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THE GENERALIZED EIGENVALUE POLYNOMIAL FOR THE ANISOTROPIC HARPER EQUATION

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Abstract. The derivation of the energy bands characterizing the Harper equation proceeds in terms of a suitable energy polynomial. The general form of this polynomial is presented in some more detail, now by accounting for the influence of the anisotropy parameter. The wavefunction can then be written down in an explicit manner. The dependence of the energy bands on the anisotropy parameter is also displayed.

Key words: energy bands, generalized energy polynomial, Harper-equation.

1. INTRODUCTION

The quantum-mechanical description of tight-binding electrons on two dimensional lattices with nearest-neighbor hoppings threaded by transversal and homogeneous magnetic fields is still a fascinating problem. In this context one gets faced with the so-called Azbel-Hofstadter problem [1,2], which results in the Harper equation written down time ago [3]. This is a second order discrete equation exhibiting the form:

$$\phi_{n+1}e^{i\alpha_1} + 2\Delta\cos\left(2\pi\beta n + \alpha_2\right)\phi_n + \phi_{n-1}\,e^{-i\alpha_1} = \varepsilon\phi_n\,, \qquad (1)$$

where n is an integer, α_1 and α_2 are the Brillouin phases relying on the first unit cell, whereas $\beta = P/Q$ is the commensurability parameter expressing the number of magnetic flux quanta per unit cell. Here we restrict ourselves to rational values of this parameter, in which case P and Q are coprime integers. The anisotropy parameter discriminating between the metallic $\left(0<\Delta<1\right)$ an insulator $\left(\Delta>1\right)$ [4] phases is denoted by Δ.

Our main emphasis in this paper is on the derivation of the general form of the energy polynomial, which opens the way to the derivation of wavefunction coefficients. We then have the opportunity to generalize the results presented before for $\Delta=1$ [5] towards arbitrary Δ values. Moreover, having obtained the energy polynomial leads to the density of states (DOS), as shown before for

$Q = 1-8$ [6]. Related Lyapunov exponents [7] as well as Δ-dependent generalizations of Green functions [8] can also be established.

The energy polynomial referred to above, say $P^{(Q)}(\varepsilon,\Delta)$, is a polynomial of degree Q, which is independent of Brillouin phases, but which produces energy bands *via* [9]:

$$P^{(Q)}(E,\Delta) = \Lambda \equiv 2\cos Q\alpha_1 + 2\Delta^Q \cos Q\alpha_2 . \tag{2}$$

The energy bands can then be established by accounting for the inequalities:

$$-2-2\Delta^Q \le P^{(Q)}(E,\Delta) \le 2+2\Delta^Q \tag{3}$$

where the equality signs are responsible for the band-edges. One would then obtain a number of Q bands, the central ones being adjacent for even Q values.

A recursive method for the computation of $P_k^{(Q)}(E,\Delta)$ can be derived by resorting to the secular equation [9, 10], or by using the transfer matrix approach [2]. It is understood that both methods are heavy tractable for large Q values. We shall then proceed further by establishing the general form of the energy polynomial relying on the present $\Delta \neq 1$-choice, *i.e.*, by resorting to the three term recurrence relations characterizing the generalized Δ-dependent but q-symmetrized Harper equation [11].

2. PRELIMINARIES CONCERNING THE Q-SYMMETRIZED HARPER EQUATION WITH ANISOTROPY

The form of the Harper equation for the midband $(\Lambda = 0)$ symmetric gauge has been discussed before for $\Delta = 1$ [12, 13]. Such formulae have been updated by accounting for the anisotropy parameter. This results in the generalized q-difference equation [11]:

$$i\left(\frac{1}{z} + \Delta q z\right)\psi(qz) - i\left(\frac{z}{q} + \frac{\Delta}{z}\right)\psi\left(q^{-1}z\right) = \varepsilon\psi(z) \tag{4}$$

where $q = \exp(i\pi\beta) = \exp(i\pi P/Q)$ is the pertinent deformation parameter. Concrete results have been established in some detail for $\Delta = 1$ [14, 15], whereas the $\Delta \neq 1$-case referred to above has been discussed recently [11]. Now the wavefunction is expressed in terms of the Laurent sums

$$\psi(z) = \sum_{i=-Q}^{Q-1} C_n z^n \tag{5}$$

where $C_{-1} = 0$ and $C_0 = 1$. Inserting Eq. (5) into Eq. (4) leads us to the three term recurrence relation:

$$i\left(q^{n+1} - \Delta q^{-(n+1)}\right)C_{n+1} + i\left(\Delta q^{n} - q^{-n}\right)C_{n-1} = \varepsilon C_n\,, \tag{6}$$

which serves as a starting point for the present investigations, too.

