Dimer-Type Correlations and Band Crossings in Fibonacci Lattices

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Fibonacci system with both diagonal and off-diagonal disorder is mapped to a model with dimer type ‘defects’. The model exhibit resonance transition corresponding to zero reflectance condition resulting in extended states in the system. These Bloch-type states reside on the line of inversion symmetry of the energy spectrum and include states at the band crossings. The resonant states at the band crossings are related to the harmonics of the sine wave and have transmission coefficient equal to unity in quasiperiodic limit. This is in contrast to other resonant states where the transmission coefficient oscillates. An exact renormalization scheme confirms the fact that all resonant states are Bloch type waves as they are described by periodic attractors of the renormalization flow.

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Fibonacci systems have emerged as an interesting class of quasiperiodic systems exhibiting self-similar fractal wave functions as well as Bloch-type extended states. In earlier studies, interest in these systems was due to the fact that they exhibit cantor spectrum and power-law decaying wave function and hence are in between periodic and random systems. Recent interest in the Fibonacci systems is due to the possibility of extended states as was first discussed briefly by Wu et al. It was argued that the Fibonacci systems with both diagonal and off-diagonal quasiperiodic order are similar to the binary alloy model which is dual to the dimer model. Therefore Fibonacci system should exhibit the resonance predicted for the binary alloy model. Recently, Macia et al. discussed the existence of extended states in these systems by imposing the condition of commutativity of two non-equivalent blocks of transfer matrices. They obtained an explicit expression for the transmission coefficient for a finite size Fibonacci system and characterized these states as extended critical due to the fact that in the quasiperiodic limit the states have transmission coefficient (T) which oscillates as the size of the system is varied. They argued that the quasiperiodic order play a key role in determining the extended states which is in constrast to the analysis of Wu et al where the existence of extended states is due to a resonance condition unaffected by the long range quasiperiodic order in the system.

In this paper, the Fibonacci lattices with both diagonal and off-diagonal disorder are mapped to the lattices with dimer-type defects. Therefore, our results put the Fibonacci systems on the same footing as the lattices with dimer type correlations and hence, the origin of extended states in this system is traced to the resonance transition corresponding to a destructive intereferece of the reflected wave between the two neighboring sites of the dimer defect. Using this mapping, we derive the resonance condition and establish the fact that the extended states as discussed by Wu et al are identical to the propagating states discussed by Macia et al.

The fact that the extended states of the Fibonacci system are in fact Bloch waves on a decimated lattice is further confirmed by an exact renormalization group (RG) scheme. Novel result of our studies is the relationship between the resonant states and the states where the energy bands cross. We show that the resonant states at the band crossings are fully transmitting states (T = 1) in the quasiperiodic limit and are described by the wave functions that are related to the harmonics of the sine wave with fundamental Bloch number equal to the golden mean. Therefore, unlike the rest of states with oscillating T, these states have a special property namely for Fibonacci sizes the perfect transmission limit is well defined.

We consider a tight binding model (TBM) with both diagonal and off-diagonal disorder,

\[ t_{n+1} \psi_{n+1} + t_n \psi_{n-1} + \epsilon_n \psi_n = E \psi_n, \]

The Fibonacci system that we study is obtained by generating a Fibonacci sequence from two symbols s and b by the substitution \( s \rightarrow b \) and \( b \rightarrow bs \). The corresponding onsite potential takes two values \( \epsilon_s \) and \( \epsilon_b \). The resulting lattice can be viewed as made up of \( bbs \) and \( sbs \) types of sub blocks. The off-diagonal couplings are of two types corresponding to two possible nearest-neighbors and are denoted as \( t_{bs} \) and \( t_{bb} \). We choose \( t_{bs} = 1 \) and \( t_{bb} = \gamma \) as shown in figure 1.

In order to map the Fibonacci system to a dimer model, we decimate all the s sites of the lattice with onsite potential \( \epsilon_s \). The remaining b type sites renormalize in two different ways depending upon whether it belongs to \( bbs \) block or \( sbs \) block. As shown in figure 1, the resulting decimated lattice can be viewed as a pure r type lattice with d type defects that always appear in pairs. The renormalized onsite potential for the regular and dimer sites will be denoted as \( \epsilon_r \) and \( \epsilon_d \) and the coupling within the dimers is denoted as \( \gamma \). It turns out that the dimers are connected to each other and rest of the lattice by a coupling of unit strength. The renormalized onsite potential as well as couplings depend upon \( E \) and are related to the corresponding bare values of the parameters by the following equations.
\[ E_x = (E_0 E_x - 1) \]  
\[ E_d = (E_0 E_x - 2) \]  
\[ \gamma = \gamma E_x \]

Here \( E_x \equiv E - \epsilon_x \), where \( x = s, b, r, d \).

