Time-Dependent Transport in Low-Dimensional Systems—A Numerical Solution Using the Nonequilibrium Green’s Functions

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Abstract—In this paper, we present a novel numerical solution to analyze time-dependent transport in low-dimensional systems, such as one-dimensional (1-D) quantum dot and quasi-one-dimensional (Q1D) carbon nanotube systems, by using the nonequilibrium Green’s functions (NEGF). The novelty of proposed approach is to jointly handle the NEGF in both the time-domain and the real-space-domain in a recursive fashion. The time-domain recursive approach is a straightforward approach to solve time-dependent transport problems, while the real-space recursive approach makes the calculations feasible for arbitrary-length 1-D and Q1D systems. To verify our proposed algorithm, we apply this method to explore the transient and ac transport properties of a sample 1-D quantum-dot array system. We will present in this paper the simulated electrical current curves, $J(t)$, in response to various pulses and sinusoid waveforms. From these simulation results, we can obtain the delay and distortion information. We will then discuss how the length of a quantum-dot array and the hopping energy affect the transport behavior. The knowledge we gain from this project will help researchers to evaluate the hopping energy affect the transport behavior. The knowledge will then discuss how the length of a quantum-dot array and the hopping energy affect the transport behavior. The knowledge can also benefit the making of time-dependent 1-D and Q1D nanoelectronic devices.

Index Terms—AC transport properties of nanodevices, nonequilibrium Green’s function, transient.

I. INTRODUCTION

UNDERSTANDING electron transportation in mesoscopic systems is a very interesting research topic, which has drawn a great deal of research interest [1]–[7]. Researchers can make various nonsilicon devices, such as molecular switches [8], [9] and carbon nanotube interconnections [10], [11]. The theoretical calculation of the transient and ac characteristics in these one-dimensional (1-D) or quasi-one-dimensional (Q1D) systems is a timely research subject. About ten years ago, nonequilibrium Green’s function (NEGF) formalism was proposed to calculate carrier transport in mesoscopic systems [2]. An effective numerical method to compute time-dependent transport in the low-dimensional systems, however, has not yet been developed. Compared to the steady-state transport, the challenge of applying the NEGF to solve time-dependent transport is that the NEGF $G(t_F, t_I)$ depends on its two time variables, $t_I$ and $t_F$. (Here, $t_I$ and $t_F$ stand for the initial and the final time in the Green’s function, respectively) An analytic solution is hard to obtain by using only the Fourier transform. Using the wideband limit (WBL) approximation for electrodes, the researchers presented their ac transport calculation results for resonant-tunneling devices with single or double energy levels by utilizing the NEGF method [12], and obtained the corresponding $\tilde{J}(\omega)$ curves. The WBL approximation, however, neglects the details about the density of states (DOS) in the electrodes; thus the simulation results of the devices’ transport properties may not be accurate. Several research groups proposed to apply advanced approaches beyond the WBL approximation [7]. One group recently proposed to use a time-domain decomposition (TDD) technique to directly solve the NEGF [13]. According to the electron lifetime inside the device, the researchers eliminated the negative infinity in the NEGF equations. If the electron lifetime is set correctly, the TDD results fit very well with the analytic solutions. The approach we propose in this paper is based on this TDD technique.

Another challenge when calculating the time-dependent transport characteristics is to handle an arbitrary-length conductor between the electrodes in low-dimensional systems. The sample conductor can be a 1-D molecular chain or a Q1D carbon nanotube. In this paper, we present a novel quantum-mechanical calculation method to handle the time-dependent transport problem in arbitrary-length low-dimensional mesoscopic systems. We propose to recursively solve the NEGF jointly in both the time-domain and the real-space-domain. For the time-domain recursive approach, our method can handle electrodes with an arbitrary-shaped DOS. In our simulations, we utilize a dynamically allocated data-structure, which enables us to compute currents in response to input signals of any time duration. For the real-space recursive approach, we can calculate the transport properties within variable-length 1-D or Q1D materials. Conventional numerical approaches can handle the transport problem only in either the equilibrium or the steady-state state. By jointly applying these two approaches, we can solve the time-dependent NEGF and obtain the corresponding currents $\tilde{J}(t)$. Compared with a direct combination of TDD technique and real-space solving Green’s function technique, our approach will require much less memory and be less time-consuming, thus making the calculation more feasible for the 1-D or Q1D systems.