3. EXPLICIT REALIZATIONS OF ENERGY POLYNOMIALS

Let us introduce the quotations

$${}_{q}^{\Delta}[n] = i\left(\Delta q^{n} - q^{-n}\right), \tag{7}$$

$${}_{q}[n]^{\Delta} = i\left(q^{n} - \Delta q^{-n}\right), \tag{8}$$

and

$$\left({}_{q,\Delta}[n]\right)^2 = \left({}_{q}^{\Delta}[n]\right)\left({}_{q}[n]^{\Delta}\right) = -\left(\Delta q^{n} - q^{-n}\right)\left(q^{n} - \Delta q^{-n}\right). \tag{9}$$

Accordingly, Eq. (6) exhibits the form

$${}_{q}[n+1]^{\Delta}\, C_{n+1} + {}_{q}^{\Delta}[n] C_{n-1} = \varepsilon C_n\,. \tag{10}$$

One readily sees that under complex conjugation one has

$${}_{q}^{\Delta}[n] = \left({}_{q}[n]^{\Delta}\right)^{*}, \tag{11}$$

in which case (see also [5])

$${}_{q}^{\Delta=1}[n] = {}_{q}[n]^{\Delta=1} = \mathrm{i}\left(q^{n} - q^{-n}\right) = {}_{q}[n] = -2\sin\left(2\pi\beta n\right), \tag{12}$$

if $\Delta = 1$. Proceeding by recursion and choosing $n > 0$ yields

$$C_1 = \frac{\varepsilon C_0 - \left({}_{q}^{\Delta}[0]\right)C_{-1}}{{}_{q}[1]^{\Delta}} = \frac{\varepsilon}{{}_{q}[1]^{\Delta}}, \tag{13}$$

$$C_2 = \frac{\varepsilon C_1 - \left({}_{q}^{\Delta}[1]\right)C_0}{{}_{q}[2]^{\Delta}} = \frac{\varepsilon^2 - \left({}_{q,\Delta}[1]\right)^2}{\left({}_{q}[1]^{\Delta}\right)\left({}_{q}[2]^{\Delta}\right)}, \tag{14}$$

$$C_3 = \frac{\varepsilon C_2 - \left({}_{q}^{\Delta}[2]\right)C_1}{{}_{q}[3]^{\Delta}} = \frac{\varepsilon^3 - \varepsilon\left(\left({}_{q,\Delta}[1]\right)^2 + \left({}_{q,\Delta}[2]\right)^2\right)}{\left({}_{q}[1]^{\Delta}\right)\left({}_{q}[2]^{\Delta}\right)\left({}_{q}[3]^{\Delta}\right)}, \tag{15}$$

$$C_5 = \frac{\varepsilon C_4 - \left({}_{q}^{\Delta}[4] \right) C_3}{{}_{q}[5]^{\Delta}} =$$

$$= \frac{\varepsilon^5 - \varepsilon^3 \left(\left({}_{q,\Delta}[1] \right)^2 + \left({}_{q,\Delta}[2] \right)^2 + \left({}_{q,\Delta}[3] \right)^2 + \left({}_{q,\Delta}[4] \right)^2 \right)}{\left({}_{q}[1]^{\Delta} \right)\left({}_{q}[2]^{\Delta} \right)\left({}_{q}[3]^{\Delta} \right)\left({}_{q}[4]^{\Delta} \right)\left({}_{q}[5]^{\Delta} \right)} + \tag{16}$$