Next we look for a Bloch wave solution on the renormalized lattice. We consider Bloch wave solution where a propagating wave \( e^{i2\gamma n k} \) at site \( n \) with Bloch number \( k \) undergoes phase shifts as it encounters the dimer defects. Let \( \Omega_d \) be the phase shift between the pure lattice sites and the dimers and \( \Omega_{dd} \) be the phase shift within the dimer. It should be noted that there is no additional phase shift between two dimers. Substituting these traveling wave solutions in the renormalized TBM determines the phase shifts. A simple algebra requiring the phase shifts to be real (corresponding to nondecaying wave) determines the resonance condition,

\[ E = \frac{(\epsilon_b - \gamma^2 \epsilon_s)}{(1 - \gamma^2)} \]  
\[ (E - \epsilon_b)(E - \epsilon_s) = 4 \cos^2(k\pi) \]

By eliminating \( E \), we obtain

\[ (\epsilon_b - \epsilon_s) = \frac{2}{\gamma}(1 - \gamma^2) \cos(k\pi) \]

The resonance condition we obtain is identical to that of Wu et al [3] for binary alloy. Furthermore, for \( \epsilon_0 = -\epsilon_s = \alpha \), it reduces to the commutativity condition obtained by Macia et al [4]. Therefore, we conclude that the extended critical states of Macia et al [5] are in fact the resonant states. The renormalization analysis [6] discussed later on in this paper will provide a confirmation of the fact that the resonance condition is globally valid. Therefore, for the parameter values at which the resonance condition is satisfied we have Bloch wave solutions on the decimated sites. However, on the original lattice, the Bloch waves exist only on the \( b \) sites and the wave attenuates on \( s \) sites and then recovers back on \( b \) sites whenever resonance condition is satisfied.

The resonance criterion shows that the off-diagonal disorder, namely \( \gamma \) different from unity is crucial for obtaining extended states in the system. It is interesting to note that the off-diagonal disorder \( \gamma \) also determines the line of inversion symmetry, \( E(n, \alpha) = -E(F_N - n, -\alpha) \) for the spectral plot as shown in figure 2. Here \( F_N \) is the size of the system. This line of inversion symmetry coincides with the line where the resonance condition is satisfied. The striking feature of this spectral plot is the existence of band crossings which form a subset of resonant states. It turns out that at the band crossings corresponds a discrete set of energies with Bloch number \( k = n\sigma \) where \( n \) is an integer. Using the expression of the transmission coefficient given by Macia et al [5] \( T = \frac{1}{(1 + c^2 \sin(F_N \pi \ell))} \), where \( c \) is a function of parameters of the system, we see that these states corresponds to \( T = 1 \) as the size of the system \( F_N \) approaches \( \infty \). It should be noted that this approach to quasiperiodic limit is using Fibonacci sizes only. Therefore, the states at the band crossings have a well defined quasiperiodic limit.

This is in contrast to the rest of the resonant states where \( T \) oscillates between its minimum value (corresponding to \( \sin(F_N \pi k) = 1 \)) and the maximum value equal to unity, as the size of the system changes.

It turns out that the resonant states at the band crossings are related to the harmonics of the sine wave when expressed in terms of a continuous variable \( \theta = \{n\sigma + \phi_0\} \) (where the brackets denote the fractional part and \( \phi_0 \) is an arbitrary constant) except for a discontinuity at \( \sigma^2 \).

\[ \psi_n(\theta) = \sin(n\theta \pi), 0 \leq \theta < \sigma^2 \]
\[ = \frac{1}{\gamma} \sin(n\theta \pi), \sigma^2 \leq \theta < 1 \]

In contrast to \( n \)-even case, for \( n \)-odd, the wave function is a double valued function of \( \theta \). This analytical expression was first observed in our numerical computation of the wave function and is shown in figure 3.

The discrete onsite potential \( \epsilon_n \) of the Fibonacci system can be viewed as a two-step function of the variable \( \theta \) with a discontinuity at \( \theta = \sigma^2 \) where the potential jumps from -\( \alpha \) to \( \alpha \). The states at the band crossings share the discontinuity of the on-site potential. This characteristic is true for all resonant states including those that do not correspond to the band crossings. Such states are typically described by a wave function which is a multivalued function of \( \theta \) with a discontinuity at \( \sigma^2 \).

The nature of discontinuity in the wave function can be understood from our figure 1. As we discussed earlier, at resonance, the Bloch wave solutions exist on the decimated model with \( r \) and \( d \) type sites after the \( s \) sites have been eliminated. It is precisely at these \( s \) sites that the wave first decays in amplitude by \( \gamma \) and then recovers. Therefore, at resonance, although we have Bloch waves on the decimated model, the original lattice consists of waves that decays but recovers again. Therefore, for infinite systems these waves are always fully propagating modes and there is no net attenuation.