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II. PROPOSED METHODOLOGY

A 1-D or Q1D system, in principle, can be separated into three regions: the left ($L$) and the right ($R$) electrodes and the central conductor ($C$). To compute the transient ac characteristics, we apply a time-variant input signal to the left electrode at time $t = t_0$. By jointly solving for the NEGF in both the time and the real-space domain recursively, we can obtain both the injection current $J_L(t)$ (the current passing from the left electrode into the central conductor) and the response current $J_R(t)$ (the current passing from the central conductor into the right electrode). Next, we will present the procedure to calculate $J_R(t)$ (we can obtain the injection current density $J_L(t)$ similarly). In general, we can express the Hamiltonian of a low-dimensional system as

$$H = H_e + H_C + H_T.$$ \hfill (1)

Here, $H_e$ is the electrodes’ Hamiltonian

$$H_e = \sum_{\kappa = L, R} \varepsilon_{\kappa\alpha} c_{\kappa\alpha}^{\dagger} c_{\kappa\alpha}$$ \hfill (2)

where $c_{\kappa\alpha}$ and $c_{\kappa\alpha}^{\dagger}$ are the single-electron annihilation and creation operators at the $k$ level energy in the electrode $\alpha$ respectively, and $\varepsilon_{\kappa\alpha}$ is the corresponding eigenenergy. $H_C$ is the conductor’s Hamiltonian. We can further divide the conductor $C$ into $N$ principal layers (indexed by numbers $1, 2, \ldots, N - 1$ and $N$). In the tight-binding representation, we can express $H_C$ as

$$H_C = \sum_{i=1}^{N} \sum_{\beta} \varepsilon_{i\beta} d_{i\beta}^{\dagger} d_{i\beta} + \sum_{i=1}^{N-1} \sum_{\beta, \gamma} (V_{i\beta\gamma} d_{i\beta}^{\dagger} d_{i+1\gamma} + h.c.)$$ \hfill (3)

where $d$ and $d^{\dagger}$ are single-electron operators in the conductor, and $\beta, \gamma$ are the energy levels on layer $i$ and $i+1$, respectively. The first term in (3) represents the intralayer Hamiltonian of the conductor, with $\varepsilon_{i\beta}$ the eigenenergy on layer $i$, and the second term represents the interlayer Hamiltonian, with $V_{i\beta\gamma}$ the coupling strength between eigenlevels on layer $i$ and layer $i+1$. The last term, $H_T$ in (1), describes the coupling between the conductor and the two electrodes

$$H_T = \sum_{k, \beta} \ldots (V_{kL,1\beta} c_{kL1\beta}^{\dagger} d_{1\beta} + V_{kR,N\beta} c_{kR,N\beta}^{\dagger} d_{N\beta} + h.c.).$$ \hfill (4)

Here $V_{kL,1\beta}$ denotes the coupling strength between electronic state $k$ on the left electrode and the $\beta$ state on the leftmost Layer 1 of the conductor, while $V_{kR,N\beta}$ denotes that between the $\gamma$ state on the rightmost layer $N$ and the $k$ state on the right electrode. Thus, the first term in (4) characterizes hopping from the conductor to the left electrode, the second term characterizes that from the conductor to the right electrode, and the third, Hermitian conjugates of the former two terms, represents the reversed processes.

