Electron delocalization and multifractal scaling in electrified random chains

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Electron localization property of a random chain changing under the influence of a constant electric field has been studied. We have adopted the multifractal scaling formalism to explore the possible localization behavior in the system. We observe that the possible localization behavior with the increase of electric field is not systematic and shows strong instabilities associated with the local probability variation over the length of the chain. The multifractal scaling study captures the localization aspects along with strong instability when the electric field is changed by infinitesimal steps for a reasonably large system size.

KEYWORDS : localization, multifractal scaling, random chain

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Electronic states are exponentially localized in one-dimensional (hereafter 1D) random chains and the envelope of the wave function, \( \phi(x) \sim \exp(-\alpha x) \) for \( x \to \infty \) where \( \alpha \) is the inverse of localization length \( \alpha \). This localization nature of electronic states can be changed through application of a constant electric field and as a result electronic states exhibit some kind of different localized nature over the sample size. The problem of electronic states and localization in a random chain in the presence of a constant electric field is still a matter of controversy and is yet to be fully understood. In the past, the possibility of existence of non-exponential localization or localization/delocalization transition in electrified chain has been addressed. The deviation from exponential localization has been also claimed through the numerical study of electronic transmittance.

However, the localization mechanism can be understood more rigorously within the multifractal scaling analysis of the electronic wave functions without any a priori assumption of exponential localization nature and the existence of localization length. The multifractal scaling formalism has been invoked in the recent past to analyze the nature of electronic states in the vicinity of the mobility edge, and also for characterization of critical nature of electronic states in 1D Fibonacci quasiperiodic systems. Generally speaking, in all of the above examples, wave functions exhibit a rather involved oscillatory behavior displaying strong fluctuations. As a consequence the notion of envelope wave function or lyapunov exponent which has been successful in studying both the extended and exponentially localized states, is no longer suitable to the states in examples above. On the other hand multifractal scaling formalism has been found to be very useful to characterize the spatial fluctuating pattern of the wave functions which are neither Bloch like homogeneously extended state nor the exponentially decaying one. The same scaling analysis has been successful to extrapolate in the extreme limits also. So, it naturally appears that the possible delocalization behavior that we are going to address in this Letter can also be understood through the same scaling analysis.

The aim of this Letter is to report our investigation on how does localization nature is influenced by switching on a constant electric field through numerical study of electronic wave functions for a reasonably large array of \( \delta \)-function random potentials having a bi-modal distribution. The choice of this type of potential has been justified in the past both from its experimental relevances as well as from the pure academic interest. We start with the Schrödinger’s equation for the electrons in a random chain in presence of a constant electric field:

\[
\left[ -\frac{d^2}{dx^2} + \sum_{n=1}^{N} V_n \delta(x - na) - Fx \right] \Psi(x) = E \Psi(x) \quad (1)
\]

where the units are such that \( (\hbar^2 = 2m_e = 1) \) \( m_e \) is the effective mass of electron. The electric field induced force \( F \) is expressed in unit of \( \frac{h^2}{2m_e a^3} \), \( a \) is the lattice spacing and \( V_n \) is the strength of the \( n \)-th potential barrier (taking the value \( V_A \) or \( V_B \) randomly). \( F \) is the product of electric field by the electronic charge. The lattice constant \( a \) is taken unity throughout this calculation.

One can map the above Eq.(1) to a finite difference equation by approximating the potential \( Fx \) by a step function in-between the \( \delta \)-functions. Within this approximation, the solutions in-between the \( \delta \)-function potentials are now plane waves instead of Airy functions. The corresponding Poincare map is:

\[
\begin{align*}
\left[ -\frac{d^2}{dx^2} + \sum_{n=1}^{N} V_n \delta(x - na) - Fx \right] \Psi(x) &= E \Psi(x) \\
\end{align*}
\]
\[ \Psi_{n+1} = A_n \Psi_n + B_n \Psi_{n-1} \]  
(2)

The coefficients \( A_n \) and \( B_n \) are given by:

\[
A_n = \left[ \cos k_{n+1} + \frac{k_n}{k_{n+1}} \sin k_{n+1} \cos k_n + V_n \frac{\sin k_{n+1}}{k_{n+1}} \right]
\]

\[
B_n = -\frac{k_n}{k_{n+1}} \left( \frac{\sin k_{n+1}}{\sin k_n} \right)
\]

(3)

with \( k_n = (E + nF)^{1/2} \) and \( \Psi_n = \Psi(x = n) \). Now in order to solve the equation iteratively for a reasonably large system size one can consider the initial values for \( \Psi_1 = \exp(-iE^{1/2}a) \) and \( \Psi_2 = (-2iE^{1/2}a) \). \( E \) being the incident electron energy before it reaches the region where the electric field is applied.

