Ambiguity Free Characterization of Metal-Insulator Transition in Disordered Fermionic Systems

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Abstract

Unambiguous characterization of metal insulator transition in disordered system is an important problem. One of the most widely used indicator to do this characterization is inverse participation ratio (IPR). IPR can capture the signature of metal insulator transition but it is not free of ambiguity. However, a much more effective and unambiguous approach to identify an insulating or metallic state is to use a localization tensor which is based on the idea of Kohn's localization. We have studied the one-dimensional Aubry-Andrè model with cosine modulated disorders. We have used both rational and irrational modulation of the disorder potential to show that it is easier to conclude about the electronic state if localization tensor is used for characterization.

Introduction

- The problem of random non-magnetic potential in real materials were first considered by P. W. Anderson.
- One of the important conclusion of his work was that in 1D an arbitrarily weak disorder is sufficient to localize all the eigenstates of non-interacting many-body fermionic system. This makes the system insulating.
- In contrast to this, in Aubry-Andrè (AA) model the disorders have been distributed over a 1D lattice following a cosine modulation.
- Surprisingly, if the potential modulation is irrational, electrons in AA model do not localize until the disorder strength reaches a critical value.
- Inverse participation ratio (*IPR*) is widely used to study metal (delocalized) to insulator (localized) transition (MIT). IPR captures the essence of MIT in most cases.
- But, *IPR* is not a very unambiguous and efficient approach to study MIT and characterize the metallic and insulating states in every situation.
- Another mathematical quantity known as localization tensor (*LT*) is discussed below, which is free of any kind of ambiguity in characterizing MIT.
- *LT* was originally developed by Resta and Sorella in late 90′*s* and used extensively to characterize MIT in case of different type of disorders.
- Details of *IPR* and *LT* methods are discussed below with AA model having rational and irrational modulation of the disorder potential.

Aubry Andrè Model

- This is a tight-binding model with on site incommensurate potential energy $cos(2\pi bi + \phi)$.
- Periodicity on a finite lattice is quite difficult to maintain with sinusoidal potential. Thus, this model is known as a disordered model.

$$H = \sum_{i=1}^{L-1} t(c_{i+1}^{\dagger} c_i + H.c) + W \sum_{i=1}^{L} cos(2\pi bi + \phi) c_i^{\dagger} c_i$$

- t is the hopping amplitude from site i to site $i+1$ and L is the size of the system (Lattice sites).
- $c^{\dagger}, c$ are the fermionic creation and annihilation operators respectively.
- W is the strength of disorderedness.
- ϕ is an arbitrary phase varying from $(0, 2\pi)$.
- b can have both rational and irrational values.

For a Half-filling system number of fermions should be equal to the size of the system in 1D i.e., $L = N$.

Energy Spectrum (E_n)

- The single particle energy spectrum for AA model studied by N. Roy with irrational value of **b** for different disorder strength.
- Considering both the rational and irrational values of **b**, one can observe the effect of disorder in non-interacting fermionic system.