$$+ \frac{\varepsilon \left(\left({}_{q,}[1] \right)^2 \left({}_{q,\Delta}[3] \right)^2 + \left({}_{q,\Delta}[1] \right)^2 \left({}_{q,\Delta}[4] \right)^2 + \left({}_{q,\Delta}[2] \right)^2 \left({}_{q,\Delta}[4] \right)^2 \right)}{\left({}_{q}[1]^{\Delta} \right)\left({}_{q}[2]^{\Delta} \right)\left({}_{q}[3]^{\Delta} \right)\left({}_{q}[4]^{\Delta} \right)\left({}_{q}[5]^{\Delta} \right)},$$

and

$$C_6 = \frac{\varepsilon^6 - \varepsilon^4 \left(\left({}_{q,\Delta}[1] \right)^2 + \left({}_{q,\Delta}[2] \right)^2 + \left({}_{q,\Delta}[3] \right)^2 + \left({}_{q,\Delta}[4] \right)^2 + \left({}_{q,\Delta}[5] \right)^2 \right)}{\left({}_{q}[1]^{\Delta} \right)\left({}_{q}[2]^{\Delta} \right)\left({}_{q}[3]^{\Delta} \right)\left({}_{q}[4]^{\Delta} \right)\left({}_{q}[5]^{\Delta} \right)\left({}_{q}[6]^{\Delta} \right)} +$$

$$+ \frac{\varepsilon^2 \left(\left({}_{q,\Delta}[1] \right)^2 \left({}_{q,\Delta}[3] \right)^2 + \left({}_{q,\Delta}[1] \right)^2 \left({}_{q,\Delta}[4] \right)^2 + \left({}_{q,\Delta}[1] \right)^2 \left({}_{q,\Delta}[5] \right)^2 \right)}{\left({}_{q}[1]^{\Delta} \right)\left({}_{q}[2]^{\Delta} \right)\left({}_{q}[3]^{\Delta} \right)\left({}_{q}[4]^{\Delta} \right)\left({}_{q}[5]^{\Delta} \right)\left({}_{q}[6]^{\Delta} \right)} + \tag{17}$$

$$+ \frac{\varepsilon^2 \left(\left({}_{q,\Delta}[2] \right)^2 \left({}_{q,\Delta}[4] \right)^2 + \left({}_{q,\Delta}[2] \right)^2 \left({}_{q,\Delta}[5] \right)^2 + \left({}_{q,\Delta}[3] \right)^2 \left({}_{q,\Delta}[5] \right)^2 \right)}{\left({}_{q}[1]^{\Delta} \right)\left({}_{q}[2]^{\Delta} \right)\left({}_{q}[3]^{\Delta} \right)\left({}_{q}[4]^{\Delta} \right)\left({}_{q}[5]^{\Delta} \right)\left({}_{q}[6]^{\Delta} \right)} -$$

$$- \frac{\left({}_{q,\Delta}[1] \right)^2 \left({}_{q,\Delta}[3] \right)^2 \left({}_{q,\Delta}[5] \right)^2}{\left({}_{q}[1]^{\Delta} \right)\left({}_{q}[2]^{\Delta} \right)\left({}_{q}[3]^{\Delta} \right)\left({}_{q}[4]^{\Delta} \right)\left({}_{q}[5]^{\Delta} \right)\left({}_{q}[6]^{\Delta} \right)}.$$

The concrete results established in this manner exhibit typical structures which can be readily generalized towards even and odd n-values as follows:

$$C_{n \text{ even}} = \Bigg[\varepsilon^n - \varepsilon^{n-2} \sum_{i=1}^{n-1} \left({}_{q,\Delta}[i] \right)^2 + \varepsilon^{n-4} \sum_{i=1}^{n-3} \sum_{j=i+2}^{n-1} \left({}_{q,\Delta}[i] \right)^2 \left({}_{q,\Delta}[j] \right)^2 -$$

$$- \varepsilon^{n-6} \sum_{i=1}^{n-5} \sum_{j=i+2}^{n-3} \sum_{k=j+2}^{n-1} \left({}_{q,\Delta}[i] \right)^2 \left({}_{q,\Delta}[j] \right)^2 \left({}_{q,\Delta}[k] \right)^2 + \tag{18}$$

