Comment on "Role of a New Type of Correlated Disorder in Extended Electronic States in the Thue-Morse Lattice"

The Letter by Chakrabarti, Karmakar, and Moitra [1] provided a novel and useful method to show the existence of extended electronic states in aperiodic one-dimensional chains like the Thue-Morse (TM) lattice and the important fact that the extended characters "owe their origin to a peculiar short range correlation among the atoms at every length scale." Nevertheless, the mechanism they demonstrated and the results they reached are not so novel as their method. The numeric result [2] and the analytical illustration [3] of so claimed extended characters have been presented previously. We also have to point out the incompleteness of their Letter. They claimed that the transfer matrices T_n and $\overline{T}_n$ [see Eq. (2)] can never be made equal at some value of energy for even values of n [see the text after Eqs. (6) of [1]]. Thus they have omitted a great part of extended electronic states. In addition, they did not clarify the number of distinct energy values that can be found from the condition $\alpha_{n-2}(E) = 0$ [Eq. (8) of [1]]. In this Comment, we would like to point out that for any integer value of $n > 2$ there are 2^{n-2} distinct energy values at which both T_n and $\overline{T}_n$ are equal to identity matrix, leading thus to extended electronic states.

Following [1], let us write the transfer matrices in terms of identity matrix I and three Pauli matrices σ_x, σ_y, and σ_z, i.e.,

$$\begin{aligned} M_A &= \alpha_A I + \beta_A \sigma_x + \gamma_A \sigma_y + \delta_A \sigma_z\,, \\ M_B &= \alpha_B I + \beta_B \sigma_x + \gamma_B \sigma_y + \delta_B \sigma_z\,, \end{aligned} \tag{1}$$

where $\alpha_{A(B)} = \delta_{A(B)} = (E - \epsilon_{A(B)})/2$, $\beta_{A(B)} = 0$, and $\gamma_{A(B)} = -i$. Denoting by T_n and $\overline{T}_n$ the transfer matrices for the nth order TM lattices S_n and $\overline{S}_n$, respectively, i.e.,

$$\begin{aligned} T_n &= M_A M_B M_B M_A M_B M_A M_A M_B \ldots\,, \\ \overline{T}_n &= M_B M_A M_A M_B M_A M_B M_B M_A \ldots\,, \end{aligned} \tag{2}$$

each being a product of 2^n matrices, for even n, one has

$$\begin{aligned} T_n &= \alpha_n I + \gamma_n \sigma_y + \delta_n \sigma_z, \\ \overline{T}_n &= \alpha_n I + \gamma'_n \sigma_y + \delta'_n \sigma_z\,, \end{aligned} \tag{3}$$

(see Eqs. (5) of [1]). As T_n and $\overline{T}_n$ can be resolved in terms of T_{n-2} and $\overline{T}_{n-2}$ by

$$T_n = T_{n-2}\overline{T}_{n-2}\overline{T}_{n-2}T_{n-2}, \quad \overline{T}_n = \overline{T}_{n-2}T_{n-2}T_{n-2}\overline{T}_{n-2}\,,$$

which originate from the inflation rules of the TM chain, for even n, one can, after some algebra, rewrite T_n and $\overline{T}_n$ as

$$\begin{aligned} T_n &= \alpha_n I + \alpha_{n-2} A \sigma_y + \alpha_{n-2} B \sigma_z\,, \\ \overline{T}_n &= \alpha_n I + \alpha_{n-2} A' \sigma_y + \alpha_{n-2} B' \sigma_z\,, \end{aligned} \tag{4}$$

where A, B, A', B' are polynomials of finite order in terms of energy E. It is important to notice that the common factor $\alpha_{n-2} \equiv \mathrm{Tr}(T_{n-2})/2$ appear in the coefficients of σ_y and σ_z in both T_n and $\overline{T}_n$. In addition, when $\alpha_{n-2} = 0$, one has $\alpha_n = 1$ [see Eq. (5) below] besides $\gamma_n = \delta_n = \gamma'_n = \delta'_n = 0$. As a result, for even values of n, T_n and $\overline{T}_n$ can simultaneously become identity matrices. Noticing that the infinite TM lattice is only an aperiodic TM sequence of nth order ones, S_n and $\overline{S}_n$, one concludes that there will be no decay of wave functions throughout the entire infinite TM lattice at such energy values, i.e., the electronic states are extended at energy values satisfying $\alpha_{n-2} = 0$ [1,2].

Now we turn to clarify the number of distinct energy values leading to $\alpha_n(E) = 0$. For convenience and without any loss of generality, let us assume that $\epsilon_A = V$ and $\epsilon_B = -V$. From the trace map for the transfer matrices of the TM lattice [4],

$$x_{n+1} = x_{n-1}^2(x_n - 2) + 2, \qquad n \geq 2\,, \tag{5}$$

where $x_n \equiv 2\alpha_n$, and the initial conditions are given by $x_1 = E^2 - V^2 - 2$, $x_2 = x_1^2 - 4V^2 - 2$, one obtains

$$x_{n+1} = x_n^2 - 2 - 4V^2 \prod_{i=2}^{n}(2 - x_i), \qquad n \geq 2\,. \tag{6}$$

Define two intervals on energy value as I_1: $-E_2^* \leq E \leq -E_1^*$; I_2: $E_1^* \leq E \leq E_2^*$, where $E_1^* = \sqrt{V^2 + 1} - 1$ and $E_2^* = \sqrt{V^2 + 1} + 1$. With reference to the initial conditions and Eq. (6), $x_n(E) \leq 2$, with E within I_1 or I_2 for any n. As a result, for any energy value $E^{(n)}$ that satisfies $x_n(E^{(n)}) = 0$, one can derive from Eq. (6) $x_{n+1}(E^{(n)}) < -2$. Any energy value $E^{(n-1)}$ leading to $x_{n-1}(E^{(n-1)}) = 0$ will give rise to $x_{n+1}(E^{(n-1)}) = 2$ [see Eq. (5)]. With these characteristics of $x_n(E)$ in mind, it is not difficult to show that $x_n(E) = 0$ has 2^n distinct real roots, each of which corresponds to an extended electronic state in the infinite TM lattice. There are thus an infinite number of extended electronic states inside the energy intervals I_1 and I_2 on the infinite TM lattice.

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