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LETTER TO THE EDITOR

New types of frequency dependence of hopping conductivity on a hierarchical lattice

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Abstract. By a real-space renormalization-group method, we have calculated the dynamic hopping conductivity of a one-dimensional hopping system with hierarchically distributed transition rates. Our numerical results show that the conductivity can display rather different types of low- and high-frequency behaviour as the value of the hierarchical parameter R is varied.

Studies concerning hopping on one-dimensional (1D) systems have shown that the distribution of the transition rates is important in establishing the qualitative behaviour of the system's response to an external electric field with frequency ω [1, 2]. The low-frequency expression for AC hopping conductivity $\sigma(\omega)$, which is of great importance in hopping, is regular for periodic chains, e.g. the real part of the conductivity $\text{Re}[\sigma(\omega)] - \sigma(0) \sim \omega^2$ as $\omega \rightarrow 0$ for periodic binary chain [1, 2]. The expression becomes non-analytic when the transition rates are distributed randomly, e.g. $\text{Re}[\sigma(\omega)] - \sigma(0) \sim \omega^{1/2}$ in the limit $\omega \rightarrow 0$ for random binary chain [1, 2]. The intermediate case, the transition rates being arranged in deterministic aperiodic sequence such as on the Fibonacci lattice and the Thue-Morse lattice has also been studied [3]. For the 1D Fibonacci quasiperiodic lattice, the low-frequency dependence of $\text{Re}[\sigma(\omega)]$ is shown to be of the new form $\omega^2(1 - \text{const} \times \ln \omega)$ as $\omega \rightarrow 0$, which is non-analytic but not random-like [2]. For the 1D Thue-Morse lattice, it is shown that $\text{Re}[\sigma(\omega)]$ behaves similarly to that of the ordinary periodic chain, i.e. $\text{Re}[\sigma(\omega)] - \sigma(0) \sim \omega^2$ [2]. Now a natural question is whether or not the hopping conductivity of a hierarchical lattice, which is another type of deterministic aperiodic system and has attracted much attention recently (see [4] for a review), will show any different type of frequency behaviour.

The model treated here is similar to that in [3]. Electrons are localized around the isoenergetic sites in the lattice, and an electron may hop from one site to either of those adjacent. The hopping rate W_n between the sites n and $n+1$ is given by

$$W_n = \begin{cases} 1 & n = 2l + 1 \\ R^k & n = 2^k(2l + 1) \end{cases} \quad (1)$$

where R is a parameter characterizing the hierarchy. The spacings between the adjacent sites d_n are set to be 1 for simplicity. When a spatially constant electric field $E = E_0 e^{i\omega t}$

is applied along the line of the hierarchical lattice, the hopping conductivity is determined by taking the spatial average of the current flowing between pairs of adjacent sites and can be written as

$$\sigma = \frac{1}{EL} \sum_n I_n \tag{2}$$

where L is the length of the chain and the 'elementary currents' I_n , representing the thermally averaged rate at which charge is transferred between the n th site and the $(n + 1)$ th or the current flowing between the sites n and $n + 1$, are the solution of the following Miller-Abrahams (MA) equations

$$\left(\frac{i\omega}{W_n} + 2 \right) I_n = I_{n+1} + I_{n-1} + i\omega E. \tag{3}$$

Owing to the 'inflation symmetry' of the system, the above MA equations can be solved by a decimation process as in [5]. To do so, we divide the hierarchical lattice into two sublattices consisting of the odd number sites and the even number sites, respectively. Then the MA equations take the more general form

$$\begin{cases} \varepsilon_1 I_n = \gamma I_{n-1} + I_{n+1} + i\omega E h_1 & \text{for odd } n \\ \varepsilon_n I_n = I_{n-1} + \gamma I_{n+1} + i\omega E h_2 & \text{for even } n \end{cases} \tag{4}$$

which can be cast into the same form before and after the decimation procedure. Clearly, the original set of MA equations (3) is a special case of (4) with

$$\varepsilon_n = 2 + \frac{i\omega}{W_n} \quad h_1 = h_2 = 1 \quad \gamma = 1. \tag{5}$$