In order to calculate $J_R(t)$, we further separate the central conductor into two parts: the remaining $N - 1$ layers (or block $B$). The system now consists of four pieces, $L, B, N, \text{ and } R$, from left to right. The response current is expressed as \hfill (5)

$$J_R(t) = \frac{2e}{h} \Re \text{Tr} \left[ V_{R,N} G_{N,R}^{R}(t, t) \right].$$

$V_{R,N}$ denotes the coupling between layer $N$ and electrode $R$. The full Green’s function $G_{N,R}^{R}(t, t)$ describes the propagation of electrons from electrode $R$ to layer $N$ at time $t$. By utilizing the contour Green’s function technique, we can expand $G_{N,R}^{R}(t, t)$ as

$$G_{N,R}^{R}(t, t) = \int_{-\infty}^{t} dt' [G_{N}^{R}(t, t') V_{N,R} g_{R}^{<}(t', t) + G_{N}^{<}(t, t') V_{N,R} g_{R}^{<}(t', t)].$$ \hfill (6)

Here, $g_{R}^{<}(t')$ represents the free lesser (the advanced) Green’s function of the right electrode $R$ and $G_{N}^{<}(t, t')$ satisfy the Dyson equation and the Keldysh equation [15], respectively

$$G_{N}^{<}(t, t') = g_{N}^{<}(t, t') + \int_{t'}^{t} dt_1 \int_{t_1}^{t_1} dt_2 g_{N}^{<}(t, t_1) \times \sum_{\gamma} \sum_{\gamma'} (V_{1\gamma} g_{N}^{<}(t_1, t_2) G_{N}^{<}(t_2, t') V_{1\gamma'} g_{N}^{<}(t_1, t') + G_{N}^{<}(t_2, t') V_{1\gamma'} g_{N}^{<}(t_1, t')) \sum_{\gamma} \sum_{\gamma'} (V_{1\gamma} g_{N}^{<}(t_1, t_2) G_{N}^{<}(t_2, t') V_{1\gamma'} g_{N}^{<}(t_1, t') + G_{N}^{<}(t_2, t') V_{1\gamma'} g_{N}^{<}(t_1, t')).$$ \hfill (7)

Here $\Sigma_{N}$ is the retarded (lesser) self-energy of layer $N$, and it takes the coupling between layer $N$ and all the other parts in the system into account. Considering the coupling to the left and right parts of layer $N$ separately, we can get

$$\sum_{N} \langle t, t' \rangle = V_{N,N-1} G_{N-1,R}^{L+B}(t, t') V_{N-1,N} + V_{N,R} g_{R}^{<}(t, t') V_{R,N}.$$ \hfill (9)

$G_{N}^{L+B}(t, t')$ in (9) represents the Green’s function of layer $N-1$, when we consider the coupling between electrode $L$ and the other layers within block $B$. We have two ways to solve (6)–(8): 1) applying the Fourier transform to convert Green’s functions in the frequency-domain and then making further approximations to simplify these equations and 2) directly discretizing Green’s functions and solving the resulting linear equations.

By utilizing the propagator properties of Green’s functions, we can solve Green’s functions at the current time based on the summation of those previously calculated values. We, therefore, can recursively solve the integral (6), (7), and (8), in the time domain. In other words, we can calculate every Green’s function along the discretized time axis based on the previous values. By utilizing this numerical integral technique, we can discretize (7) and rearrange the equation as shown in (10) at the bottom of the next page, in which $t_m = t_0 + m \cdot \Delta t$, and $\Delta t$ is the discretized step along the time-axis.
In this paper, we employ the time-domain recursive technique to solve the NEGF. We set $G^r$ with a small $t_F$ initially, and then we update $G^r$ with a larger $t_F$ based on the previously calculated results. At the beginning of our calculation, we set $t_F$ equal to $t_0$. Calculating $G^r$ at $t_F = t_0$, however, needs $G^r$ with $t_F$ less than $t_0$. We can obtain these $G^r$ easily by using the equilibrium or steady-state Green’s functions. The NEGF $G^r$ for $t_F < t_0$ are calculated recursively one after another until the input signal ends.

