current $I(t)$ curves, we also show the total equilibrium spectral function of the system ($V_L = V_R = 0$) in the inset of figure 8. By referring the figure, one can see that with the increase of $\gamma$ the oscillation of the dynamical current changes dramatically, with some features of the quantum phase transition clearly shown. In the regime of small $\gamma$, the direct first-order coupling $(\gamma)$ is much stronger than the induced second-order antiferromagnetic spin coupling ($J = 4 \gamma^2 / U$) between two impurities. As a consequence, the ground state of the systems is the degenerate Kondo singlet states of individual impurity, with the equilibrium spectral function showing a single peak at $\omega = 0$. The behavior of the current oscillation in this case is analogous to the single impurity one, as already confirmed in figure 7. Besides, a new feature called the ‘$\gamma$-enhanced Kondo effect’
can be seen in figure 8, which is shown by an increased amplitude but equal frequency in the oscillation of the dynamical current (compare the $I(t)$ curves of $\gamma = 0$ and 0.1 meV). We will report our detailed study on the $\gamma$-enhanced Kondo effect elsewhere. In the regime of large $\gamma$, the spin–spin coupling $J$ dominates, which locks the ground state as a spin-singlet state between two impurities. The Kondo peak of the equilibrium spectral function at $\omega = 0$ thus disappears, and consequently the current oscillation is suppressed, as shown in figure 8 (see the $I(t)$ curve of $\gamma = 0.4$ meV).

In the regime of medium $\gamma$, the crossover of the phase transition between the above two ground states takes place. By referring to figure 8, we can find two interesting features of the current oscillation: 1) although the peak of spectrum function at $\omega = 0$ has already changed to a dip, the double peaks in the transition window still cause oscillations of current with smaller amplitude; and 2) the frequency of the current oscillation for the double-peak and single-peak states is almost the same, but the phase is exactly reversed (compare the $I(t)$ curves of $\gamma = 0.1$ and 0.2 meV for detail).

4. Summary

In summary, we have investigated the time-dependent transport properties of single and double quantum-impurity systems based on the hierarchical equations of motion. In the Kondo regime, the dynamical current in both cases is found to be oscillating due to the temporal coherence of electrons tunneling through the device, which shares the same mechanism as the single-level resonance without e–e interactions but shows some different characteristics.

For single quantum-impurity systems, the temperature has an inhibitory effect on the oscillations of dynamic current through its suppression to the Kondo effects. The amplitude of the current oscillations is found to be enhanced by the band width $W$ of the leads but attenuated by the e–e interaction $U$ in the Kondo regime. The reason for the latter phenomenon is that the e–e interaction will partly weaken the Kondo effects at fixed temperature $T$ by means of inducing a smaller distance between $T$ and $T_K$. We find the steady-state current decreases with the increase of $U$ for both cases of $T < T_K$ and $T > T_K$. On the other hand, the frequency of the current oscillation is found to be almost independent of $T$, $W$ and $U$.

For parallel-coupling double quantum-impurity systems, the steady current is approximately twice the single one and the oscillation of $I(t)$ shows similar behaviors to the single one, but with two- to three-times larger amplitudes. With the increase of the inter-impurity coupling $\gamma$, the system undergoes a quantum phase transition process from the degenerate Kondo singlet states of individual impurity to singlet spin states formed between two impurities. Reflecting on the dynamical current, the oscillation of the current exhibits enhanced characters due to the ‘$\gamma$-enhanced Kondo effect’ at low $\gamma$ limit, while the oscillation will be subdued at the other limit (with large $\gamma$). These characteristics may be observed in experiments.
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