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A Floquet–Green's function approach to mesoscopic transport under ac bias

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Abstract

The current response of a mesoscopic system under a periodic ac bias is investigated by combining the Floquet theorem and the nonequilibrium Green's function method. The band structure of the lead under ac bias is fully taken into account by using appropriate self-energies in an enlarged Floquet space. Both the retarded and lesser Green's functions are obtained in the Floquet basis to account for the interference and interaction effects. In addition to the external ac bias, the time-varying Coulomb interaction, which is treated at the self-consistent Hartree–Fock level, provides another internal ac field. The numerical results show that the time-varying Coulomb field yields decoherence and reduces the ringing behavior of the current response to a harmonic bias.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

With the fast development of technology, people are now empowered to fabricate conductors on the mesoscale and nanoscale [1]. The linear or nonlinear response of the mesoscopic system to an external driving field can be used to reveal the underlying physics in the quantum regime [2–6]. Comparing with the stationary field, a time-varying one can provide an effective way to modulate the quantum phase of wavefunctions [7]. For chaotic quantum dots, this modification of phase evolution gives rise to a variety of mesoscopic phenomena ranging from the conductance fluctuations [8–10] to the dynamical localization [11, 12]. The ac effect on these properties can be statistically described by the diagrammatic Green's function method or using random matrix theory [13]. For small open quantum dots, time-dependent transport has been studied by the nonequilibrium Green's function method [6, 7]. There, a general expression for the current under an arbitrary ac field is expressed in terms of double-time functions which are nontrivial for either analytical or numerical simulations. As a matter of fact, the solutions of those general formulas rely on approximations such as the wide-band limit. However, this approximation becomes inapplicable in situations, such as that of molecular electronics, where the system response is sensitive to the band structure.

Recently, particular interest has been attracted by the quantum charge/spin pumping [14, 15], where a dc current is generated by a periodic driving field at zero dc bias. Fortunately, instead of having to solve an arbitrary nontrivial time-dependent Schrödinger equation, the periodic condition imposed by the ac field makes the power of the Floquet theorem available [16–19]. By combining the Floquet theorem and the scattering matrix method [20], the quantum pumping of charge or spin current beyond the adiabatic limit has been investigated. More recently, a retarded Floquet–Green's function [21] was derived in the wide-band limit for investigating the transport properties of molecular wire driven by an ac field. A coherent suppression of the current and shot noise by the ac field is predicted, though the validity of the wide-band limit on the molecular scale is unclear. To circumvent the wide-band approximation, a more general treatment of the lead structure was then proposed [22, 23] by using a tight-binding description of the *static* lead.

Although the quantum interference in these studies is well accounted for, the nonequilibrium distributions and interaction effects are much less studied. As a matter of fact, in these studies, only the retarded Floquet–Green's function is needed to find the current or noise properties. The nonequilibrium occupation in the conductor which may be important in the presence of interaction effects is not characterized. Moreover,

the ac field in previous studies is confined to the conductor regime which may origin from either an oscillating gate voltage or a microwave (infrared) laser. However, if the system is driven out of equilibrium by an oscillating bias as in [7], a direct application of the formalisms mentioned above becomes improper since electrons in the lead are no longer equilibrium; instead their energies as well as phases can vary with time.

In this work, with the help of the Floquet theorem and nonequilibrium Green's function method, the general formula for time-dependent transport proposed by Jauho *et al* [7] is reformulated using the Floquet–Green's functions for periodic ac bias. With the Floquet theorem to hand, we work in an enlarged Hilbert space to bypass the nontrivial double-time functions in time-dependent phenomena. Both the retarded and the lesser Floquet–Green's functions are obtained from the Keldysh equation in the time domain to account for the interaction effect. The ac bias in leads is well incorporated in the formalism by the appropriate self-energies beyond the wide-band approximation. The Coulomb interaction is self-consistently included under the Hartree–Fock approximation. As an example, the Floquet–Green's function formalism is applied to investigate the transport properties of quantum dots in the presence of harmonic bias.

