Spectral features of one dimensional phononic quasicrystals

Anupam Saha¹, Moumita Dey¹ and Santanu K Maiti²

¹Department of Physics, Adamas University, Barasat-Barrackpore Road, Kolkata-700 126, West Bengal, India
²Physics and Applied Mathematics Unit, Indian Statistical Institute, 203 Barrackpore Trunk Road, Kolkata-700 108, India

Abstract. We make an in-depth analysis of phonon frequencies and phononic eigenstates for one-dimensional phononic lattices. The results are analyzed for two different types of lattices, depending on whether the spring constants are uniform or aperiodic. For the first case, we find usual band structures with extended states, while several non-trivial features are obtained for the latter one. We find the eigenfrequencies by solving the set of coupled equations involving the motions of different atoms in the chain. The frequency spectrum reveals a fractal like behaviour and the fractality gradually decreases with the increase of the strength of the aperiodic modulation. The nature of different phonon states is characterized by calculating inverse participation ratio. A finite transition from conducting to non-conducting phase is obtained upon the variation of the modulation strength. We hope the results studied here can easily be tested in a suitable setup.

1. Introduction

Quasiperiodic lattices have been the object of intense research over many years and known to exhibit different non-trivial signatures [1-12] in transport phenomena in mesoscopic regime especially due to the existence of atypical gapped spectrum. A large amount of works has been done in the context of electronic localization considering many quasicrystals [1-12], as localization phenomenon has always been a classic problem since its prediction by P. W. Anderson [13] in 1958 and still relevant. In the seminal work, Anderson had shown that for a 1D system all the energy eigenstates are (exponentially) localized, when the lattices are arranged in a ‘random’ sequence, irrespective of the strength ($W$) of the randomness, which yields the critical point $W_c = 0$. This critical point gets changed when the sites are arranged in a specific sequence which is neither perfect, nor completely disordered one, rather it bridges the gap between these two types and they are known as ‘correlated or deterministic disordered’ systems. One example of such correlated disordered systems is Aubry-Andre or Harper (AAH) model where the site energies and/or hopping integrals are modulated in the cosine form [1,5-7]. The non-trivial topological phase of matter makes the AAH model truly unique. One of the key features is the charge pumping and most importantly it is done without any dissipation by adiabatically changing the physical parameters describing the system [5]. Such a prediction of dissipationless...
transmission is undoubtedly a breakthrough work and moreover it has recently been verified experimentally using photonic superlattices with AAH modulations [5].

Now similar to photonic superlattices, interest has rapidly grown up in phononic superlattices [14-17] as well aiming to have anomalous signature in elastic or sound wave propagation. For proper manipulation of phonon transmission, the understanding of phonon frequency spectrum is the foremost requirement. Till date, to the best of our knowledge, very few works have been reported in this line of work and essentially it triggers us to further probing. Considering a one-dimensional phononic lattice, with AAH type modulation, we explore (i) spectral properties and (ii) nature of phononic eigenstates under different input conditions. The eigenfrequencies are obtained by solving the equations of motion of different atoms following Hooke’s law where the nature of phononic states is characterized by investigating Inverse Participation Ratio (IPR) [10,18]. IPR provides a suitable measure whether a state is extended or not as it is directly associated with the participation at different lattice sites [10,18]. We hope that the present analysis gives some basic spectral features of a quasiperiodic phononic lattice that can be extended in more complicated systems.

The work is arranged as follows. Following the brief introduction (Sec. 1), in Sec. 2 we present the model and theoretical formulation for finding the phonon frequencies and characterizing the localization properties of different phonon states. All the essential results are presented and thoroughly discussed in Sec. 3. Finally we conclude our findings in Sec. 4.

2. Quantum system and Theoretical framework

Let us begin with Fig.1 where atoms are arranged to form a 1D chain and they are connected by springs. Each atom can oscillate about its equilibrium position. If \( u_n \) be the displacement of \( n \)-th atom, then following Hooke’s law we write the force equation as

\[
F_n = C_{n+1}(u_{n+1} + u_n) + C_n(u_{n-1} - u_n)
\]

(1)

![Figure 1: One dimensional phononic lattice where atoms are connected by springs. \( u_n \) is the displacement of the atom at \( n \)-th site from its equilibrium position.](image)

Assuming, \( u_n = e^{i\omega t} \) Eq. (1) can be rewritten as,

\[
\left(M_n\omega^2 - v_n\right)u_n = -c_{n+1}u_{n+1} - c_nu_{n-1}
\]

(2)

Where, \( M_n \) is the mass of atom, \( \omega \) is the phonon frequency and \( v_n = \left(C_n + C_{n+1}\right) \).

