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Butterflies and likewise: properties of tridiagonal periodic Hamiltonians

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Abstract. We present a general model for modulated lattices particularly suitable for the investigation of the moments of the density of states and establish an interpretation of the dependence on the modulation parameter which avoids the occurrence of unphysical incommensurability effects. The final result is an exact interpretation of the influence of an inevitably finite resolution on the system characteristics. We conclude by presenting some specialized results for Harper's equation in the context of this model.

1. Motivation

Typical of the problems in question is the tridiagonal Hamiltonian, which describes a chain of harmonic oscillators. This system is represented by a recurrence law that connects the elongations f_n of three successive oscillators in the chain.

A general form of this recurrence law is

$$(\omega - a_n)f_n = b_{n-1}f_{n-1} + b_n f_{n+1} \tag{1}$$

where ω is the eigenfrequency, the b_n are nearest-neighbour couplings (spring constants), while the a_n represent a self-coupling or the influence of a background field.

The coefficents b_r, a_r are real numbers determined as functions of the site-label n by

$$a_n = a(\mathrm{e}^{\mathrm{i}2\pi n\Phi}) \tag{2}$$

$$b_n = b(\mathrm{e}^{\mathrm{i}2\pi n\Phi}) \tag{3}$$

where Φ is a fixed real number. This yields a Hermitian Hamiltonian.

One specialization of this Hamiltonian yields Harper's equation [1] with

$$b_n = \mathrm{e}^{\mathrm{i}k_x} \tag{4}$$

$$\begin{aligned} a_n &= \mathrm{e}^{\mathrm{i}k_y + \mathrm{i}2\pi n\Phi} + \mathrm{e}^{-\mathrm{i}k_y - \mathrm{i}2\pi n\Phi} \\ &= 2\cos(k_y + 2\pi n\Phi). \end{aligned} \tag{5}$$

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Harper's equation emerges from a tight-binding model which describes a two-dimensional electron gas in a periodic potential subject to a perpendicular magnetic field. The quantity Φ is determined by the ratio of the magnetic length and the period length of the periodic potential [2] and the k_x, k_y are the components of the two-dimensional lattice wavevector. We further assume the Landau gauge $\boldsymbol{A} = B(0, x, 0)$. This model recently gained new attention, as it coincides with a mean-field approach to the so-called anyon problem on a square lattice [3]. A discussion of special results for this problem can be found in [4].

Other specializations of this recurrence law are realized in simple models for longitudinally modulated spin magnets [5, 6] with

$$a_n = 0 \tag{6}$$

$$b_n = b(\mathrm{e}^{\mathrm{i}2\pi n\Phi + \Delta}) \tag{7}$$

where Φ is again determined by the ratio of the two relevant length scales, namely the lattice spacing along the direction of the spin modulation and the modulation wavelength. Δ is a phase shift, representing the influence of a probe on the system, e.g. the momentum transfer of a neutron beam to the system.

In general, the existence of two characteristic length scales in a system defines a modulated lattice. One length defines the lattice spacing and the other a modulation wavelength.

2. Introduction

In order to explain the problem we want to address, let us have a closer look at Harper's equation.

Hofstadter has carried out extensive studies of this model on a square lattice, investigating the change in the spectrum of the energy states caused by changes in the parameter Φ [2]. The Φ-dependent spectrum which he obtained shows an appealing resemblance to a butterfly and is generally known as the Hofstadter butterfly. An explanation of his findings has been given much attention, but it is still incomplete.

The most intriguing aspect of this model lies in the way Φ influences the appearance of the spectrum. The spectrum is bounded and consists of an integer number N of discrete bands.

To understand the way Φ enters the problem consider the parameter $\mathrm{e}^{\mathrm{i}2\pi\Phi}$ introduced in (2) and (3). The values of $(\mathrm{e}^{\mathrm{i}2\pi\Phi})^n$ lie on the unit circle, and are dense on its circumference except when Φ is rational, $\Phi = M/N$ say. In that case the unit circle is split into N arcs, and we pass M times round the unit circle while we mark the N distinct endpoints of translations by $2\pi\Phi$.

In the formalism presented later N will be found to determine the genuine dimensionality of the problem, represented by a polynomial θ of degree N.

As found by Hofstadter and others, N determines the number of bands in the energy spectrum and this result is confirmed by symmetry considerations. (The translatory unit cell of the square lattice is extended to a unit cell of the modulated lattice by 'multiplication' by N.)

This result nevertheless has odd consequences. Taking $\Phi = \frac{1}{3}$ results in three arcs. If we now change Φ to $\Phi' = \frac{1}{3} \pm 1/3^r$ the first three translations closely resemble the previous case. Taking the entity of endpoints however does not suggest any close

relationship. All cases with Φ with denominator 3^{-r} appear the same. Furthermore as $r \to \infty$ as Φ' approaches Φ, we even seem to lose similarity. Allowing $|\Phi - \Phi'|$ to take on irrational values even worsens the result.

