Breakup of a Dimer: A New Approach to Localization Transition

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(74v, 2021)

Within the framework of tight binding models, aperiodic systems are mapped to a renormalized lattice with a dimer defect. In models exhibiting metal-insulator transition, the dimer acts like a resonant cavity and explains the existence of the ballistic transport in the system. The localization in the model can be attributed to the vanishing of the coupling between the two sites of the dimer. Our approach unifies Anderson transition and resonance transition and provides a new formulation to understand localization and its absence in aperiodic systems.

PACS numbers: 72.15.Rn+72.15-v

The existence of metal-insulator transitions due to quantum interference in correlated disordered systems is a fascinating subject. The origin of this resonant transition can be understood from the textbook examples of the quantum mechanics of a barrier in the continuum problem and from a simple dimer model in the case of a discrete lattice. The resonance transition where the metallic phase with ballistic transport is due to zero reflectance at the two sites of the dimer provides a simple mechanism to understand localization and its absence in systems with short range correlation. Recently, this transition was verified in experiments in superlattices [4].

In this letter, we present a universal approach to understand metal-insulator transitions by unifying Anderson transition with the resonance transition. Our formulation is applicable for any aperiodic system with reflection symmetry described by a nearest-neighbor tight binding model (TBM). In this paper we will confine ourselves to sinusoidal potentials which are further modulated by a Gaussian profile. The purpose of the Gaussian modulation is two-fold: as explained below, it provides a useful means to motivate and illustrate our ideas even though our results and conclusions are valid in the limit where the width of the Gaussian goes to infinity. Secondly, it facilitates the study of the pure Gaussian systems that have been the subject of recent studies due to its possible application as efficient energy band-pass filters in semiconductor superlattices. Finally, the case of sinusoidal potential further modulated by a Gaussian profile includes the famous Harper equation exhibiting Anderson localization as a limiting case.

The model system under consideration here is a TBM describing an eigenvalue problem with energy $E$,

$$\psi_{m+1} + \psi_{m-1} - E_m \psi_m = 0. \quad (1)$$

The $E_m = E - \epsilon_m$ is the diagonal term containing the aperiodic onsite energy $\epsilon_m$. This model also describes the Schrodinger equation for an array of $\delta$-function Kronig-Penny potential barriers,

$$-\frac{\hbar^2}{2M} \psi''(x) + \sum \epsilon_m \delta(x-ma) \psi(x) = E \psi(x). \quad (2)$$

This is due to the fact that the Poincare map associated with the model is a TBM with $E_m = \frac{\epsilon_m \sin(K)}{K} - \cos(K)$. Here $K$ is the Bloch vector related to the energy as $E = \hbar^2 K^2/2M$.

We choose $\epsilon_m$ to be sinusoidal potential which is further modulated by a Gaussian,

$$\epsilon_m = 2\lambda \cos[2\pi \mu(m-m_0)] \exp[-\frac{(m-m_0)^2}{2\sigma^2}]. \quad (3)$$

Here $\lambda$ is the strength of the potential, $\sigma$ is the width of the Gaussian profile and $\mu$ is an irrational number chosen to be the inverse golden-mean $\mu = \sqrt{5} - 1$. In this paper, we will describe our results for the pure Gaussian model ($\mu = 0$), the Harper equation ($\sigma \rightarrow \infty$) and also for the $\delta$-function barriers Eq. The last case closely resembles the recent study of Gaussian modulated Kronig-Penny model [3] and is also currently under experimental investigation in superlattices.

The basic idea underlying our approach can be understood for any localized defect with finite spatial extent. For aperiodic systems such as Harper equation where the aperiodicity exists throughout the lattice, we introduce Gaussian modulation so that the system can be viewed as a lattice with a localized defect. However, as shown below, the $\sigma \rightarrow \infty$ limit is well defined and therefore Gaussian modulation, although not needed, is useful in understanding the decimation scheme described below.