Another challenge we still face by using our previous method is that $-\infty$ in the integral of (6) and (8) makes the discretization of these integrals impossible. Here, we substitute $-\infty$ with electron lifetime $\tau$ within the central conductor [14]. This replacement is valid because electrons in the central conductor can escape to the electrodes during the propagation in an open system. As the time difference between $t_F$ and $t_f$ increases, the Green’s functions of the central conductor gradually approach to zero. In order to calculate the Green’s functions with a final time index $t_F$, we need to compute only the Green’s function that meets the requirement of $|t_F - t_f| \leq \tau$. After we limit the low-end in the integrals and discretize the Green’s functions, we can calculate the response current as

$$J_R(t_n) = \frac{2e}{h} \text{Re} \text{Tr} \left\{ \sum_{m=t_n-\tau}^{t_n} d\bar{G}_N^r(t_n, t_m) \times V_{N,R} \bar{G}_R^r(t_m, t_n) + G_N^r(t_n, t_m) \times V_{N,R} \bar{G}_R^r(t_m, t_n) \right\}. \quad \text{(11)}$$

From (11), we observe that the current at point time $t_n$ depends on the Green’s functions $G_N(t_F, t_f)$ when $t_F = t_n$ and $t_n - \tau \leq t_f \leq t_n$. We can use two-dimensional (2-D) arrays $G[(t_n - \tau, \ldots, t_n - \tau : 0]$ to store the calculated results. The first term in the array has time index $t_F$, while the second term has index $t_f-t_F$. This data-structure is dynamic because we need to calculate the Green’s functions with $t_F = t_n+1$ and $t_n+1 - \tau \leq t_f \leq t_n+1$ as we proceed to calculate the current at time $t_{n+1}$. We then store these results into the array while clearing up those with time index $t_F = t_n - \tau$. In our computation, the memory requirement is determined by electron lifetime $\tau$ and the discretization step $\Delta t$ instead of the duration of the input signals. This dynamic data-structure significantly reduces the memory requirements, especially when the input signals last for a long time.

Next, we will discuss how to calculate the self-energy $\Sigma$. We can calculate the first term in (9) $G_{N-1}^{L+B,r}(t) \approx$ by using the Lattice Green’s function technique [16]. We compute $G^B$ in the real-space initially and then calculate $G_{N-1}^{L+B}$ based on $G^L$ and $G^B$. This approach has several advantages. 1) Since the time-dependent signal is applied to the left electrode $L$, Green’s functions $G^L$ are time-dependent, but $G^B$ are not. This result means that $G^B$ denotes the equilibrium or steady-state transport and can be calculated simply. 2) Because block $B$ is composed of $N-1$ identical layers in 1-D or Q1D materials, we can compute $G^B$ recursively. Suppose that block $B$ has $2^n$ layers, and each layer has a given free Green’s function, we first calculate the Green’s functions for the two neighboring layers, and then we can compute the four neighboring layers based on the previous results. This process can continue until we calculate the $G^B$ with $n$ recursive steps. As a matter of fact, $G^B$ at any layer $N$ can always be obtained after $(\log_2(N - 1))$ steps $(N - 1 = \sum_{i=0}^{n-1} 2^i)$.

For simplicity, we can neglect the time indexes and express $G_{N-1}^{L+B,r}$ and $G_{N-1}^{L+B,c}$ in a compact form

$$G_{N-1}^{L+B,r} = G_{N-1}^{r} + G_{N-1}^{B,r} V_1 L G_{N-1}^{r} V_1 G_{N-1}^{L+B,r}, \quad \text{(12)}$$

$$G_{N-1}^{L+B,c} = G_{N-1}^{r} + G_{N-1}^{B,c} V_1 L G_{N-1}^{c} V_1 G_{N-1}^{L+B,c}. \quad \text{(13)}$$

Here,

$$G_{N-1}^{L+B,r} = G_{N-1}^{B,r} V_1 L G_{N-1}^{r} V_1 G_{N-1}^{L+B,r}, \quad \text{(14)}$$

$$G_{N-1}^{L+B,c} = G_{N-1}^{B,c} V_1 L G_{N-1}^{c} V_1 G_{N-1}^{L+B,c}, \quad \text{(15)}$$

$$G_{N-1}^{L+B} = G_{N-1}^{B} + G_{N-1}^{L+B} V_1 L G_{N-1}^{r} V_1 G_{N-1}^{L+B}. \quad \text{(16)}$$

In the above equations, $G_{N-1}^{L+B}$ is the advanced Green’s function, which describes the propagation of electrons from Layer $N-1$ to Layer 1 when we consider the coupling of layers 1 and $N-1$ with electrode $L$ and block $B \cdot G^{L+B}$. and $G^{L+B}$ are the retarded Green’s functions. From (12)–(16), we observe that $G_{N-1}^{L+B,r}$ and $G_{N-1}^{L+B,c}$ depend on $G_{N-1}^{B,r}, G_{N-1}^{B,c}, G_{N-1}^{L+B}$ and $G_{N-1}^{B}$, $G_{N-1}^{L+B}$. These variables can be calculated by using the same recursive method introduced previously.