For a N site phononic chain, we get N coupled equations like Eq. (2), and solving them we obtain the eigenfrequencies and eigenenergies.

Now, the incomensuration effect can be added in a system in different ways, either in the spring constant considering identical masses or in the masses [19] taking uniform spring constant or in both. In the present study we impose the modulation only in the spring constant keeping the masses identical.
as a matter of simplification. Hence, considering Cosine modulations, spring constants can be expressed as,

\[ C_n = C_0 \left[ 1 + \lambda \cos(2\pi bn) \right] \]

Here, \( C_0 \) being the spring constant in absence of any modulation, \( \lambda \) is the modulation strength, \( b \) is a constant parameter which can be a rational or irrational number \([18,20]\). When \( b \) is rational (i.e., in the form of \( 1/q \), \( q \) being a nonzero number), the system becomes a periodic one with periodicity \( q \). On the other hand, for an irrational value of \( b \), the system becomes aperiodic. In this present work, we critically examine the spectral properties of such systems where the modulations are given through aperiodic form.

Now, in order to characterize the localization properties of such a phononic super lattice we calculate the Inverse Participation Ratio (IPR) of individual phonon states. For any particular state \( |\psi_p\rangle \), IPR is defined as \([10,18]\),

\[ IPR|_p = \frac{\sum_n |u_{p,n}|^4}{\left( \sum_n |u_{p,n}| \right)^2} = \sum_n |u_{p,n}|^2 \]

where \( u_{p,n} \)'s are the wave amplitudes of \( p \)-th state at \( n \)-th site. Finally we calculate the Average Inverse Participation Ratio (AIPR) to predict the localization properties of the full system. AIPR is defined as, \( AIPR = \left( \frac{1}{N} \sum_{p=1}^{N} IPR|_p \right) \).

AIPR \( \rightarrow 0 \) means the states are extended in nature, whereas for the localized ones AIPR \( \rightarrow 1 \). AIPR very closed to 1 is achieved only in the asymptotic limit \([10,18]\).

3. Quantum system and Theoretical framework

The primary aims of our work are to analyze the spectral properties and localization behavior of a 1D phononic lattice under different input conditions. Before presenting the results let us briefly mention the parameter values those are kept unchanged throughout the numerical calculations. The spring constant amplitude \( C_0 \) is fixed at 1, and we set, \( M_n = M = 1 \) \( \forall \ n \) for the sake of simplification, as those are constant factors. As already mentioned, the parameter \( b \) can be commensurate (in the form of \( 1/q \)) or an incommensurate one. Unless stated otherwise we choose the incommensurate value of \( b \) as \( b = (1 + \sqrt{5})/2 \), the Golden Mean.

We begin our discussion by referring Fig. 2 where phonon frequencies are shown for 3 commensurate values of \( b \) considering a 200-site phononic lattice with \( \lambda = 0.5 \). The results are quite interesting. For \( b = 1 \) (\( q = 1 \)), a continuous band is obtained throughout the frequency window, like what we get for the electronic case since in this situation the system is fully perfect and behaves like a monoatomic chain. All the diagonal elements \( v_n \) (see Eq. (2)) are same and the non-zero elements associated with the spring constants are also same. As a result of this a continuous, gapless spectrum is obtained. Now, as we make \( b = 1/2 \) (i.e., \( q = 2 \)), all the diagonal elements remain identical, while the non-zero off diagonal elements achieve two different values. Under this situation, the system looks like a
monoatomic lattice with two different kinds of bonds (viz, short and long). Because of this a band splitting takes place providing a large gap between the bands.

Figure 2: Phonon frequencies for a 200-site phononic chain for three different values of $b$, which are (i) $b = 1$, (ii) $b = \frac{1}{2}$ (iii) $b = \frac{1}{3}$. For better viewing we draw a vertical line of identical height at each eigenfrequency. Here, we set, $\lambda = 0.5$.

The spectrum becomes somewhat interesting when we set $b = 1/3$ (i.e., $q = 3$). For this case, both the diagonal and non-zero off-diagonal elements acquire two different types of values similar to the binary lattice with (say,) long and short bonds. As a result of this more sub-bands appear in the frequency spectra.

Figure 3: Eigenfrequencies of an incommensurate 1D phononic lattice for three different values of $\lambda$, where, (a) $\lambda = 0.5$, (b) $\lambda = 1.5$ and (c) $\lambda = 2.5$. The other parameters are $N = 200$ and $b = (1+\sqrt{5})/2$.