We envision perfectly transmitting phase in all aperiodic systems to be described by Bloch states on some renormalized lattice. In aperiodic systems where the defects are spatially confined to only some parts of the lattice, Bloch wave amplitudes are attenuated or amplified due to various quantum interferences only in the neighborhood of these defects. (See figure 1) We eliminate such sites from the model by decimating them. The resulting renormalized model will have solutions that are Bloch waves at all sites in the metallic phase. We like to emphasize that we decimate all sites which is in contrast to previous use of decimation for random systems where every other site is decimated. However, the basic idea of decimating all sites is similar in spirit to that
of Fibonacci decimation used in quasiperiodic systems where one eliminates all but Fibonacci sites so that the renormalized lattice may exhibit translational invariance in Fibonacci space.

Figure 2 outlines the decimation process. We begin by eliminating the central site $m_0$ of the symmetric defect. This leads to a renormalized model consisting of a dimer with coupling between the two sites as $\gamma_1 = 1/E_0$ and the onsite energy $E_1 = E_1 - \gamma_1$. We now begin the iterative process by decimating this dimer. At the $n^{th}$ step, we obtain a new lattice with renormalized dimer with onsite energies denoted as $E_{n+1}$ and the renormalized coupling between the 2-sites of the dimer as $\tilde{\gamma}_{n+1}$. This iterative decimation scheme results in a two-dimensional driven map for $\gamma - \tilde{E}$ where the $E_n$ containing diagonal disorder of the bare model provides the driving term,

$$\tilde{\gamma}_{n+1} = \frac{\gamma_n}{E_n^2 - \tilde{\gamma}_n^2},$$

$$\tilde{E}_{n+1} = E_{n+1} - (1 + \tilde{\gamma}_{n+1}\tilde{\gamma}_n)/\tilde{E}_n. \quad (4)$$

It should be noted that the parameters of the model are included in $E_{n+1}$. This 2-dimensional map contains the complexity of various interference effects within the Gaussian profile, manifesting itself in the energy dependent coupling and onsite potential. We would like to emphasize again that the map has a well defined limit for $\sigma$ equal to $\infty$. Therefore, Gaussian profile is not necessary in obtaining the mapping of the aperiodic model to the dimer model. The dynamics of the map depend upon $\sigma$: the finite value of $\sigma$ provides damping in the map with the consequence that the renormalization group (RG) flow settles on attractors while, in the limit of $\sigma \rightarrow \infty$, there are no attractors in the map.

The usefulness of this map emerges from the fact that the changes in the parameters $\lambda$ are reflected in the significant changes in the trajectories of the map for both finite as well as for the infinite value of $\sigma$. Figure 3 shows how the metal-insulator transition in the pure Gaussian case manifests itself in terms of the variation in the RG attractor as $\lambda$ is varied. In the subcritical phase, where the lattice has a transmission coefficient $T$ equal to unity, a symmetric period-2 limit cycle describes the RG flow for the renormalized coupling $\gamma$ while the dynamics of $\tilde{E}$ is governed by a fixed point. Away from the transition point, the RG attractor exhibits very regular oscillatory pattern consisting of symmetric lobes and divergences which is periodic in $\lambda$ with periodicity equal to $\frac{1}{\sigma}$. The fact that the total number of lobes or divergences is equal to $\sigma$ suggests that each lobe owes its existence to a particular site within the Gaussian profile where the sites near the center contributing at smaller values of $\lambda$. However, the quantitative understanding of almost equally spaced lobes and its physical significance remains eluded to us at present.

As we approach the transition point, the symmetric 2-cycle of $\gamma$ losess its symmetry, degenerates to a fixed point (seen in the figure 3 where the lobes cross) and then continues as an asymmetrical period-2 attractor. On the other hand, the fixed point describing the $\tilde{E}$ values becomes a 2-cycle. At the transition, $\gamma$ approaches zero with a power-law decay resulting in a broken dimer. The localized phase is characterized by an exponential vanishing of the the coupling with a characteristic length which is found to be related to the localization length $\xi$, of the localized wave function, $\tilde{\gamma}_n \approx \exp(-2\alpha/\xi)$. It turns out that in the localized phase, $\tilde{E}$ continues to be described by a period-2 fixed point exhibiting divergences where the spacing between two successive divergences increases as $\lambda$ increases.