$$+ \ldots - \prod_{i=1}^{n-1} \left({}_{q,\Delta}[i] \right)^2 \Bigg] \frac{1}{\prod_{i=1}^{n} \left({}_{q}[i]^{\Delta} \right)}$$

and

$$C_{n\ \mathrm{odd}} = \Bigg[\varepsilon^n - \varepsilon^{n-2} \sum_{i=1}^{n-1} \left({}_{q,\Delta}[i] \right)^2 + \varepsilon^{n-4} \sum_{i=1}^{n-3} \sum_{j=i+2}^{n-1} \left({}_{q,\Delta}[i] \right)^2 \left({}_{q,\Delta}[j] \right)^2 - $$
$$ - \varepsilon^{n-6} \sum_{i=1}^{n-5} \sum_{j=i+2}^{n-3} \sum_{k=j+2}^{n-1} \left({}_{q,\Delta}[i] \right)^2 \left({}_{q,\Delta}[j] \right)^2 \left({}_{q,\Delta}[k] \right)^2 + $$
$$ + \ldots + \varepsilon \sum_{i=1}^{2} \sum_{j=3}^{4} \sum_{k=5}^{6} \cdots \sum_{l=n-2}^{n-1} \left({}_{q,\Delta}[i] \right)^2 \left({}_{q,\Delta}[j] \right)^2 \left({}_{q,\Delta}[k] \right) \ldots \tag{19}$$
$$ \ldots \left({}_{q,\Delta}[l] \right)^2 \Bigg] \frac{1}{\prod_{i=1}^{n} \left({}_q[i]^\Delta \right)},$$

respectively.

The complementary $n < 0$-domain can be handled in terms of the identities

$$ {}^{\Delta}_{q}[n] = -{}_q\left[|n|\right]^\Delta , \tag{20}$$

and

$$ {}_q[n]^\Delta = -{}^{\Delta}_{q}\left[|n|\right]. \tag{21}$$

where $|n| = -n$. One would then obtain the concrete realizations

$$C_{-2} = \frac{\varepsilon C_{-1} - {}_q[0]^\Delta C_0}{{}^{\Delta}_{q}[-1]} = \frac{(1-\Delta)}{{}_q[1]^\Delta}, \tag{22}$$

$$C_{-3} = \frac{\varepsilon C_{-2} - \left({}_q[-1]^\Delta \right) C_{-1}}{{}^{\Delta}_{q}[-2]} = -(1-\Delta) \frac{\varepsilon}{\left({}_q[1]^\Delta \right)\left({}_q[2]^\Delta \right)}, \tag{23}$$

$$C_{-4} = \frac{\varepsilon C_{-3} - \left({}_q[-2]^\Delta \right) C_{-2}}{{}^{\Delta}_{q}[-3]} = (1-\Delta) \frac{\varepsilon^2 - \left({}_{q,\Delta}[2] \right)^2}{\left({}_q[1]^\Delta \right)\left({}_q[2]^\Delta \right)\left({}_q[3]^\Delta \right)}, \tag{24}$$

$$C_{-5} = \frac{\varepsilon C_{-4} - \left({}_q[-3]^\Delta \right) C_{-3}}{{}^{\Delta}_{q}[-4]} = -(1-\Delta) \frac{\varepsilon^3 - \varepsilon\left(\left({}_{q,\Delta}[2] \right)^2 + \left({}_{q,\Delta}[3] \right)^2 \right)}{\left({}_q[1]^\Delta \right)\left({}_q[2]^\Delta \right)\left({}_q[3]^\Delta \right)\left({}_q[4]^\Delta \right)}, \tag{25}$$

$$C_{-6}=\frac{\varepsilon C_{-5}-\left({}_{q}[-4]^{\Delta}\right)C_{-4}}{{}_{q}^{\Delta}[-5]}=$$
$$=(1-\Delta)\frac{\varepsilon^{4}-\varepsilon^{2}\left(\left({}_{q,\Delta}[2]\right)^{2}+\left({}_{q,\Delta}[3]\right)^{2}+\left({}_{q,\Delta}[4]\right)^{2}\right)+\left({}_{q,\Delta}[2]\right)^{2}\left({}_{q,\Delta}[4]\right)^{2}}{\left({}_{q}[1]^{\Delta}\right)\left({}_{q}[2]^{\Delta}\right)\left({}_{q}[3]^{\Delta}\right)\left({}_{q}[4]^{\Delta}\right)\left({}_{q}[5]^{\Delta}\right)} \tag{26}$$

