Quantum transport in nano-devices with a time-varying switch and a time-dependent gate

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The quantum transport properties of systems with time-varying components can be calculated using time-dependent nonequilibrium Green's functions (TD-NEGF) techniques [1]. In this paper, we study how the particle current behaves in linear chain systems with a dynamical interleads coupling [2] and when a time-dependent gate voltage is applied. An illustration of two linear chain leads with an interleads coupling that can be dynamically switched on is shown in Fig. 1. For an abrupt step-like switch-on (at time $t = 0$), the current would initially overshoot the expected steady-state value, oscillate and decay as a power-law, and eventually settle into a steady-state value (see Fig. 2). The power-law parameters for the decaying transient current depends on the value of the applied bias voltage between the two leads, the strength of the coupling between sites in the leads, and the speed of the switch-on. The device can further be modeled by an equivalent series resistor-inductor-capacitor (RLC) circuit as shown in Fig. 1(c). Such an RLC circuit, however, contain components that have time-dependent properties, i.e., dynamical resistance, inductance, and capacitance.

Instead of a step-like switch-on, the interleads coupling can also be considered to vary sinusoidally in time. This can be thought of as rocking the right lead in Fig. 1(a) back and forth thereby modulating the interleads coupling. Our results (see Fig. 3) show that the current does not exactly follow the sinusoidal form of the interleads coupling. In particular, the maximum current does not occur whenever the leads are exactly aligned. The location of the maximum current depends on the value of the bias potential between the leads, the strength of the couplings between sites in the leads, and the interleads coupling.

The TD-NEGF technique can also be employed in the study of nano-devices with a time-varying applied gate potential [3]. Shown in Fig. 4 is a linear chain system wherein the channel is acted upon by a time-dependent gate voltage $V_g(t)$. The reaction of the current to the gate potential depends on the dynamical form of $V_g(t)$. For a gate potential in the form of a rectangular pulse (see Fig. 5), the current reacts (but not instantaneously) to either an increasing or a decreasing gate potential. Furthermore, a relaxation time is required for the current to settle back to a steady-state value.

In summary, in this paper we present our studies and results on linear chain systems undergoing dynamical changes either through a time-varying switch-on or a time-dependent gate potential. We use TD-NEGF to numerically determine the dynamical current. In systems experiencing a step-like switch-on, the transient current initially overshoots the expected steady-state value and then decays as a power-law. In systems with a sinusoidally changing interleads coupling, the current does not exactly follow the sinusoidal form of the coupling and the maximum current does not occur whenever the leads are exactly aligned. In systems where a time-dependent gate potential is applied, the current reacts to a changing gate potential.

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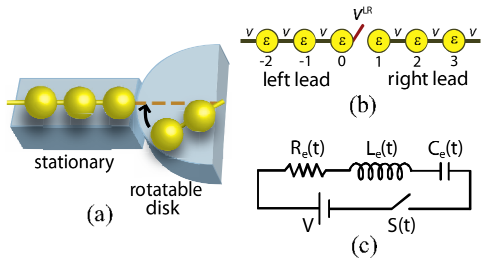

Fig. 1. (a) An illustration of a system with a time-varying coupling between the leads. The left lead is stationary and the right lead is on a rotatable disk that can be turned to align both leads. (b) A representation of the two leads and the dynamical coupling. (c) An equivalent circuit containing components with dynamical properties.

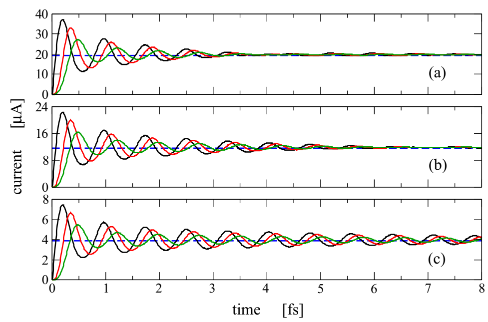

Fig. 2. The time-varying current through the leads after the interleads coupling is switched on. The coupling is switched on abruptly at time $t = 0$ (black lines), gradually in the form of a hyperbolic tangent with driving frequency $\omega_d = 0.5[1/\mathrm{t}]$ (red lines), and $\omega_d = 0.25[1/\mathrm{t}]$ (green lines), where $[1/\mathrm{t}] = 10^{16}$ rad/s. The source-drain potentials are (a) $U_{ds} = 0.5$ eV, (b) $U_{ds} = 0.3$ eV, and (c) $U_{ds} = 0.1$ eV. The blue dashed lines are the expected values of the steady-state current.

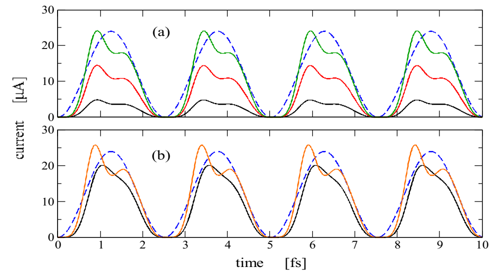

Fig. 3. The dynamical current in an oscillator with driving frequency $\omega_d = 0.25$ $[1/\mathrm{t}]$. In (a) the source-drain bias potentials are $U_{ds} = 0.1$ eV (black), 0.3 eV (red), and 0.5 eV (green). The value of the nearest-neighbor coupling used is $v = -2.7$ eV. In (b) the bias potential is $U_{ds} = 0.5$ eV. The amplitude of the interleads coupling is varied to values-2.1 eV (black) and -3.0 eV (orange). The blue dashed lines exhibit the sinusoidal variation (in time) of the interleads coupling.

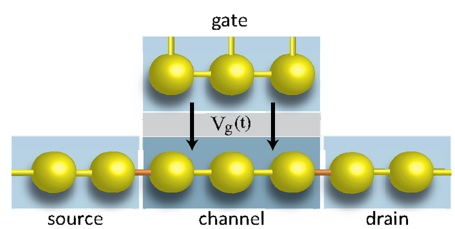

Fig. 4. An illustration of a linear device with a gate that exerts a time-varying potential $V_g(t)$ to the channel. There is no direct connection between the gate and the channel.

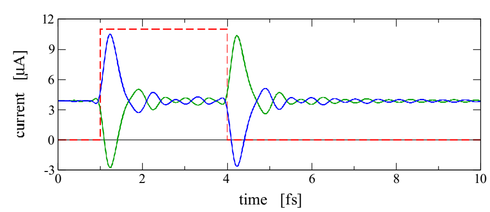

Fig. 5. The current when a gate potential pulse acts on a 3-site channel. The shape of the gate pulse is illustrated by the red dashed line. The blue line is the current when the gate potential pulse is -0.1 eV while the green line is when the gate potential pulse is $+0.1$ eV. The source-drain bias potential is $+0.1$ eV.