This paper is organized as follows. In section 2, the Floquet–Green's function formalism is presented for a driving system represented by a tight-binding Hamiltonian. General expressions for the current and the retarded and lesser Floquet–Green's function are presented. As an example, we apply the formalism to the ac transport of a quantum dot with Coulomb interaction in section 3. The quantum response to a harmonic ac bias is displayed and the Coulomb effect on the ac response is discussed. Finally, a brief summary is presented.

2. Theory and formalism

2.1. The Hamiltonian and the general expression for the current

The model system studied here is a one-dimensional quantum wire. It is composed of an interacting central site ($i = 0$) with its left ($i < 0$) and right ($i > 0$) leads. The tight-binding Hamiltonian with nearest-neighbor hopping can be given by

$$H_d = \sum_{i\sigma} \epsilon_\alpha(t) c^\dagger_{i\sigma} c_{i\sigma} + \sum_{\langle ij\rangle\sigma} t_\alpha c^\dagger_{i\sigma} c_{j\sigma} + U c^\dagger_{0\uparrow} c_{0\uparrow} c^\dagger_{0\downarrow} c_{0\downarrow}, \quad (1)$$

where $c^\dagger_{i\sigma}$ ($c_{i\sigma}$) is the electron creation (annihilation) operator at site i with spin index σ ($\sigma = \uparrow$ or $\downarrow$) and the Coulomb interaction in the central site is accounted for by a charging energy U. ϵ_α and t_α are the on-site energy and the nearest-neighbor hopping term where $\alpha =$ L, R or C, represent the left ($i, j < 0$), right ($i, j > 0$) and central parts ($i * j = 0$) respectively. Suppose a time-periodic bias is applied to the system [7]; the on-site energy ϵ_i then becomes time varying with the same period T. For simplicity, the ac strengths in the αth parts are assumed to be uniform but may not be equal to each other. This ac bias will make the electron energy become time dependent and keep the occupation unchanged. The on-site energy ϵ_α can then be expressed in the Fourier expansion due to the periodicity as $\epsilon_\alpha(t) = \epsilon^0_\alpha + \sum_k V^\alpha_k e^{ik\Omega t}$, where ϵ^0_α is the static energy and $\Omega = 2\pi/T$. In order to make the Coulomb interaction term more tractable, we adopt the Hartree–Fock approximation [24], i.e., the replacement $U c^\dagger_{0\uparrow} c_{0\uparrow} c^\dagger_{0\downarrow} c_{0\downarrow} \to U(n_\uparrow c^\dagger_{0\downarrow} c_{0\downarrow} + n_\downarrow c^\dagger_{0\uparrow} c_{0\uparrow})$ was introduced, where $n_\sigma = \langle c^\dagger_{0\sigma} c_{0\sigma}\rangle$ is the on-site population with spin σ. In the presence of a time-dependent field, it should be determined self-consistently as a function of time. As the Hamiltonian is periodic in the time domain, the evolution of the whole system should be a periodic function with the same periodicity. Therefore, the time-dependent Coulomb potential which depends on the occupation can be expressed in the Fourier expansion as $U n_{\bar\sigma}(t) c^\dagger_{0\sigma} c_{0\sigma} = \sum_k U_k e^{ik\Omega t} c^\dagger_{0\sigma} c_{0\sigma}$. As a consequence, the time-dependent response is due to the interplay between the external ac bias and the Coulomb interaction. As the spin degeneracy is conserved in the Hamiltonian, we will drop the spin index and the unit $\hbar = 1$ is used in the following for simplicity.