and

$$C_{-7}=\frac{\varepsilon C_{-6}-\left({}_{q}[-5]^{\Delta}\right)C_{-5}}{{}_{q}^{\Delta}[-6]}=$$
$$=-(1-\Delta)\left[\frac{\varepsilon^{5}-\varepsilon^{3}\left(\left({}_{q,\Delta}[2]\right)^{2}+\left({}_{q,\Delta}[3]\right)^{2}+\left({}_{q,\Delta}[4]\right)^{2}+\left({}_{q,\Delta}[5]\right)^{2}\right)}{\left({}_{q}[1]^{\Delta}\right)\left({}_{q}[2]^{\Delta}\right)\left({}_{q}[3]^{\Delta}\right)\left({}_{q}[4]^{\Delta}\right)\left({}_{q}[5]^{\Delta}\right)\left({}_{q}[6]^{\Delta}\right)}+\right. \tag{27}$$
$$\left.+\frac{\varepsilon\left(\left({}_{q,\Delta}[2]\right)^{2}\left({}_{q,\Delta}[4]\right)^{2}+\left({}_{q,\Delta}[2]\right)^{2}\left({}_{q,\Delta}[5]\right)^{2}+\left({}_{q,\Delta}[3]\right)^{2}\left({}_{q,\Delta}[5]\right)^{2}\right)}{\left({}_{q}[1]^{\Delta}\right)\left({}_{q}[2]^{\Delta}\right)\left({}_{q}[3]^{\Delta}\right)\left({}_{q}[4]^{\Delta}\right)\left({}_{q}[5]^{\Delta}\right)\left({}_{q}[6]^{\Delta}\right)}\right].$$

Generalizing typical patterns exhibited by Eqs.(22)–(27) one gets faced with generalized formulae like

$$\begin{aligned}C_{-n\ \text{even}}=(-1)^{n}(1-\Delta)\Bigg[&\varepsilon^{n-2}-\varepsilon^{n-4}\sum_{i=2}^{n-2}\left({}_{q,\Delta}[i]\right)^{2}+\\&+\varepsilon^{n-6}\sum_{i=2}^{n-4}\sum_{j=i+2}^{n-2}\left({}_{q,\Delta}[i]\right)^{2}\left({}_{q,\Delta}[j]\right)^{2}-\\&-\varepsilon^{n-8}\sum_{i=2}^{n-6}\sum_{j=i+2}^{n-4}\sum_{k=j+2}^{n-2}\left({}_{q,\Delta}[i]\right)^{2}\left({}_{q,\Delta}[j]\right)^{2}\left({}_{q,\Delta}[k]\right)^{2}+\\&+\ldots-\prod_{i=2}^{n-2}\left({}_{q,\Delta}[i]\right)^{2}\Bigg]\frac{1}{\prod_{i=1}^{n-1}\left({}_{q}[i]^{\Delta}\right)}\end{aligned} \tag{28}$$

and

$$C_{-n\ \text{odd}}=(-1)^{n}(1-\Delta)\Bigg[\varepsilon^{n-2}-\varepsilon^{n-4}\sum_{i=2}^{n-2}\left({}_{q,\Delta}[i]\right)^{2}+$$

$$+\varepsilon^{n-4}\sum_{i=2}^{n-4}\sum_{j=i+2}^{n-2}\left({}_{q,\Delta}[i]_{q,\Delta}[j]\right)^2-$$
$$-\varepsilon^{n-6}\sum_{i=2}^{n-6}\sum_{j=i+2}^{n-4}\sum_{k=j+2}^{n-2}\left({}_{q,\Delta}[i]\right)^2\left({}_{q,\Delta}[j]\right)^2\left({}_{q,\Delta}[k]\right)^2+\ldots+\varepsilon\sum_{i=2}^{3}\sum_{j=4}^{5}\sum_{k=6}^{7}\cdots \tag{29}$$
$$\left.\cdots\sum_{j=n-4}^{n-2}\left({}_{q,\Delta}[i]\right)^2\left({}_{q,\Delta}[j]\right)^2\left({}_{q,\Delta}[k]\right)^2\cdots\left({}_{q,\Delta}[l]\right)^2\right]\frac{1}{\prod_{i=1}^{n-1}\left({}_q[i]^{\Delta}\right)}$$

in which $n > 0$.