The localization transition discussed above is a resonant transition where the metallic phase is described by Bloch wave solutions which undergo real phase shifts as they encounter the dimer defect. In the localized phase, these phase shifts become imaginary. Imposing this condition on the solutions of therenormalized system determines the condition for the perfect transmission. We express this condition in terms of a function $f$ defined as

$$f_n(\lambda, \sigma, E) = 1 - \tilde{\gamma}_n^2 + \tilde{E}_n(\tilde{E}_n - E_n). \quad (5)$$

Figure 4 shows the variation in $f_n$ and the transmission coefficient $T$ for the Kronig-Penny model Eq. (3) as the energy $E$ is varied. We see that the condition for the vanishing of this function coincides with the condition for perfect transmission. We would like to point out that the transmission coefficient was calculated in a rather simple way by using the renormalized dimer. This requires multiplying only two transfer matrices in contrast to usual calculations where one needs to multiply all transfer matrices on an aperiodic lattice.

The existence of a band of conducting states in Gaussian modulated lattices as discussed above (which is consistent with the previous related study) is a very desirable feature of a lattice making it a useful filter. Attempts are underway to make such filters using superlattices. This should be contrasted with the dimer-type defects where the metal-insulator transition is obtained by fine tuning the parameter to obtain the resonant energy close to the Fermi energy. We would like to point out that the metal-insulator transition and a band of perfectly transmitting states in Gaussian system can also be understood by heuristic arguments of asymptotic property of ”constancy” of the potential. Due to the finite width of the potential, the model has a constant potential asymptotically. This property is crucial in determining the $E$, which is the global property. This argument leads to extended states if $E > 2 - 2\lambda$ and localized states for $E < 2 - 2\lambda$. This condition is found to be true in our numerical simulations for large values of $\sigma$.

We next discuss the case of the pure Harper equation obtained in the limit $\sigma \rightarrow \infty$ in the driving term for the two-dimensional map. The sub-critical phase is not an

\[ \text{Figure 4: Variation in } f_n \text{ and transmission coefficient } T. \]
attractor. As $\lambda$ increases, the RG trajectories become more and more complex (see figure 5) and eventually collapse to a vertical line corresponding to $\gamma \to 0$ at the onset to localization transition. The localized phase is again characterized by an exponentially decaying coupling of the dimer with length scale which is equal to half the localization of the Harper equation. The metallic phase in Harper equation is thus described in terms of resonance due to the dimer and the Anderson localization is due to the breaking of this dimer.

Recently, the existence of extended states in supercritical Frenkel-Konterova (FK) model and in Fibonacci lattices was shown to be due to dimer-type correlations using decimation schemes that were model dependent. The novel aspect of the work described here is the universal nature of our approach: the 2-dimensional map Eq. (4) can be used to study localization or its absence in systems with short range correlations such as dimer defects, FK and Fibonacci models with long range correlations as well as in Harper equation. Our most important result is the picture of the localized phase as a phase with the broken dimer. Although the present framework is developed only for the TBM type systems, it is possible to extend our method to study localization in 2-dimensional models as well as for systems with long range interaction. The new methodology developed here will have applications in many other areas including dynamical localization in kicked rotors as well as the transition to strange nonchaotic attractors (SNAs) in quasiperiodically driven maps.

The research of IIS is supported by National Science Foundation Grant No. DMR 097535. IGC would like to thank for the hospitality during his visit to George Mason University. We would like to thank Bala Sundaram for his useful comments on this paper.

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FIG. 1. The wave function for sinusoidally modulated Gaussian case. We have Bloch wave with $K = 1/2$ outside the Gaussian profile. The points in the wave function are not joined for clarity. Here $\lambda = 0.5$ and $\sigma = 1000$.

FIG. 2. The Gaussian modulated lattice and the iterative decimation process.

FIG. 3. The variation in the asymptotic values of the renormalized coupling $\gamma_n$ and $E_n$ for $\sigma = 100$. There are few isolated points in the localized phase near the transition where $\gamma_n$ may diverge. Note that $\tanh$ is used to display the behavior at $\pm\infty$.

FIG. 4. The band of resonant energies corresponding to perfect transmission for $\delta$-function potential Kronig-Penny model. Here $\lambda = 10$ and $\sigma = 100$.

FIG. 5. RG trajectory for $\lambda = 0.992$ for $E = 0$ case for the Harper equation.
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