In the presence of a time-varying field, the time-translational invariance is broken. The functions are no longer all determined by the difference of the two time labels as in the stationary case. Instead, they depend on the two time labels separately. The widely used retarded (r)/advanced (a) and lesser ($<$) Green's functions are defined as

$$G^{r/a}_{ij}(t, t') = \mp i\Theta(t - t')\langle\{c_i(t), c^\dagger_j(t')\}\rangle, \quad (2)$$

$$G^<_{ij}(t, t') = i\langle c^\dagger_j(t') c_i(t)\rangle. \quad (3)$$

As the system is driven by a time-varying field, the current is a function of time. For the tight-binding Hamiltonian discussed above, the current from the left lead can be given by

$$J_L(t) = 2 \cdot 2e t_{-1,0}\, \mathrm{Re}[G^<_{0,-1}(t, t)], \quad (4)$$

where the first factor 2 is due to spin degeneracy and the displacement current is neglected [7]. By using the analytic continuation rules, the lesser Green's function can be written as

$$G^<_{0,-1}(t, t') = \int d\tau [G^r_{00}(t, \tau)\Sigma^<_L(\tau, t') + G^<_{00}(t, \tau)\Sigma^a_L(\tau, t')] \quad (5)$$

where the self-energies due to the coupling between the central dot and the semi-infinite left lead are given by

$$\begin{aligned} \Sigma^a_L(t, t') &= t_{0,-1} G^a_{-1,-1}(t, t') t_{-1,0} \\ \Sigma^<_L(t, t') &= t_{0,-1} G^<_{-1,-1}(t, t') t_{-1,0}. \end{aligned} \quad (6)$$

Here, $G_{-1,-1}(t, t')$ is the surface Green's function of the semi-infinite lead in time domain.

The current from the left lead to the central dot becomes

$$J_L(t) = 4e\, \mathrm{Re} \int d\tau\, [G^r_{00}(t, \tau)\Sigma^<_L(\tau, t) + G^<_{00}(t, \tau)\Sigma^a_L(\tau, t)]. \quad (7)$$

This is nothing but the general expression for time-dependent current [7] in the tight-binding Hamiltonian.

2.2. Floquet–Green's functions and the current expression

Let $O_{ij}(t,t')$ represent the double-time Green's function or self-energy. Its Fourier transform can be defined as

$$O_{ij}(t,\epsilon) = \int \mathrm{d}t'\, \mathrm{e}^{\mathrm{i}\epsilon(t-t')} O_{ij}(t,t'). \tag{8}$$

In the case of periodic ac bias, the function $O_{ij}(t,\epsilon)$ is a periodic function with the same period frequency Ω. Now, we make use of the periodicity of the ac field to bypass the nontrivial double-time formalism.

Due to its periodicity, it is more convenient to work within the Floquet space $\mathcal{R}\otimes\mathcal{T}$, where $\mathcal{R}$ is the real space and $\mathcal{T}$ is the space of time-periodic functions with the set of Floquet bases $|k\rangle = \exp(-\mathrm{i}k\Omega t)$ with $k \in Z$ [17]. The basis in this enlarged space can be given by $|i,k\rangle = |i\rangle \otimes |k\rangle$, where $|i\rangle$ is the localized state at site i. This leads to the following expansion:

$$O_{ij}(t,\epsilon) = \sum_k \mathcal{O}^k_{ij}(\epsilon)\mathrm{e}^{-\mathrm{i}k\Omega t}. \tag{9}$$

The expansion coefficient $\mathcal{O}^k_{ij}(\epsilon)$ in equation (9) can be viewed as the projection of the function O on the orthogonal basis in Floquet space: $\mathcal{O}^k_{ij}(\epsilon) = \langle i,k|\hat{O}(\epsilon)|j,0\rangle$. A useful relation between the projections with different Floquet indices is given by the relation $O_{ik;jk'}(\epsilon) = O_{i(k-k');j0}(\epsilon + k'\Omega)$. Equations (8) and (9) are important and will be used frequently in the following derivations. They connect the functions in Floquet space with their time evolution.