The transmittance corresponding to the array of random \( \delta \)-function potential is given by:

\[
T = \left( \frac{k}{k_1} \right) \left( \frac{|\Psi_{N+2} - \Psi_{N+3} \exp(-i k_1)|^2}{|\Psi_{N+2} - \Psi_{N+3} \exp(-i k_1)|^2} \right)
\]

(4)

with

\[ k = E^{1/2} \quad \text{and} \quad k_1 = (E + FL)^{1/2} \]

and \( L = Na \).

We now analyze the pattern of local probability density \( |\Psi_n|^2 \) along the chain through its multifractal scaling relation of \( \alpha \) and \( f(\alpha) \), where \( \alpha \) stands for the scaling exponent and \( f(\alpha) \), the corresponding distribution function. We have used the mathematical prescription suggested by Chabbra and Jensen for its simplicity and success in correctly evaluating the quantities \( \alpha \) and \( f(\alpha) \) directly through the normalized measure without any numerical instability. Let us define the required normalized measure in our study by:

\[
P_i = \frac{|\Psi_i|^2}{\sum_{i=1}^{N} |\Psi_i|^2}
\]

where the scaling behavior of \( P_i \sim N^{-\alpha} \) for \( N \to \infty \).

According to Chabbra and Jensen if we define the \( q \)-th moment of the probability measure \( P_i \) by \( \mu_i(q, N) \) where

\[
\mu_i(q, N) = \frac{P_i^q}{\sum_{i=1}^{N} P_i^q}
\]

then a complete characterization of the fractal singularities can be made in terms of \( \mu_i(q, N) \). The expression for the distribution function of scaling exponent \( \alpha \) can be written as:

\[
f(\alpha) = \lim_{N \to \infty} \frac{1}{\log N} \sum_{i=1}^{N} \mu_i(q, N) \log \mu_i(q, N)
\]

(5)

and the corresponding singularity strength of the measure is obtained by:

\[
\alpha = \lim_{N \to \infty} \frac{1}{\log N} \sum_{i=1}^{N} \mu_i \log P_i.
\]

(6)

One can infer on the nature of electronic states for large \( N \) based on the following observation:

1. \textit{Extended nature} \( \alpha_{\text{min}} \to 1, f(\alpha_{\text{min}}) \to 1, \alpha_{\text{max}} \to 1, f(\alpha_{\text{max}}) \to 1 \).

2. \textit{Localized nature} \( \alpha_{\text{min}} \to 0, f(\alpha_{\text{min}}) \to 0, \alpha_{\text{max}} \to \infty, f(\alpha_{\text{max}}) \to 1 \).

This property is usually manifested by rectangular two-hump form of \( f(\alpha) \) curve with a sparse distribution of points in between.

3. \textit{Critical nature} \( \alpha \) vs \( f(\alpha) \) curves closely overlap on one another with the increase of system size.

4. \textit{Power-law nature} \( \alpha - f(\alpha) \) curve deviates slowly from one another with the increase of system size in contrast to the strong deviation as seen in the exponential decay.

We now define a simple way the degree of localization. We consider \( \Delta_n = (\alpha_{\text{max}} - \alpha_{\text{min}}) \) as a measure of degree of localization. This can distinguish clearly an extended state from a localized state for a sufficiently large system size \( N \). Also, one can investigate the change in the nature of states brought about due to the change of some external parameters, e.g., electric field.

In figure (1) we have shown the spatial pattern of local probability variation along the chain for a localized state in both zero and finite electric field. The upper curve exhibits the delocalized pattern in the presence of electric field \( F = 1.25 \times 10^{-5} \) unit. The corresponding localized and delocalized behavior of the electronic transmittance data have been been presented for both the zero as well as for a finite electric field in figure (2). In figure (3), we have shown \( (\alpha - f(\alpha)) \) plots for both the zero and the finite field value \( 2 \times 10^{-5} \). In the zero field case the plot shows in \( f(\alpha) \) a two-hump form corresponding to the exponential localization. This is due to the fact that \( (\alpha - f(\alpha)) \) spectrum is densely populated on the extreme left and on the right but the region in-between is very sparse. On the other hand, for finite electric field, the \( (\alpha - f(\alpha)) \) data gather in a relatively narrow region on the curve having a convex shape. This indicates that the change in localization behavior shows an overall delocalization trend which is exhibited through the more spatial extension of the state over the sample and hence resulting in the contraction of the \( \alpha - f(\alpha) \) spectrum.

Next we investigate further whether this delocalization pattern can change systematically as we change the electric field through small steps of the order of \( 10^{-8} \) unit for a sufficiently large system size.