Next let us rescale the coefficients derived above as

$$C_n=\begin{cases}\dfrac{\tilde{C}_n}{\prod_{i=1}^{n}\left({}_q[i]^{\Delta}\right)}, & n>0\\[2ex] \dfrac{(1-\Delta)\tilde{C}_{|n|}}{\prod_{i=1}^{|n|-1}\left({}_q[i]^{\Delta}\right)}, & n<0\end{cases} \tag{30}$$

We have to realize that at this stage of our calculations an additional eigenvalue condition like [11]

$$\tilde{C}_{-Q}=\frac{\mathrm{e}^{i\pi(Q-1)}}{q^{\mathrm{Q}}}\tilde{C}_Q, \tag{31}$$

is needed. This opens the way to derive the energy polynomial by virtue of the equation

$$P^{(Q)}(E,\Delta)=\tilde{C}_Q-(1-\Delta)^2\,\tilde{C}_{-Q}. \tag{32}$$

which represents the main result of this paper. Now, the following comments are in order. First, inserting $\Delta = 1$ reproduces precisely general energy polynomials written down before [5]. Second the coefficients of ε^{Q} and ε^{Q-2} are given by 1 and $-Q(1-\Delta)$, respectively, whereas the free term, say C_f, is given by

$$C_f=\begin{cases}0, & Q=\text{odd}\\ 2\left(1+\Delta^{Q}\right), & Q=\text{even}\end{cases}. \tag{33}$$

4. THE INFLUENCE OF THE ANISOTROPY PARAMETER ON THE ENERGY

Having obtained the general form of the energy polynomial we are ready to establish the influence of the anisotropy parameter on the energy bands in terms of Eq. (32). It is clear that one deals with Q energy bands which are ordered $E_1 < E_2 < \ldots < E_{Q-1} < E_Q$, now for arbitrary Δ-values. The central two bands are touching again for even Q-values, so that $E = 0$ is doubly degenerate. The energy-reflection symmetry $E_j = -E_{Q-j+1}$ [16, 17] is also preserved.

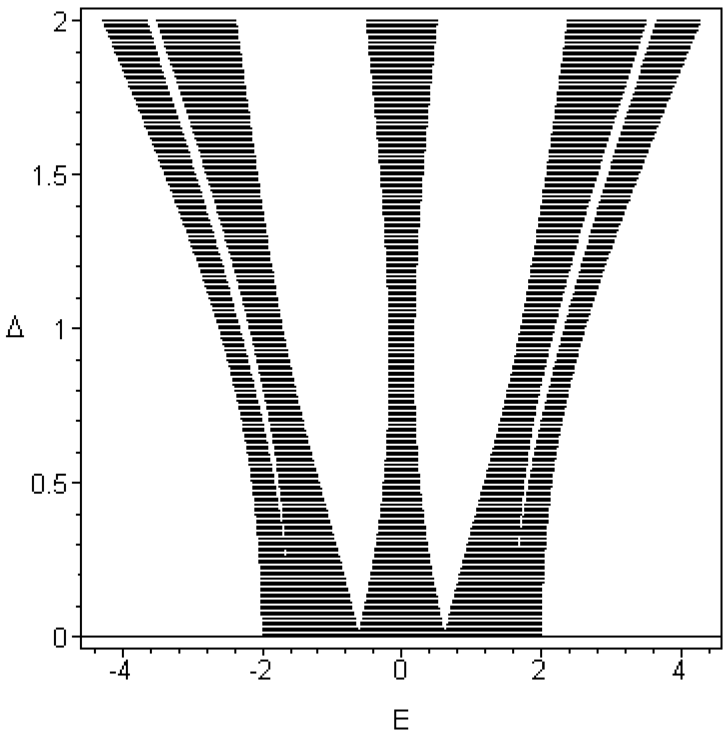

Fig. 1 – The anisotropy Δ dependence of the energy bands for $P = 2$, $Q = 5$.