Now, we will derive the Floquet–Green's functions, i.e. the Green's function in Floquet space, as well as the self-energies. Instead of starting from its time evolution, the retarded Floquet–Green function can be more conveniently found from the resolvent [19, 21–23] as $\mathcal{G}^{\mathrm{r}} = \lim_{\eta\to 0} 1/(\epsilon + \mathrm{i}\eta - \mathcal{H})$, where the Floquet Hamiltonian $\mathcal{H}$ is defined as $\mathcal{H}(t) = H(t) - \mathrm{i}\hbar\partial/\partial t$, Its matrix element in the Floquet space $\mathcal{R}\otimes\mathcal{T}$ can be found from

$$\mathcal{G}^{\mathrm{r}}_{i,k;j,k'}(\epsilon) = \langle i,k|\mathcal{G}(\epsilon)|j,k'\rangle. \tag{10}$$

The advanced Floquet–Green's function is given by the conjugate transpose of the retarded Floquet–Green's function as $\mathcal{G}^{\mathrm{a}} = [\mathcal{G}^{\mathrm{r}}]^{\dagger}$. This relation can be verified by noting the relation $G^{\mathrm{a}}_{ij}(t,t') = [G^{\mathrm{r}}_{ji}(t',t)]^*$.

Although the Floquet–Green's function is straightforward from its resolvent definition, it is not realistic to obtain the retarded Floquet–Green's function by direct matrix inversion since the resolvent $\mathcal{G}^{\mathrm{r}}$ is defined for infinite degrees of freedom. In real calculations, we use the self-energies to take the coupling between the central dot and the semi-infinite leads into account. Meanwhile, once the accuracy is fulfilled, the infinite Floquet state is truncated to make the calculation feasible. As the leads are driven by periodic ac bias, the retarded or advanced self-energies should be determined in the enlarged space $\mathcal{R}\otimes\mathcal{T}$ to contain the ac effect. If there is no ac bias in the lead, the Floquet Hamiltonian in the lead is trivially diagonal to the Floquet index k. The band structures for different Floquet indices are identical except for the energy shift. However, if the ac strength is nonzero, the Floquet states in the lead will couple to each other and complicate the band structure. For the stationary situation, a well established tool for finding the surface Green's function is the recursive iteration method [25, 26]. Fortunately, the power of the recursive iteration method is still available here for calculating the surface Floquet–Green's function, as well as the Floquet self-energies, though the space has been enlarged. For example, the present Floquet Hamiltonian of the αth lead is given in the Floquet space as

$$\langle i,k|\mathcal{H}_\alpha|j,k'\rangle = (\epsilon^0_\alpha - k\hbar\Omega)\delta_{kk'}\delta_{ij} + V^\alpha_{k'-k}\delta_{ij} + t_\alpha\delta_{kk'}\delta_{i,j\pm1}. \tag{11}$$

We note that the Floquet self-energy obtained by the recursive iteration method is numerically exact and beyond the wide-band limit. It contains the fine structure of the lead due to its internal degree of freedom as well as the ac bias. Figure 1 shows the numerically obtained self-energy for semi-infinite wire in the presence and absence of an ac field. The upper panel of figure 1 shows the real and imaginary parts of $[\mathcal{E}^{\mathrm{L,r}}_{00}]_{00}$ which are obtained with the harmonic ac bias $V(t) = 1.2\cos(0.2t)$ and $t_\alpha = 1$. For comparison, the self-energy in the absence of an ac field is displayed in the lower panel of figure 1. It is obvious that the ac field has modified the self-energy profile, especially at the band edges, dramatically.