The second term in (9) can be written as

$$V_{N,R} \bar{G}_R^r(t, t') V_{R,N} = \sum_{k \in R} V_{N,k} g_{k}^{r}(t, t') V_{k,N}$$

$$= \int d\varepsilon_k V_N(\varepsilon_k) \rho(\varepsilon_k) g_{k}^{r}(t, t') V_N^{+}(\varepsilon_k) \quad \text{(17)}$$

$$G_N(t_m, t_m) = \begin{cases} \frac{1}{4} \left[ G_N(t_m, t_m) \sum_{j=1}^{\text{N}} G_N(t_m, t_m) \right] G_N(t_m, t_m) & (n = 0) \\ \frac{1}{4} \left[ G_N(t_m, t_m) \sum_{j=1}^{\text{N}} G_N(t_m, t_m) \right] G_N(t_m, t_m) + 2 \sum_{j=1}^{\text{N}} G_N(t_m, t_m) G_N(t_m, t_m) + 2 \sum_{j=1}^{\text{N}} G_N(t_m, t_m) G_N(t_m, t_m) + 2 \sum_{j=1}^{\text{N}} G_N(t_m, t_m) G_N(t_m, t_m) & (n \geq 1) \end{cases} \quad \text{(10)}$$
where \( g_k^R(t, t') = -i \theta(t - t') e^{-i \varepsilon_k (t - t')} \) and \( g_k^L(t, t') = i e^{-i \varepsilon_k (t - t')} f(\varepsilon_k - \mu_R) \cdot \rho_R(\varepsilon_k) \) is the density of states (DOS) in the right electrode, and \( f \) is the Fermi distribution function.

It is worth pointing out that the free Green’s function at the left electrode differs from the one at the right electrode because the time-dependent signal is applied only to the left electrode. We can treat this time-dependent signal by using the adiabatic approximation. For instance, when applying a time-dependent voltage with the bias \( \Delta V(t) \) to the left electrode, the single-particle energy levels at this electrode become time-dependent and are in the range of \( \varepsilon_k^L \) to \( \varepsilon_k^L + \Delta V(t) \), but the occupation of the individual state \( k \) remains the same. The free Green’s functions of the electron states in the left electrode now become

\[
 g_k^R(t, t') = -i \theta(t - t') e^{-i \varepsilon_k (t - t')} \exp\left\{ -i \int_{t'}^{t} d\tau \Delta V(\tau) \right\},
\]

\[
 g_k^L(t, t') = i e^{-i \varepsilon_k (t - t')} f(\varepsilon_k - \mu_L) \exp\left\{ -i \int_{t'}^{t} d\tau \Delta V(\tau) \right\},
\]

As our previous discussion demonstrates, the joint time-domain and real-space-domain recursive technique is an effective way to calculate time-dependent transport characteristics in low-dimensional systems with arbitrary length. To verify our proposed method, we compare our simulation results with those obtained by using the TDD method combined with the surface Green’s function technique. In a low-dimensional system, we assume that the central conductor contains only three dots (numbered as 1, 2, 3) and that every dot has only one energy level. We further assume that the electrodes’ energy bands are in the Lorentzian shape. At time \( t = 0 \), the energy level on dot #1 jumps from \( E_1 \) to \( E_2 \) due to some external perturbation. The numerical results are shown in Fig. 1. Our simulation results match exactly with those based on the TDD method combined with the surface Green’s function technique.