Now we focus on the spectra given in Fig.3, where the eigenfrequencies are shown for the incommensurate phononic lattice at three different values of $\lambda$. With the inclusion of irrational $b$, both the diagonal and non-zero off diagonal elements of the matrix formed by the equations of motion (see Eq. (2)), involving the spring constants become different, like disordered system but they are deterministic in nature unlike the random (uncorrelated) ones. Although the masses are uniform, the effective diagonal elements $(M \omega^2 - v_n)$ are modulated in the cosine form along with spring constants.

This is quite analogous to the generalized AAH model and the frequency spectrum looks similar to what we get in electronic eigenenergies. The spectrum is ‘gapped’ in nature which is the generic feature of an AAH system. In this context, it is relevant to note that similar kind of gapped spectrum can also be obtained in other quasicrystals, and thus, it is a robust phenomenon. The eigenfrequencies are fractal like, and the fractality gradually decreases with increasing $\lambda$. The band widths get reduced with $\lambda$ and more higher values of $\omega$ are obtained.

The characteristic features of extendedness of phononic eigenstates under different input conditions are clearly described in Fig.4. As already pointed out that for $\text{AIPR} \to 0$, we get extended behavior, while it becomes finite for the localized phase. Absolute localization yields $\text{AIPR} \to 1$, which can be achieved in the asymptotic limit, i.e., for $N \to \infty$. We compute AIPR in Fig.4 by varying either $\lambda$.
keeping $b$ as a constant (Fig.4(a)), or by changing $b$ when $\lambda$ is kept constant (Fig.4(b)) or by varying both $b$ and $\lambda$ (Fig.4(c)). In all these cases we set $N = 100$. The results are really interesting and significant as well. From the AIPR- $\lambda$ curve (Fig.4(a)), it is observed that beyond a critical $\lambda$ (say, $\lambda_c \approx 1$), a transition takes place. Below $\lambda_c$, AIPR is very close to zero which reveals extended behavior of the phononic states. But for $\lambda > \lambda_c$, all the states starts to get localized. Thus, a delocalization to localization transition is clearly obtained by tuning the modulation strength $\lambda$. This phase transition is analogous to the electronic phase transition in the AAH lattices. But, the most notable feature that is observed here is the ‘delocalizing’ tendency of the phononic states in the limit of higher $\lambda$ (Fig.4(a)) where AIPR tends to decrease with increasing $\lambda$. It can be physically explained as follows. With the inclusion of cosine modulation in spring constants the system behaves like a generalized AAH model as the diagonal elements are also modulated. So, we can say that the deterministic disorders are there both in the diagonal and off diagonal sectors. As a result of this, the states get localized with increasing $\lambda$ (for weak $\lambda$). When $\lambda$ is quite large, the effective spring constants increases which circumvents the localization caused by the non-uniform effective masses. An analogous delocalizing behavior in the context of electronic eigenstates has also been reported in a generalized AAH model very recently [18].

Figure 4: Dependence of AIPR of a 1D phononic lattice on (a) $\lambda$, when $b$ is fixed at golden mean value, (b) $b$, when $\lambda$ is fixed at 1, and (c) $b$ and $\lambda$ (density plot). Here we set $N = 100$.

Figure 4(b) describes the variation of AIPR with $b$ for a fixed $\lambda$ a nice oscillatory pattern is exhibited which clearly indicates that multiple transitions from one phase to another phase can be obtained. This is somewhat related to the multiple switching action.

The results presented in Figs. (a) and (b) raise an obvious question like what will be the nature of AIPR when we simultaneously vary $b$ and $\lambda$. The answer is given in Fig. 4(c) where the density plot of AIPR is shown as functions of $b$ and $\lambda$. Almost for the entire region AIPR seems to be very low, but there are some specific zones associated with $b$ and $\lambda$ for which AIPR reaches to a large value which essentially suggests the localized behavior. From this spectrum, we can thus easily select $b$ and $\lambda$ to have an extended phase or the localized one.

4. Closing Remarks

In the present work we have studied spectral properties of a one-dimensional phononic lattice. Both the commensurate and incommensurate forms have been taken into account, where the
eigenfrequencies have been calculated by solving the coupled equations involving the equations of motions of different atoms. For the commensurate lattices we have the usual band splitting depending on the unit cell, whereas the frequency spectrum exhibits fractal like feature for the incommensurate ones. The fractality gets reduced with increasing the modulation strength. We have also examined the characteristic features of different phononic eigenstates under different input conditions. A sharp transition from extended to localized phase has been observed. Together with this, we have also found a delocalizing behavior even when we increase the modulation strength. Our analysis can easily be extended to investigate the spectral peculiarities in multi-stranded phononic ladders in presence of quasiperiodic modulations.

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