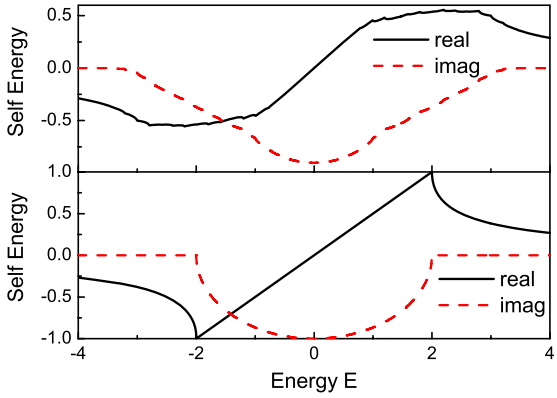

Figure 1. Self-energy profiles for the one-dimensional semi-infinite tight-binding model in the presence (upper panel) and absence (lower panel) of a harmonic ac field. The upper level shows the element $[\mathcal{E}^{\mathrm{L,r}}_{00}]_{00}$ of the self-energy matrix in Floquet space. The energy unit is chosen as the hopping term $t_\alpha = 1$. The ac frequency $\Omega = 0.2$ and its strength $V = 1.2$.

With the retarded Floquet self-energy to hand, the Floquet Green's function of the central dot can be found from

$$\mathcal{G}^{\mathrm{r}}_{00}(\epsilon) = \frac{1}{\epsilon - \mathcal{H}_0 - \mathcal{E}^{\mathrm{L,r}}_{00} - \mathcal{E}^{\mathrm{R,r}}_{00}}, \tag{12}$$

where $\mathcal{H}_0 = \epsilon_{\mathrm{C}}(t)c^\dagger_0 c_0 - \mathrm{i}\hbar\partial/\partial t$ and $\mathcal{E}^{\alpha,\mathrm{r}}_{00}$ is the retarded Floquet self-energy of the central dot due to its coupling to the αth lead. For the present Hamiltonian, the matrix element of the Floquet Hamiltonian is given by $\langle 0,k|\mathcal{H}_0|0,k'\rangle = (\epsilon^0_{\mathrm{C}} - k\hbar\Omega)\delta_{kk'} + (V^{\mathrm{C}}_{k'-k} + U_{k'-k})$. The last two terms represent the ac driving fields in the central dot where V^{C} arises from *external* ac bias while U originates from the *internal* Coulomb interaction. The Coulomb field U must be obtained self-consistently as discussed in the following.

One next needs to have the lesser Green's function $G^<_{00}(t,t')$ in Floquet space. This double-time function is given by the Keldysh equation as [6, 7]

$$G^<_{00}(t,t') = \int \mathrm{d}t_1 \int \mathrm{d}t_2\, G^{\mathrm{r}}_{00}(t,t_1) \times \sum_{\alpha=\mathrm{L,R}} \Sigma^{\alpha,<}_{00}(t_1,t_2) G^{\mathrm{a}}_{00}(t_2,t'), \tag{13}$$

with the lesser self-energy due to the αth lead

$$\Sigma^{\alpha,<}_{00}(t,t') = -\int \mathrm{d}t_1\, f_\alpha(t-t_1)(\Sigma^{\alpha,\mathrm{r}}_{00}(t_1,t') - \Sigma^{\alpha,\mathrm{a}}_{00}(t_1,t')), \tag{14}$$

where $f_\alpha(t) = \int \mathrm{d}\epsilon\, f_\alpha(\epsilon)\mathrm{e}^{-\mathrm{i}\epsilon t}/2\pi$ is the Fourier transform of the Fermi energy $f_\alpha(\epsilon)$ in the αth lead since we have assumed an equilibrium distribution in the leads [7]. $\Sigma^{\alpha,\mathrm{a}}_{00}$ is the advanced self-energy due to coupling to the αth lead. The choice of the ac bias in the lead is quite subtle as discussed in [7]. We introduce the ac bias according to the gage proposed by Jauho *et al* [7]. The ac bias makes the electron energy time dependent while the occupation function in the lead remains unchanged. Therefore, the Fermi function in the time domain $f_\alpha(t)$ is still a function of the time difference in the present study. The lesser self-energy in the time domain can also be decomposed in the Floquet basis. After some algebra, the lesser self-energy in the Floquet basis $\mathcal{E}^<_{00} = \sum_{\alpha=\mathrm{L,R}} \mathcal{E}^{\alpha,<}_{00}$ is given by