In figure (4) we have shown the plot of degree of localization \( \Delta_n \) with the electric field for two large system sizes, \( N = 10^8 \) (upper curve) and \( N = 2 \times 10^9 \) (lower curve).
curve). In both the plots we see that $\Delta \alpha$ exhibits strong instability throughout the whole regime of electric field from a very low to as high as $10^{-5}$ unit. We have observed that for both the two system sizes, the order of deviation in $\Delta \alpha$ from its previous step is of the order of unity whereas the value of $\Delta \alpha$ itself is of the same order. Also the fluctuating pattern of $\Delta \alpha$ with $F$ for the both the two system sizes is almost the same. In figure (5) we have shown again the variation of the degree of localization, i.e., $\Delta \alpha$ with the electric field for a different set (cf. Figure 4) of potential parameters. Here the order of fluctuations in $\Delta \alpha$ corresponding to two large systems, i.e., $75 \times 10^3$ and $1.7 \times 10^4$ number of atoms have been presented. The order of fluctuations appear to be quite significant and it is nearly unity in the both the cases over a wide region of the electric field as shown in the figure through covering the fluctuating zone between the horizontal lines.

We think this kind of instability has its intrinsic origin in the restructuring of the different states in a complicated manner and each of them is highly sensitive even for an infinitesimal change in the applied electric field. This can be also understood as due to the competing nature of the potential $F n$ and the disordered $\delta$-potentials in the large system size. However, if one neglects this fluctuation through some brute force methods, it shows only an apparent simple delocalization effects due to the increase of electric field.

In conclusion, we have shown that the change of localization aspects due to the increase of a uniform electric field is not simply an overall delocalization but the localization property is very sensitive with respect to an infinitesimal change of electric field giving rise to a strong instability in the degree of localization. This instability aspect in the localization/delocalization is present for all reasonably large lengths for an appropriate set of parameters and is due to the combined effects of disorder potential and the electric field induced linear potential. At sufficiently large length scale the states change depending upon the restructuring of the spectrum from its previous form and hence the localization property of a particular state in a given field will change drastically giving rise to a state of modified localized nature. P. Biswas would like to thank the Council of Scientific and Industrial Research (CSIR) for financial assistance in the form of a senior research fellowship.

FIG. 1. Local probability (in log-scale) vs system size ($N$) in unit of $10^4$ number of sites. The parameters are: $V_A = 1.25$ units, $V_B = 1.4$ units, $c = 0.01$, $N = 4 \times 10^5$ for electric field $F = 2.0 \times 10^{-5}$ (upper) unit and $N = 5.6 \times 10^4$ for zero field (lower) with the energy of the incoming electron $E = 1.4890$ units in both cases. The data in the upper curve has been given a constant shift of 20 units in the log-scale for convenience of comparison.

FIG. 2. Transmittance $T$ (in log-scale) vs size ($N$) for the set of parameters as in figure 1. The plot is made up to a length of $4 \times 10^5$ number of sites for $F = 2.0 \times 10^{-5}$ (upper curve) and up to $5 \times 10^4$ number of sites in the zero field case (lower curve).
\[ f(\alpha) \]

\[ \alpha \]

\[ F = 0, 2 \times 10^{-5} \]

FIG. 3. \( \alpha \) vs \( f(\alpha) \) plot for finite (\( F = 2 \times 10^{-5} \) unit) as well as zero electric field for the local probability variation (\(|\Psi_n|^2\)) over the chain of length \( N = 4 \times 10^5 \). The other parameters are the same as in figure (1).

\[ f(\alpha) \]

\[ \alpha \]

\[ F = 0, 2 \times 10^{-5} \]

FIG. 4. The degree of localization (\( \Delta_\alpha \)) vs electric field (\( F \)) for the two different system sizes \( 10^5 \) (thick line) and \( 2 \times 10^5 \) (dashed line). The parameters are \( V_A = 1.25 \) units, \( V_B = 1.4 \) units, \( c = 0.01 \), and for incoming energy \( E = 1.4890 \) units. Once again, for comparison, we plot the negative of \( \Delta_\alpha \) for system size \( 2 \times 10^5 \) (dashed line).

\[ f(\alpha) \]

\[ \alpha \]

\[ F = 0, 2 \times 10^{-5} \]

FIG. 5. The degree of localization (\( \Delta_\alpha \)) vs electric field (\( F \)) for a different set of potential parameters. The thick and the dashed line corresponds to system size \( 7.5 \times 10^4 \) and \( 1.7 \times 10^5 \) with other parameters, \( V_A = 5.15 \) units, \( V_B = 5.34 \) units, and \( c = 0.05 \), and energy \( E = 5.6025 \) units.

\[ f(\alpha) \]

\[ \alpha \]

\[ F = 0, 2 \times 10^{-5} \]

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