So let us choose another approach. When we fix some 'resolution', i.e. some interval around the endpoints of a translation, we find that there is a perfect agreement between a certain number of translations $\mathcal{N}$ in both cases, which corresponds to the resolution applied. Nevertheless, the errors per translation accumulate and exceed the fixed resolution interval sufficiently far from the set origin. This observation is independent of the rational or irrational nature of the deviation between Φ and Φ'. Furthermore, we find that a process taking Φ' to Φ results in $\mathcal{N} \to \infty$ for all finite resolutions. Hence this 'constructive' approach yields some suggestive way to picture the kind of continuous behaviour to be expected from modulated systems and highlights the importance of a finite resolution in the discussion. As this can be negligibly small, its presence supports the physical nature of the problem rather than presenting a problem by itself.

We find that, whenever we are only interested in an essentially finite system, we should be able to find suitable rational approximations to Φ, depending on a given required resolution for the result. If N is now the number of lattice sites the possible approximations are primarily provided in a $1/N$ grid, but can then be extended to non-integer values for the numerator. This accesses all possible Φ values of the finite sized system, while the dimensionality of the problem remains constant.

This has two consequences:

(1) every N-finite system can be described as a rational system with $\Phi = M/N$ with $M \in \mathbb{N}$ or $M \in \mathbb{R}$ as only the denominator really has to be an integer as it determines an integer quantity (the degree of θ); and

(2) as it is impractical to calculate a macroscopic system based on (1), we find that, as soon as the resolution is restricted by fluctuations or measurement commodities to a finite value, we obtain corresponding cells of size $\mathcal{N}$ in the crystal, in which an approximate calculation with a system of dimension $\mathcal{N}$ is good. If this cell size corresponds to a characteristic dimension of the system, e.g. the correlation radius, this calculation is a faithful description of the system.

3. Definition of the model

Let V denote the linear space of all doubly infinite real sequences $\boldsymbol{f} = (f_n)_{n\in\mathbb{Z}}$, and let Z be the operator given by

$$Z\boldsymbol{f} = (b_{n-1}f_{n-1} + a_n f_n + b_n f_{n+1})_{n\in\mathbb{Z}} \tag{8}$$

with a_n, b_n as previously defined, the b_n being non-zero. Our concern is with the stable solutions of the eigenvalue problem

$$Z\boldsymbol{f} = \omega\boldsymbol{f}.$$

3.1. The rational case

For fixed ω consider the corresponding eigenspace $U = \{\boldsymbol{f} : Z\boldsymbol{f} = \omega\boldsymbol{f}\}$. As $b_n \neq 0$ it is clear that f_0 and f_1 determine all f_n for $n \geq 0$; as $b_{n-1} \neq 0$ it is clear that all f_n

for $n \leq 1$ are also determined. We obtain therefore a two-dimensional eigenspace U, spanned by α, β determined by the initial conditions

$$\begin{aligned} \alpha &: \alpha_0 = 1 \\ &\quad \alpha_1 = 0 \\ \beta &: \beta_0 = 0 \\ &\quad \beta_1 = 1 \end{aligned} \tag{9}$$

and the related recurrence obtained from (1) [4, 6]:

$$f_n = (\omega - a_{n-1}) f_{n-1} - b_{n-1}^2 f_{n-2}. \tag{10}$$

When Φ is rational, the definition of a_n, b_n leads to

$$\begin{aligned} b_{n+N} &= b_n \qquad \forall n \\ a_{n+N} &= a_n \qquad \forall n \end{aligned} \tag{11}$$

for some integer number N. Suppose this is indeed the case.

If we let E denote the usual shift operator on V

$$E\boldsymbol{f} = (f_{n+1})$$

then the hypothesis of rationality yields

$$[E^N, Z] = 0$$

so that $E^N(U) \subseteq U$. As E^N and Z are simultaneously diagonalizable, let ζ denote the eigenvalues of E^N:

$$E^N \boldsymbol{f} = \zeta \boldsymbol{f}.$$

Now we can specify the condition of a stable solution by requiring $|\zeta| = 1$. This eigenvalue equation resembles Floquet's theorem and if we set $\zeta = \mathrm{e}^{\mathrm{i}Nq}$ we obtain Bloch's theorem

$$f_{n+N} = \mathrm{e}^{\mathrm{i}Nq} f_n$$

with q as the wavevector (k_x in Harper's equation).