$$\mathcal{E}^{\alpha,<}_{00}(\epsilon) = -[\mathcal{E}^{\alpha,\mathrm{r}}_{00}(\epsilon) - \mathcal{E}^{\alpha,\mathrm{a}}_{00}(\epsilon)]\mathcal{F}_\alpha(\epsilon), \tag{15}$$

where $\mathcal{F}_\alpha$ is a diagonal matrix and its matrix element with Floquet index k, k' is given by

$$[\mathcal{F}_\alpha(\epsilon)]_{k,k'} = f_\alpha(\epsilon + k\Omega)\delta_{kk'}. \tag{16}$$

$\mathcal{F}_\alpha$, which is a diagonal matrix with an energy shift between matrix elements, resembles the scalar Fermi function used in the expression for stationary self-energy.

With the lesser self-energy and the retarded and advanced Green's functions obtained above and after some calculations, the lesser Green's function defined in equation (13) can be rewritten in the Floquet basis as

$$\mathcal{G}^<_{00}(\epsilon) = \mathcal{G}^{\mathrm{r}}_{00}(\epsilon)\mathcal{E}^<_{00}(\epsilon)\mathcal{G}^{\mathrm{a}}_{00}(\epsilon). \tag{17}$$

Equation (17) is the Keldysh equation for the lesser Floquet–Green's functions. Interestingly, the appearance of equation (17) resembles greatly the Keldysh equation for stationary situations. This lesser Floquet–Green's function contains information such as the time evolution of the nonequilibrium distribution in the dot. This enables us to enclose the self-consistent procedure due to Coulomb interaction. The electron occupation number in the dot as a function of time can be written as

$$n_\sigma(t) = \mathrm{Im}\int \frac{\mathrm{d}\epsilon}{2\pi} G^<_{00}(t,\epsilon) = \mathrm{Im}\int \frac{\mathrm{d}\epsilon}{2\pi} \sum_k [\mathcal{G}^<_{00}(\epsilon)]_{k0}\mathrm{e}^{-\mathrm{i}k\Omega t}. \tag{18}$$

The Fourier expansion coefficients of $n_\sigma(t)$ determine the ac driving force produced by the Coulomb interaction.

Finally, by expressing the quantities in the current formula in terms of the Floquet basis, we arrived at the general expression for the current in the Floquet–Green's function as

$$J_{\mathrm{L}}(t) = 4e\,\mathrm{Re}\left\{\int \frac{\mathrm{d}\epsilon}{2\pi} \sum_{k,k'} [\mathcal{G}^{\mathrm{r}}_{0k;0k'}(\epsilon)\mathcal{E}^{L,<}_{k'0}(\epsilon) + \mathcal{G}^<_{0k;0k'}(\epsilon)\mathcal{E}^{\mathrm{L,a}}_{k'0}(\epsilon)]\mathrm{e}^{-\mathrm{i}k\Omega t}\right\}. \tag{19}$$

This formula is the central result of the present work. It expresses the time-dependent current in terms of the Floquet–Green's functions and their corresponding Floquet self-energies. The interaction effect as well as the ac field in the central dot can be included in the appropriate Floquet–Green's function of the central dot, while the effect of ac bias in leads is contained in the Floquet self-energy. An analogous formula can be arrived at for the current flowing to the right lead, $J_{\mathrm{R}}(t)$, though $J_{\mathrm{L}}(t)$ may not be equal to $J_{\mathrm{R}}(t)$ due to the ac driving. In the absence of an ac bias in the lead, i.e. where the ac field is confined in the dot, the Floquet self-energy due to the semi-infinite lead will be diagonal in the Floquet index k. By inserting equations (12), (15), and (17) into the current formula equation (19) and taking the time average, one can readily recover the averaged current formula given in [21]. In the above derivations, only single-channel transport is considered. However, the generalization to ac driven multi-channel cases is straightforward.