In terms of the generalized MA equations (4), the conductivity (2) for the system becomes

$$\sigma = \frac{1}{EL} \sum_n I_n h_n \tag{6}$$

where h_n takes either h_1 or h_2 , depending on whether n is odd or even. Decimating all $4n + 2$ and $4n + 3$ sites (marked by crosses in figure 1) and relabelling the remaining ones leave us with a new set of equations which is in the same form as the old one,

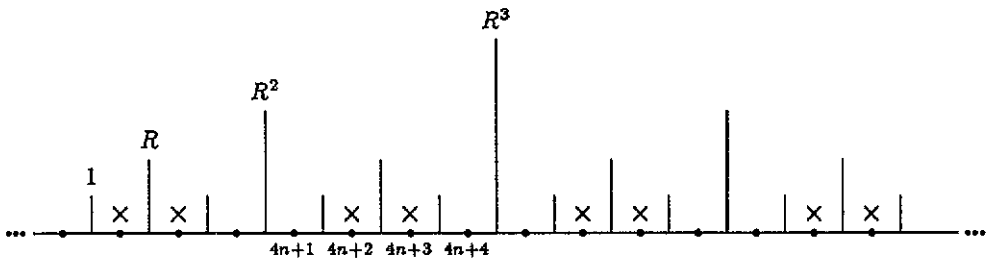


Figure 1. Schematic representation of the hierarchical lattice with a hierarchy of transition rates. The dots stand for the isoenergetic atomic sites and the vertical segments represent the transition rates between two adjacent sites. Sites with crosses are decimated during the present renormalization scheme.

except that the original parameters ε_n , h_1 , h_2 and γ are renormalized as follows

$$\begin{aligned} \varepsilon'_{n-1} &= \frac{\varepsilon_n \gamma' - \varepsilon_2}{\gamma} \quad n > 2 & \varepsilon'_1 &= \frac{\varepsilon_1 \gamma' - \varepsilon_1}{\gamma} \\ h'_1 &= \left(1 + \frac{\gamma'}{\gamma}\right) h_1 + \frac{\varepsilon_1}{\gamma} h_2 & h'_2 &= \left(1 + \frac{\gamma'}{\gamma}\right) h_2 + \frac{\varepsilon_2}{\gamma} h_1 \\ \gamma' &= \varepsilon_1 \varepsilon_2 - \gamma^2. \end{aligned} \tag{7}$$

Using (6) and (7), and after some algebra, we can show that the conductivity σ' , defined by the value of (6) on the renormalized chain, is given by

$$\sigma' = \frac{2\gamma'(h_1 + h_2)}{\gamma(h'_1 + h'_2)} \sigma - \frac{i\omega h_1^2 x}{\gamma(h'_1 + h'_2)} \tag{8}$$

where

$$x = \varepsilon_2 + \frac{2h_2}{h_1} \gamma + \left(\frac{h_2}{h_1}\right)^2 \varepsilon_1. \tag{9}$$

Thus, a straightforward iterative procedure yields

$$\sigma = \frac{h_1^{(N-1)} + h_2^{(N-1)}}{2^N \gamma^{(N-1)}} \sigma^{(N-1)} + \frac{i\omega}{4} \sum_{i=0}^{N-2} \frac{x^{(i)} [h_1^{(i)}]^2}{2^i \gamma^{(i)} \gamma^{(i+1)}} \tag{10}$$

where the variables $h_1^{(i)}$, $h_2^{(i)}$, $\gamma^{(i)}$ denote the values of h_1 , h_2 , γ after i iterations of (7) with the initial values (5), and $x^{(i)}$ is obtained by replacing in (9), h_j , ε_j ($j = 1, 2$) and γ by $h_j^{(i)}$, $\varepsilon_j^{(i)}$ and $\gamma^{(i)}$, respectively. In the following practical calculation, we shall study the infinite chain consisting of the periodic repetition of an N -order hierarchical chain of length 2^N . Such an N -order approximant to the real hierarchical chain is indeed obtained by setting the transition rates (1) with $k \geq N$ to be of the following form

$$W_n = R^N \quad n = 2^k(2l + 1) \quad \text{with } k \geq N. \tag{11}$$

The real hierarchical lattice itself is regarded as the limit of this N -order approximant as $N \rightarrow \infty$. If we start with such an N -order approximant of period 2^N , then after decimating $N - 1$ times, we are left with a simple periodic chain composed of two types of transition rates. The MA equations for such a final chain are given by

$$\begin{cases} \varepsilon_1^{(N-1)} I_n = \gamma^{(N-1)} I_{n-1} + I_{n+1} + i\omega E h_1^{(N-1)} & \text{for odd } n \\ \varepsilon_2^{(N-1)} I_n = I_{n-1} + \gamma^{(N-1)} I_{n+1} + i\omega E h_2^{(N-1)} & \text{for even } n. \end{cases} \tag{12}$$