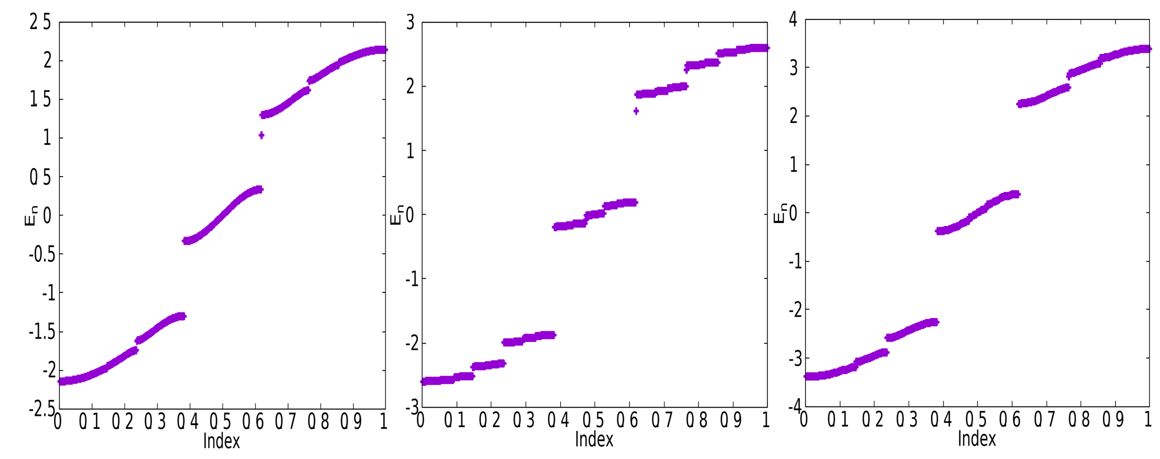

Figure: (left-right)Single particle energy spectra (E_n) for W= 1.0, 2.0, 3.0 respectively. Here N = 500, $\phi = 0$, $b = (\sqrt{5}+1)/2$.

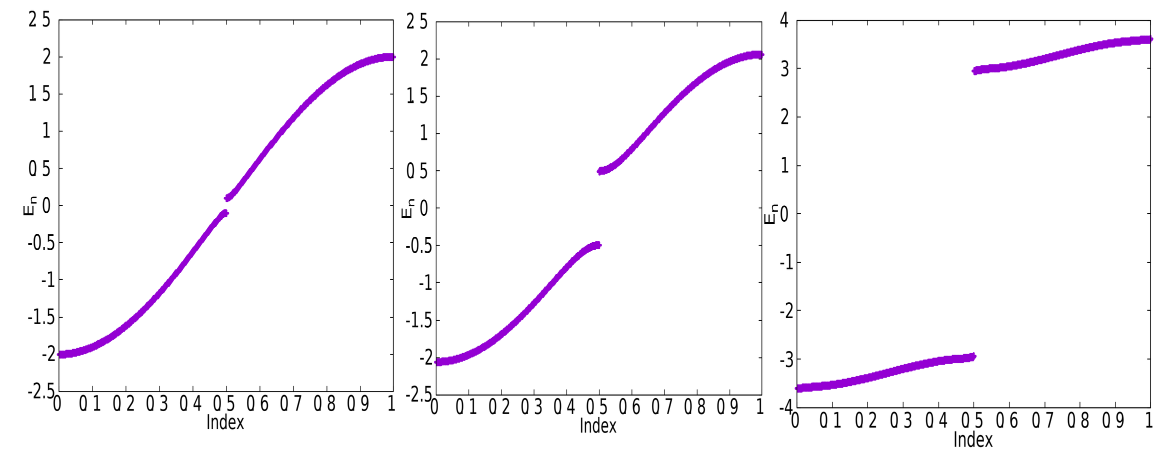

Figure: (left-right)Single particle energy spectra (E_n) for W= 0.1, 0.5, 3.0 respectively. Here N = 500, $\phi = 0$, $b = 1/2$.

Inverse Participation Ratio (IPR/I_n)

- IPR gives the spatial localization of a state.
- IPR acts as an order parameter for the Anderson localization phase transition.
- IPR tends to 0 for extended state and 1 for localized state.

$$I_n = \sum_{i=1}^{N} |\Psi_i|^4$$

where Ψ_i is the eigenstate at site $i = 1, 2, \ldots .N$ of the system.