It is interesting to make a brief comparison between the present formalism and the nonequilibrium Green's function formalism for stationary multi-channel transport which can be found in for example [6] and [7]. The similarity of the two formalisms to matrix multiplication is obvious. The main difference is in the matrix basis where the quantities for the stationary multi-channel case are expanded in the transport eigenchannels while in ac driving they are expanded in the Floquet basis. This similarity implies that each Floquet state may play, to some extent, the role of a transport channel in the presence of an ac field [2, 27].

3. Current driving by a harmonic ac bias

As an example, we numerically investigated the current response of a tight-binding wire driven by a harmonic ac bias by applying the present formalism. The left and right leads are assumed identical. The dc voltage is V, which shifts the Fermi energy of the left and right lead as follows: $\epsilon^{\mathrm{L}}_{\mathrm{F}} = \epsilon^0_{\mathrm{F}} + V/2$ and $\epsilon^{\mathrm{R}}_{\mathrm{F}} = \epsilon^0_{\mathrm{F}} - V/2$ due to symmetric coupling. Here ϵ^0_{F} is the Fermi energy at equilibrium. In the following, we fix $\epsilon^0_{\mathrm{F}} = 0$. The harmonic bias is applied to the left lead and the central dot as

$$V_{\mathrm{L/C}}(t) = V_{\mathrm{L/C}}\cos(\Omega t). \tag{20}$$

The hopping term in the leads is assumed uniform and fixed at $t_{\mathrm{L}} = t_{\mathrm{R}} = 1$ as the energy unit. The band structure of the stationary one-dimensional wire is well known to have a bandwidth of $4t_{\mathrm{L}}$. Here, the coupling between the lead and the central dot, t_{C}, may be varied. The level width of the central dot depends on this coupling. The ratio of the level width of

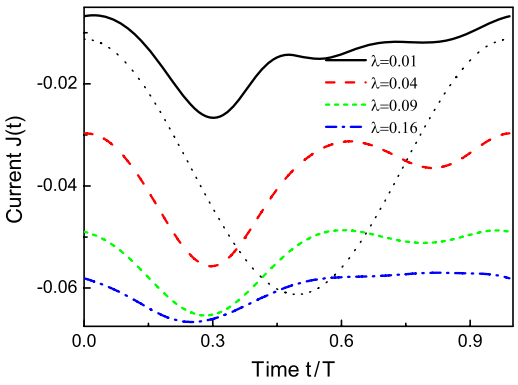

Figure 2. Time-dependent current through a wire with a single oscillating site for different level width parameters λ. The ac bias is depicted as a dotted thin line. The current is given in the units of $\hbar = 1$ and $e = 1$. The charging energy U is taken to be zero.

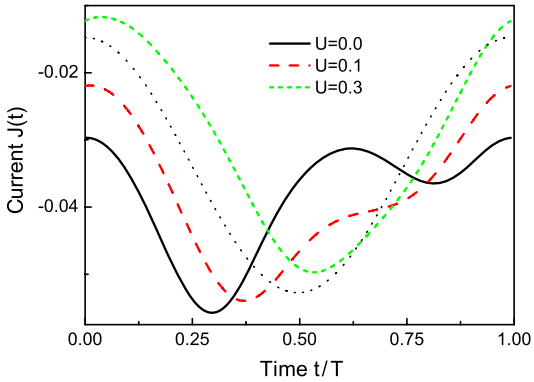

Figure 3. Time-dependent current for different Coulomb strengths U in the presence of an ac field. The ac field is depicted as a dotted thin line in the figure. The model and other parameters are the same as those for figure 2 except that we have fixed $\lambda = 0.04$.

the central dot and the bandwidth of the lead can be defined as $\lambda = (t_C/t_L)^2$. For $\lambda \ll 1$, the system approaches the wide-band limit.