Finally, we estimate the different memory requirements and time-consuming in the TDD technique and in our approach. Take the calculation of time-dependent transport in a N-dot 1-D system for example. A direct combination of the TDD and real-space solving Green’s function technique will require the treatment of \( N^2 (\tau / \Delta \tau)^2 \)-dimensional matrices (\( \tau \) is the electronic lifetime in the central conductor, and \( \Delta \tau \) is the discretized time-step), while our approach need a few 2-D arrays with length of \( \tau / \Delta \tau \). Hence, our approach is much less time-consuming and memory-consuming.

The NEGF of such a three-dot system cannot be handled directly by using the TDD technique. We use the surface Green’s function technology to express the Green’s functions needed in the computations. In this approach, we first calculate Green’s functions of dot #3 by considering the coupling between the dot and the right electrode. We get \( G_{13} = g_1^R + g_2^R V_{3,6} g_6^R V_{6,13} G_{13} \) and \( G_{13} = G_{13} V_{3,1} g_1^R V_{1,3} G_{13} \). We then calculate the Green’s functions of dot #2 by taking all the couplings on its right into account, and get \( G_{23} = g_1^R + g_2^R V_{3,2} g_2^R V_{2,3} G_{23} \) and \( G_{23} = G_{23} V_{3,1} g_1^R V_{1,3} G_{23} \). Finally, we calculate the full Green’s functions of dot #1 as \( G_1 = g_1^R + g_2^R V_{1,2} g_2^R V_{2,1} + V_{1,3} g_1^R V_{1,3} G_{13} \) and \( G_1 = G_{13} V_{3,1} g_1^R V_{1,3} G_{23} \). The numerical values of these Green’s functions are obtained by using the TDD method.

III. NUMERICAL RESULTS AND DISCUSSION

In this section, we will present our simulation results for a 1-D quantum-dot array, which couples with two symmetric electrodes. We can use this 1-D quantum-dot array to emulate switches and interconections made of low-dimensional materials. Time-dependent voltage signals are applied into the left electrode, and our goal is to calculate the injection and its response current. We choose various pulse and sinusoid waveforms as inputs. We also change the number of dots on the array and their hopping energies to explore how these parameters can influence the transport characteristics.

First, we need to estimate the electron lifetime \( \tau \) on the central conductor. This parameter can be extracted from the decay rates of the equilibrium Green’s functions \( G_N^R(\tau) \). Fig. 2 plots \( G_N^R(\tau) \) as a function of various quantum-dot numbers on the array. The electron lifetime clearly gets larger when the number of dots increases because the electron lifetime is inversely proportional to the probability of the electron escaping into the electrodes. As the number of quantum dots increases, the electrons on the
rightmost dot within the conductor have higher probability to stay in the same state as the other dots in the conductor, so the probability of escaping into the left electrode becomes smaller. This phenomenon leads to an increased electron lifetime when the number of dots within the quantum-dot array increases.

After obtaining the electron lifetime, we can now calculate the transient and ac characteristics of the 1-D quantum-dot array. The numerical results are presented in Figs. 3 and 4. Fig. 3 shows the input pulse voltage signal, and the corresponding injection and response currents as the functions of time and the number of quantum dots on the array. The calculated injection currents are almost the same for the various simulations, as shown in the insert subfigure in Fig. 3. The on-state conductance \( g_{RL} \), defined as \( g_{RL} = I_R/V_L \), is about 186.7 k\( \Omega \)-1, 197.0 k\( \Omega \)-1, and 228.2 k\( \Omega \)-1 for the 5-, 10-, and 20-dot arrays respectively, while \( g_{LL} \) is always 166.6 k\( \Omega \)-1 no matter how many dots on the array. The response currents’ delays are about 2, 4, and 8 time units for the 5-, 10-, and 20-dot arrays, respectively. These delays are proportional to the array-length. This phenomenon can be explained by the ballistic transport theory [5]. When a time-dependent signal is applied into the left electrode, the electrons get enough energy and start to move towards the central conductor. Based on the ballistic transport limit, the electron translocation time from the left electrode to the right one is proportional to the distance between them. The length of a 20-dot array is about 6 nm, and the electrons’ thermal velocity is \( 10^{0.5} \) m/s at room temperature. The electron translocation time between two electrodes is, therefore, in the order of \( 10^{-15} \) s. This result fits quite well with our simulated delays in Fig. 3.