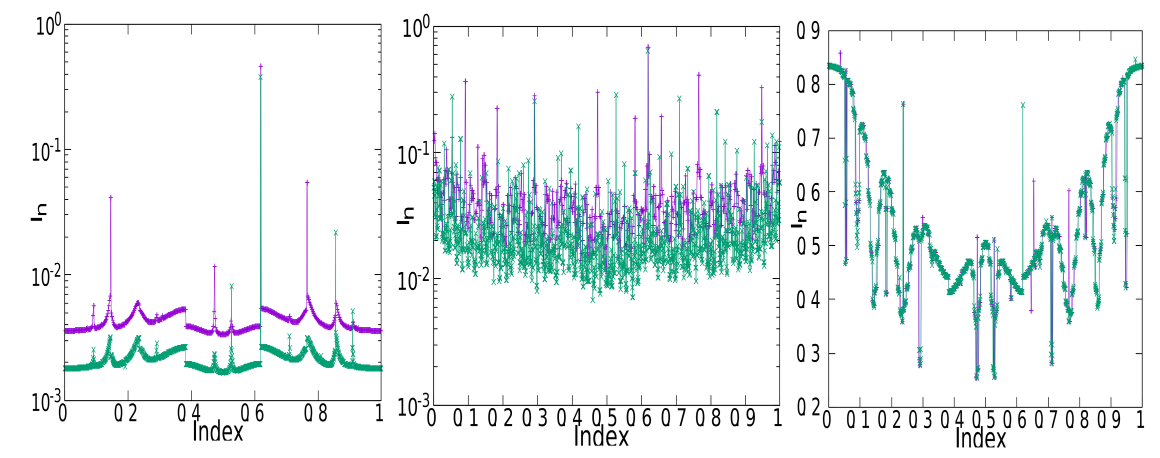

Figure: (left-right)Inverse Participation Ratio (I_n) for W= 1.0, 2.0, 3.0 respectively. Here N = 500 and 1000, $\phi = 0$, $b = (\sqrt{5}+1)/2$.

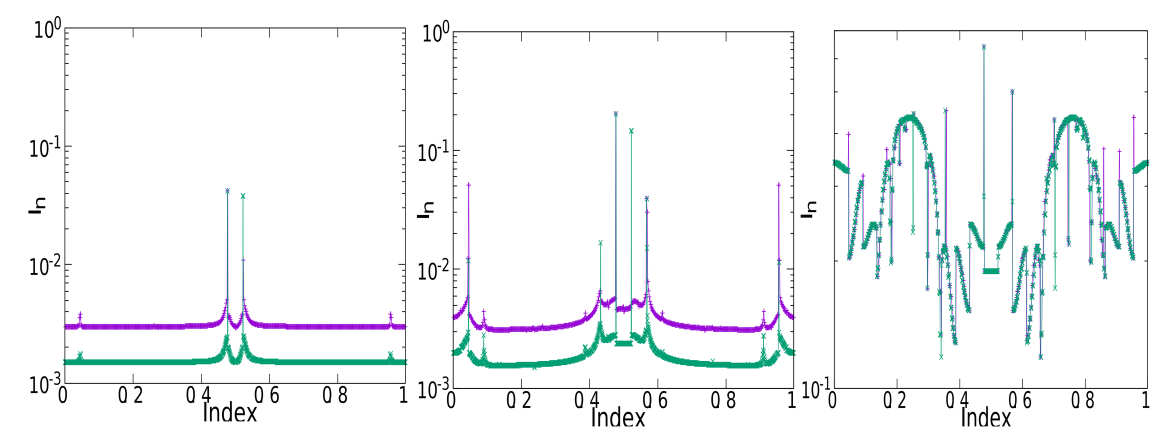

Figure: (left-right)Inverse Participation Ratio (I_n) for W= 0.1, 0.5, 3.0 respectively. Here N = 500 and 1000, $\phi = 0$, $b = 1/2$.

Conclusions

- There are various ways to study MIT and characterize metallic or insulating state. However, not all the methods are free of ambiguity.
- One of the most widely used indicator, *IPR*, is ambiguous in certain cases.
- As discussed, localization tensor λ^2 is actually a better alternative to study MIT and characterize metallic or insulating state.