By increasing λ, we may check the influence of the finite bandwidth on the ac response. In figure 2, we show the time-dependent current for different λ values in the absence of Coulomb interaction. The ac signal is indicated as a black dotted line in the figure. The dc bias is $V = 0.2$. The external ac field on the left lead is given by $V_L(t) = 0.2\cos(\Omega t)$ with the frequency $\Omega = 0.05$. The central part is driven by the same frequency but with different ac strength $V_C = 0.1$. The temperature $k_B T = 0.01$, where k_B is the Boltzmann constant. The numerical results clearly show that the current response is sensitive to the band structure. For $\lambda = 0.01$, the level width is much smaller than the bandwidth of the lead. The transport is in the wide-band limit. For this case, despite the maximum and minimum values, some oscillation appears in the current curve. This observation is in accordance with the ringing phenomenon predicted in previous studies [7] with the wide-band limit. However, our numerical results show that the ringing of the current in response to an ac bias cannot survive when the wide-band limit approximation no longer holds. As we increase the value of λ, for example to $\lambda = 0.16$ in figure 2, the level width increases to be comparable to the bandwidth. The oscillating structures disappear. The current curve becomes much smoother than that for the lower λ case.

As the Coulomb effect and other interactions in the ac response are largely ignored in previous studies, we numerically investigated the Coulomb effect on the ac response of a quantum dot. In figure 3, the current response to a harmonic bias is presented with different Coulomb interaction strengths U. The ac signal is displayed as a dotted line too. The other parameters are the same as those for figure 1 except that we have fixed $\lambda = 0.04$ and different values of U. For the given parameters, figure 3 has shown that on increasing the Coulomb strength, the fast oscillation in the current for zero Coulomb field decreases. It tends to follow the external ac field for very large Coulomb strength. This behavior can be understood as follows. The complicated oscillation behavior in the absence of Coulomb interaction arises due to the coherence of the leads and the resonant site [7]. However, the existence of a Coulomb field can effectively change the energy level as well as the electron phase evolution. The time-dependent Coulomb interaction brings decoherence into the electron dynamics. Obviously, this dephasing effect increases with the Coulomb strength. Therefore, if the Coulomb strength is large enough, the coherence of the electrons in the lead and the dot will be reduced. As a consequence, the ringing of the current response will be suppressed for large U as shown in figure 3. Therefore, to experimentally observe the ringing behavior of the current response predicted in [7], it is better to avoid strong Coulomb interactions.

4. Conclusion

In summary, a formalism obtained by combining the Floquet theorem and the nonequilibrium Green's function has been presented for studying the transport under periodic ac driving. The time-dependent current formula was obtained by using the retarded and lesser Floquet–Green's functions as well as the corresponding self-energies. Both the ac bias on the leads and the finite bandwidth effect can be taken into account in the self-energy in the Floquet space, which can be obtained via the recursive iteration method. Moreover, the Coulomb effect is accounted for in the self-consistent Hartree–Fock level. Due to the presence of the ac field, the occupations as well as the Coulomb interaction in the quantum dot become time dependent. Not only the external ac bias, but also the time-varying Coulomb field which can modulate the dot level provides another internal ac field. As an example, the present formula is applied to the transport of a quantum dot under harmonic bias. The numerical results show that the band structure of the leads and the Coulomb effect are paramount in determining the nonlinear current response to an ac bias.

The model used here is a tight-binding one-dimensional wire with harmonic oscillation. However a generalization to multi-channel transport with arbitrary periodic ac field is straightforward, by expansion of the Floquet space to include higher harmonics and the transport channels. As a trade-off, more CPU time is required. We hope the present formalism

based on a tight-binding Hamiltonian may be helpful to the study of time-dependent transport in molecular electronics where the band structure of the leads and the Coulomb effect are expected to play dominant roles. In addition, the formalism presented above can be used to investigate the transport through a tight-binding chaotic quantum dot numerically. These numerical results are believed to be complementary to the analytical perturbative approaches such as the time-dependent random matrix method [13].

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