In addition to the pulse waveform, we also apply a sinusoid voltage signal, \( V(t) = 2 \sin(\pi t) \), as an input. Fig. 4 shows the simulation results for the 5-, 10-, and 20-dot arrays, respectively. In Fig. 4, we can observe that the ac conductance \( g_{LL} \) is al-

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**Fig. 3.** Input pulse waveform and the corresponding injection and response currents as a function of the variable-length 1-D quantum-dot arrays (5, 10, and 20 dots on the array, respectively). The hopping energy between the neighboring dots is set to be one.

**Fig. 4.** Injection and response currents driven by the sinusoid voltage signal \( V = 2 \sin(\pi t) \), for 1-D 5-, 10-, and 20- quantum-dot arrays, respectively. The hopping energy between the neighboring dots is set to be one. A bias voltage of 2 V is applied to the right electrode.
ways 123.5 kΩ⁻¹ about for the arrays with various numbers of dots, while $g_{RL}$ is about 195.6 kΩ⁻¹, 178.5 kΩ⁻¹, and 248.9 kΩ⁻¹ for 5-, 10-, and 20-dot arrays, respectively. The response current delay gets larger as the number of dots on the array increases. The response current amplitude of the 10-dot array is largest among the three response currents. The calculated injection currents of the various quantum-dot arrays differ only slightly. However, we can still observe that the minimum response current of the 10-dot array is smaller than those of the 5- and 20-dot arrays. It is worth noticing that abrupt negative peaks exist at the beginning of the calculated injection current curves. We speculate that they are caused by the overshoot effect occurred in the quantum transport similar to those in the classical transport [18]. The amplitude of this transient overshoot is significantly attenuated as the electrons pass through the barrier between the conductor $C$ and electrode $R$. Compared to the injection currents, the response currents at the right electrode are much smoother.

In this paper, we also explore how the hopping energy between neighboring quantum dots affects the currents. The knowledge can be used to explain how the quantum dots’ intrinsic characteristics affect the transport properties. The numerical results are shown in Fig. 5. The profiles of the time-variant injection currents are smooth, and the response current delay is small when the hopping energy is large. For an extremely small hopping energy, such as 0.1 eV, which is used to describe a narrowband conductor, both the injection and response currents are close to zero. This result is reasonable because the hopping energy indicates how easily an electron can hop from one position to a neighboring site on the dot array. With small hopping energy, the electron flow from the electrode will pile up at the interface of the electrode and dot array when the input signal suddenly changes. This leads to the acute peaks in the injection-current profiles for small hopping energy at the edges of the input signal.

IV. CONCLUSION

In summary, we propose a novel quantum mechanical method to handle the time-dependent transport in low-dimensional systems by using the NEGF formalism. Compared with the TDD technique, the proposed numerical method can deal with time-dependent transport problems more efficiently in 1-D or Q1D systems, such as molecular switches or carbon nanotube interconnections, by recursively solving NEGF jointly in both the time domain and real-space domain. The time-domain recursive approach is a substitute for the TDD technique. It help us utilize a dynamically allocated data-structure in the computation, which can significantly reduce the memory consumption. In addition, by using the real-space recursive approach to solve NEGF, we can obtain numerical solutions with $(\log N)^2$ computation steps for a system with $N$ layers in the central conductor. The total computational memory requirement scales with $(\tau/\Delta t)^2$, and the computational time requirement scales with $(\tau/\Delta t)^4$.

Based on our proposed method, we calculate the injection and response currents $J(t)$ driven by various pulse and sinusoid signals in 1-D quantum-dot arrays. Delay and distortion informations are observed when we calculate the $J(t)$ curves. We also discuss how the quantum-dot array length and the hopping energy affect the transport behavior. The knowledge gained from this research can help researchers to understand the time-dependent transport in 1-D and Q1D systems. This knowledge can also benefit the building of nanoscale devices by using these low-dimensional materials.

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