The Δ dependence of the energy bands is rather interesting, as displayed in Fig. 1 ($P = 2$, $Q = 5$) and 2 ($P = 1$, $Q = 6$). One sees that if $\Delta = 0$ all the Q energy bands are touching, so that the band edges are doubly degenerate. For $0 < \Delta \leq 1$ the formation of the gaps can be observed, and the degeneracy is lifted. As $\Delta \to 1$ the gaps broaden and the energy bands become thinner. The largest total bandwidth, *i.e.* $W = 4$, is obtained for $\Delta = 0$.

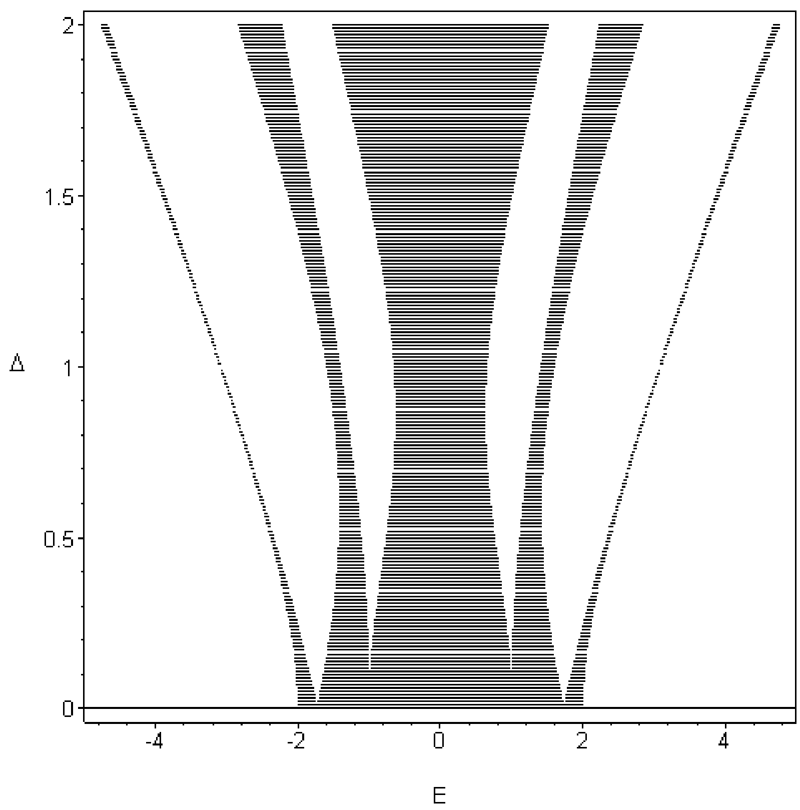

Fig. 2 – The anisotropy Δ dependence of the energy bands for $P = 2$, $Q = 5$.

In contradistinction, the smallest bandwidth case is obtained for $\Delta = 1$. The $\Delta > 1$ case is complementary, in accord with the Aubry-André symmetry $E(\Delta) = \Delta E(1/\Delta)$ [4]. Now the gaps become smaller as Δ increases, and the energy bands broaden. In the limiting case of $\Delta \to +\infty$ the energy bands cover the full real axis, and the gaps have the tendency to disappear. Note that the influence of the next nearest hopping have also been considered, but for $\Delta = 1$ only (see Fig. 8 in [9]).

5. CONCLUSIONS

In this article an easy tractable $\Delta \neq 1$ generalization of the energy polynomial characterizing the anisotropic Harper has been derived. This opens the way to establish thermodynamic properties by resorting to the DOS [6]. In addition updated calculations concerning the bandwidth, the Lyapunov exponent [7], the related Green-function [8] as well as the Hall conductance [18] can also be done without resorting to the explicit knowledge of the energy eigenvalues. Moreover, the Δ dependence of the energy bands, which is useful for a better understanding of band and gap structures, has also been displayed.

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