From (12) it is not difficult to derive

$$\sigma^{(N-1)} = \frac{i\omega}{\Delta} \{ [h_1^{(N-1)}]^2 \varepsilon_2^{(N-1)} + [h_2^{(N-1)}]^2 \varepsilon_1^{(N-1)} + 2h_1^{(N-1)} h_2^{(N-1)} [1 + \gamma^{(N-1)}] \} \tag{13}$$

with

$$\Delta = (h_1^{(N-1)} + h_2^{(N-1)}) \{ \varepsilon_1^{(N-1)} \varepsilon_2^{(N-1)} - [1 + \gamma^{(N-1)}]^2 \}. \tag{14}$$

So by iterating (7) with the initial values (5) and substituting $h_j^{(i)}$, $\varepsilon_j^{(i)}$ and $\gamma^{(i)}$ into (9), (10) and (13), we may obtain numerically the conductivity of an arbitrarily high-order approximant to the hierarchical lattice. The results for the real hierarchical lattice corresponding to the limit of $N \rightarrow \infty$ can be obtained by an extrapolation.

The first result coming out of our numerical calculation is that when $\omega \rightarrow 0$, we have exactly $\text{Re}[\sigma(\omega)] \rightarrow \sigma_0 = \sigma_0$ with [3]

$$\sigma_0 = 1/m_{-1} \quad m_{-1} = \frac{1}{2^N} \sum_n W_n^{-1} = \frac{R}{2R-1} + \frac{R-1}{2R-1} \left(\frac{1}{2R} \right)^N. \quad (15)$$

Obviously, when $R > 1/2$, $\text{Re}(\sigma)$ tends to a finite limit $\sigma_0 = (2R-1)/R$ as $\omega \rightarrow 0$ and $N \rightarrow \infty$, while for $R < 1/2$, we find $\text{Re}(\sigma) \rightarrow 0$. In order to attest this result, we have calculated $\text{Re}(\sigma)$ at frequencies as low as 10^{-60} in units of W_1 , where our numerical results still corroborate the analytical result (15) derived from a formal fluctuation expansion [3].

Next, we study the low-frequency behaviour of $\text{Re}(\sigma) - \sigma_0$ and $\text{Im}(\sigma)$ for various values of R . Since our practical numerical calculations are proceeded with finite N , we have calculated the conductivity for quite a few values of N to extrapolate the small- ω dependence of the real hierarchical system. After eliminating the ordinary period effect by an extrapolation, we observe the power-law behaviour of the conductivity at low frequencies for various values of R , i.e.

$$\text{Re}(\sigma) - \sigma_0 \sim \omega^\delta \quad \text{Im}(\sigma) \sim \omega^{\delta'} \quad (16)$$

where the exponents δ and δ' depend on R . To be specific, we shall distinguish the following cases:

(i) For $R \geq 2$, we find $\delta = 2$ and $\delta' = 1$, the conductivity possesses the same small- ω behaviour as in the binary periodic case

$$\text{Re}(\sigma) - \sigma_0 \sim \omega^2 \quad \text{Im}(\sigma) \sim \omega. \quad (17)$$

(ii) For $1 < R < 2$, the low-frequency behaviour of $\text{Im}(\sigma)$ remains ordinary as in the case of $R \geq 2$, while the exponent for the real part of the conductivity $\delta = R$, i.e.

$$\text{Re}(\sigma) - \sigma_0 \sim \omega^R \quad \text{Im}(\sigma) \sim \omega. \quad (18)$$

Thus, the crossover for a transition from ordinary to anomalous small- ω dependence of $\text{Re}(\sigma) - \sigma_0$ is observed at $R = 2$.