We have described two types of resonant states: the states which are related to all harmonics of the sine functions and have the transmission coefficient equal to unity in quasiperiodic limit and the states where the transmission coefficient oscillates as we approach quasiperiodic limit. We next seek a better characterization of the resonant states using our recently developed RG approach. This methodology provides an independent confirmation of the existence of extended states in the system. Here the extended states are distinguished from the critical states by the trivial attractor of the renormalization flow. This approach was recently used to demonstrate the existence of Bloch wave type phonon modes in the supercritical incommensurate Frenkel-Kontorova (FK) model.
Basic idea underlying the renormalization scheme for the quasiperiodic system with golden mean incommensurability is to decimate out all lattice sites except those labeled by the Fibonacci numbers $F_m$. Starting from an arbitrary initial site $n$, at the $m$th step, the decimated TBM can be written as

$$\psi(n + F_{m+1}) = c_m(n)\psi(n + F_m) + d_m(n)\psi(n). \quad (10)$$

Using the defining property of the Fibonacci numbers, $F_{m+1} = F_m + F_{m-1}$ with ($F_0 = 0, F_1 = 1$), the following recursion relations are obtained analytically for the decimation functions $c_m$ and $d_m$.

$$c_{m+1}(n) = c_m(n + F_m)c_{m-1}(n + F_m) - d_{m+1}d_m(n), \quad (11)$$

$$d_{m+1}(n) = -d_m(n)d_m(n + F_m) + c_m(n + F_m)c_{m-1}(n + F_m)c_m^{-1}(m). \quad (12)$$

These recursion relations can be iterated numerically for a large number of decimation steps limited only by the precision of the parameters and the energy $E$ and the machine precision. For resonant states, since the energies are known analytically, the asymptotic behavior of the RG flow can be obtained with very high precision. Our previous studies have shown that the extended eigenfunctions lead to an asymptotic trivial attractors of the RG flow while the critical states at the band edges are characterized by nontrivial attractors. In the localized phase, the RG flow decays to zero or becomes unbounded. Therefore, by studying the variation in the renormalization attractor as the parameters $\alpha$ and $\gamma$ are varied, we can determine the nature of eigenstates of the system.

Figure 4 shows the renormalization attractor as $\alpha$ varies for a fixed value of $\gamma$ for states corresponding to the minimum energy ($k = 0$). There exists a symmetric 4-cycle which varies continuously as the parameter $\alpha$ changes. This implies that the wave function repeats itself at every 4th Fibonacci site and hence describes a translational invariance in Fibonacci space for quasiperiodic system. The variations in the RG attractor implies that the scaling properties of the critical wave function changes continuously as the parameter $\alpha$ changes. For a special value of the parameter which satisfy the resonance condition, this nontrivial RG attractor degenerates to a trivial cycle $\pm \sigma^{-1}$, determined by the underlying incommensurability. Therefore, the existence of a crossings in the RG attractors signal the resonance transitions. Further studies of resonant states other than those at band crossing shows that all such states are described by trivial attractors of the renormalization flow. The period of these attractors vary as the parameters change but the RG flow always settle asymptotically at values which are $1, 0, \infty$ or powers of $\sigma$. For example, for for $E = -5/6$, the RG flow converges to $-1, -\sigma, -1, 0, \infty, 1, 1/\sigma, 1, 0, \ldots$

It should be noted that in contrast to the resonant states, off-resonant states are always characterized by a nontrivial RG attractors. The critical states at the band edges are characterized by a period-4 cycle while the rest of the critical states are described by strange attractors of the RG flow.

In summary, the RG analysis confirms the fact that quasiperiodic Fibonacci systems exhibit Bloch wave type solutions. Appropriate decimation scheme traces the origin of these states to hidden dimer type correlations in the system. Therefore all states that satisfy resonance condition are Bloch waves on a decimated lattice. These includes the semi transparent states of finite Fibonacci lattices discussed previously. For infinite size system, these states are fully transparent states with oscillating $T$ as there is no net attenuation. Intriguing result of our paper is the existence of extended states with Bloch number equal to the multiple of the golden mean. In contrast to rest of the resonant states, these states which reside at the band crossings have transmission coefficient equal to unity in the quasiperiodic limit. Therefore, our studies provide a clear characterization of extended states in the Fibonacci system and shows that the existence of fully propagating states is not related to the quasiperiodic long range order of the system.

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FIG. 1. Fibonacci lattice with two types of diagonal couplings defining a lattice with $b$ and $s$ types of atoms. The springs denote the coupling $\gamma$ while straight lines denote unit coupling. Renormalized lattice after the $s$ type sites are decimated. The resulting lattice can be viewed as a regular $r$ type lattice with $d$ type de wh always appear in pairs.

FIG. 2. Band spectrum as a function of $\alpha$ for a fixed $\gamma$ equal to 2 in (a) and is equal to unity in (b). The resonant states lie on the dashed line which happens to be the line of inversion symmetry and passes through the band crossings. In the absence of off-diagonal disorder, the resonance and band crossings happen at trivial value of $\alpha$.

FIG. 3. Figure shows the wave functions at four different band crossings as a function of $\theta$: (a) shows the wave function for $n = 2, 4$ which is related to the first and second harmonics of the sine wave, and (b) corresponds to $n = 1, 3$. Unlike the even $n$ case, the wave function is not a single valued function of $\theta$. The wave functions show the discontinuity of the underlying potential at golden mean.

FIG. 4. Renormalization attractor as a function of $\alpha$ showing how the period-4 limit cycle of the decimation function $c_n$ changes as $\alpha$ varies for the states corresponding to minimum energy ($k = 0$) at a fixed value of $\gamma = 2$. The existence of resonant states appears as a crossing as the nontrivial cycle degenerates to a trivial 2-cycle $\pm \sigma^{-1}$. 
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