Kohn's Localization and Localization Tensor

- A new and more comprehensive characterization of the insulating state of matter is developed by W. Khon.
- He showed the transition between an insulating and a conducting state with a physical quantity known as Khon's localization tensor.
- Using the idea of Kohn's localization we are giving a quantitative idea of the many-body localization tensor.
- In case of *metals* localization tensor *diverges* whereas in *insulators* localization tensor is *finite* in the thermodynamic limit.

$$\lambda^2 = \frac{1}{\nu N} \sum_{j,j'=1}^{N} \rho_{jj'}^2(\nu)(j - j')^2$$

where ν is the filling factor and $\rho_{jj'}^2(\nu)$ is the one-body density matrix.

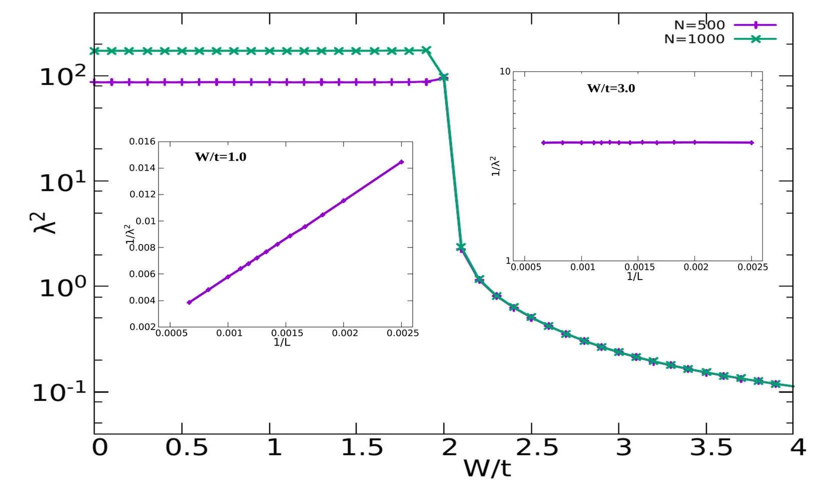

Figure: Square Localization tensor (λ^2) Vs. Disorder Strength (W/t). Here N = 500 and 1000, $\phi = 0$, $b = (\sqrt{5}+1)/2$.

- Irrational value of b, at half-filling AA model shows a MIT at a critical strength of the disorder $W/t = 2$ for any value of ϕ.
- Above result shows metallic below $W/t < 2$ and insulating for $W/t > 2$

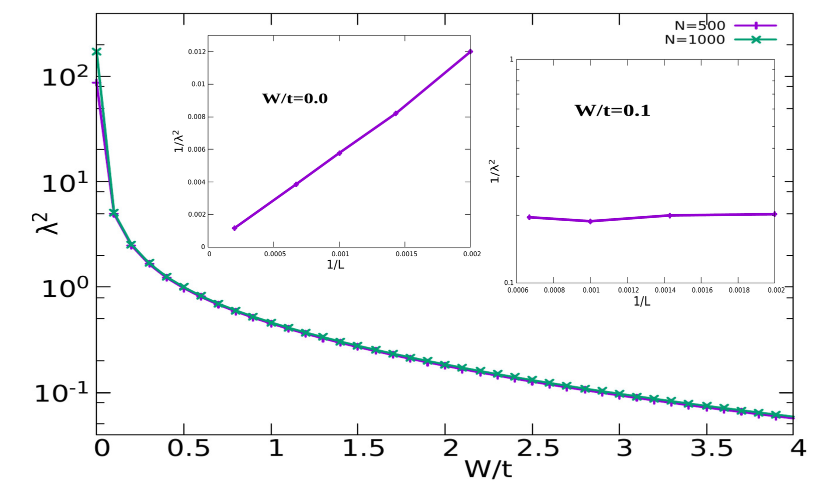

Figure: Square Localization tensor (λ^2) Vs. Disorder Strength (W/t). Here N = 500 and 1000, $\phi = 0$, $b = 1/2$.

- Rational value of b, AA model with half-filling should be insulating at any non-zero value of W/t.

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