(iii) For $1/2 < R < 1$, we find $\delta = \delta' = 2R - 1$, i.e.

$$\text{Re}(\sigma) - \sigma_0 \sim \omega^{2R-1} \quad \text{Im}(\sigma) \sim \omega^{2R-1}. \quad (19)$$

Similarly, a transition of the power-law exponent for $\text{Im}[\sigma(\omega)]$ occurs at $R = 1$, with $R = 1$ corresponding to $W_n \equiv 1$ and thus $\text{Re}(\sigma) = \sigma_0 = 1$; $\text{Im}(\sigma) = 0$.

(iv) For $0 < R < 1/2$, we have $\sigma_0 \rightarrow 0$ as $N \rightarrow \infty$ from (15). The numerical results show $\delta = \delta'$. Although we cannot give an explicit expression for the exponents δ or δ' in the context of this paper, we find $d\delta/dR < 0$, which is contrary to the case of $R > 1/2$.

(v) For $R = 1/2$, we find $\delta \sim \delta' \sim 0$. However, our numerical results show evidence that a logarithmic singularity may exist in the low-frequency behaviour, which is similar to the Fibonacci chain [3].

Finally we turn to the high-frequency behaviour of $\text{Re}(\sigma)$ and $\text{Im}(\sigma)$. As in the low-frequency case, we also find the ordinary high-frequency dependences $\text{Re}(\sigma) \rightarrow \text{const}$ and $\text{Im}(\sigma) \sim \omega^{-1}$. We believe some of these results are due to the period effect. Eliminating the period effect by an extrapolation yields the high-frequency results as follows:

(i) For $R^2 < 2$, the conductivity has the same high-frequency behaviour as in the ordinary periodic chain

$$\text{Re}(\sigma) = m_1 \quad \text{Im}(\sigma) \sim \omega^{-1} \quad (20)$$

with

$$m_1 = \frac{1}{2^N} \sum_n W_n = \frac{R-1}{R-2} \left(\frac{R}{2}\right)^N - \frac{1}{R-2} \quad (21)$$

which is consistent with the analytical expression of [2].

(ii) For $2 < R^2 < 4$, the high-frequency behaviour of $\text{Re}(\sigma)$ remains ordinary as in the case of $R^2 < 2$, while $\text{Im}(\sigma)$ displays an anomalous power-law decay, i.e.

$$\text{Re}(\sigma) = m_1, \quad \text{Im}(\sigma) \sim \omega^\beta \quad (22)$$

with

$$\beta = \frac{\ln R - \ln 2}{\ln R}. \quad (23)$$

Thus the crossover for a transition from the ordinary ω^{-1} behaviour to anomalous power-law decay behaviour of $\text{Im}(\sigma)$ is at $R = \sqrt{2}$.

(iii) For $R^2 > 4$, both $\text{Re}(\sigma)$ and $\text{Im}(\sigma)$ display the anomalous power-law growth

$$\text{Re}(\sigma) \sim \omega^\beta, \quad \text{Im}(\sigma) \sim \omega^\beta \quad (24)$$

with β given by (23). Clearly a transition for the high ω dependence of $\text{Re}(\sigma)$ occurs at $R = 2$.

(iv) For $R = 2$, from our numerical results, we conjecture that $\text{Re}[\sigma(\omega)] - \sigma_0$ and $\text{Im}[\sigma(\omega)]$ may display logarithmic growth as $\omega \rightarrow \infty$.

To summarize, we have calculated, at low and high frequencies, the dynamic hopping conductivity of a 1D system with hierarchically distributed transition rates by solving the MA equations using a real space renormalization method. It is found that both the low-frequency conductivity and the high-frequency one may display a variety of new power-law ω dependences, with the power-law exponents dependent on R . As the value of R is varied, the power-law exponents have been found to undergo several phase transitions. This new type of ω behaviour of $\sigma(\omega)$ is rather different from the previous results for the Fibonacci and the Thue-Morse aperiodic chains, where the small- ω dependence of $\sigma(\omega)$ is independent of the diluted parameter W_A/W_B associated with two different building letters and the large- ω behaviour of $\sigma(\omega)$ is independent of the transition-rate distribution [3, 5].

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