This condition restricts the values of ω. Let $\boldsymbol{f}$ be an eigenvector of E^N in U, and consider the action induced by Z on the space spanned by

$$\bar{\boldsymbol{f}} := \boldsymbol{f} \text{ modulo } (E^N - \zeta)\boldsymbol{f}$$

which is just a scalar multiplication by ω. We have, therefore,

$$(Z_\zeta - \omega I)\bar{\boldsymbol{f}} = 0 \tag{12}$$

where

$$Z_\zeta = \begin{pmatrix} a_0 & b_0 & 0 & \cdot & \cdot & \cdot & \zeta^{-1}b_{N-1} \\ b_0 & a_1 & b_1 & & & & \cdot \\ 0 & b_1 & \cdot & \cdot & & & \cdot \\ \cdot & & \cdot & \cdot & \cdot & & \cdot \\ \cdot & & & \cdot & \cdot & \cdot & 0 \\ \cdot & & & & \cdot & a_{N-2} & b_{N-2} \\ \zeta b_{N-1} & \cdot & \cdot & \cdot & 0 & b_{N-2} & a_{N-1} \end{pmatrix}. \tag{13}$$

Hence ω is a root of

$$\theta_\zeta(\omega) := \det(\omega I - Z_\zeta).$$

A Laplace expansion of this determinant (based on the 2×2 minor of the corner elements) yields [6]

$$\theta_\zeta(\omega) = \theta(\omega) + (\zeta + \zeta^{-1}) \prod_{n=0}^{N-1} b_n \tag{14}$$

where $\theta(\omega)$ is a polynomial in ω free of ζ. For convenience we write

$$\Omega = \prod_{n=0}^{N-1} b_n \tag{15}$$

and note that we can scale to $\Omega = 1$. Note that as $\mathrm{i} + \mathrm{i}^{-1} = 0$ we have $\theta(\omega) = \theta_1(\omega)$.

For every choice of ζ on the unit circle the polynomial $\theta_\zeta(\omega)$ represents the characteristic polynomial of a Hermitian matrix. There will therefore be N real roots of $\theta_\zeta(\omega)$, representing the N branches of the dispersion relation which are expected for a crystal with N atoms per unit cell.

3.2. The density of states

The equation $\theta_\zeta(\omega) = 0$ also allows calculation of the density of states $D(\omega)$. We suppose ζ to be uniformly distributed on the unit circle.

From (14) we have

$$\theta(\omega) + \Omega(\zeta + \zeta^{-1}) = 0 \tag{16}$$

so that

$$\zeta\theta'(\omega)\,\mathrm{d}\omega + \Omega(\zeta - \zeta^{-1})\,\mathrm{d}\zeta = 0 \tag{17}$$

Now

$$(\zeta - \zeta^{-1})^2 = (\zeta + \zeta^{-1})^2 - 4 \tag{18}$$

$$= \frac{\theta^2(\omega)}{\Omega^2} - 4. \tag{19}$$

Together these yield

$$\mathrm{d}\zeta = \frac{-\zeta\theta'(\omega)}{\sqrt{\theta^2(\omega) - 4\Omega^2}}\,\mathrm{d}\omega. \tag{20}$$

As ζ is uniformly distributed on the unit circle, $\zeta = \mathrm{e}^{\mathrm{i}t}$ with t uniform in $[0, 2\pi)$. In terms of this parameter t

$$\mathrm{d}t = \frac{\theta'(\omega)}{\sqrt{4\Omega^2 - \theta^2(\omega)}}\,\mathrm{d}\omega. \tag{21}$$

With $t = Nq$ from Bloch's theorem and after normalization the density of states is given by [6, 7]

$$D(\omega) = \begin{cases} \dfrac{1}{\pi N}\dfrac{|\theta'(\omega)|}{\sqrt{4\Omega^2 - \theta^2(\omega)}} & \text{when } 4\Omega^2 - \theta^2 > 0 \\ 0 & \text{otherwise.} \end{cases} \tag{22}$$

3.3. ... in terms of α and β

We now obtain an expression for $D(\omega)$ in terms of the sequences α, β which form a basis for the eigenspace U of the operator Z. To do this it will suffice to give $\theta'(\omega)$ and $(\zeta - \zeta^{-1})$ in terms of these. For convenience, set $\Omega = 1$.

The second of these is straightforward. Consider the action of $S := E^N$ on the basis vectors $\boldsymbol{\alpha}, \boldsymbol{\beta}$ of U. Let ζ_1, ζ_2 be the eigenvalues of S. As the solutions are supposed to be stable,

$$\det(S) = 1 \qquad \text{and} \qquad \zeta_2 = \zeta_1^{-1}. \tag{23}$$

Now

$$\begin{aligned} S(\boldsymbol{\alpha}) &= (\alpha_{n+N}) \\ &= \alpha_N \boldsymbol{\alpha} + \alpha_{N+1}\boldsymbol{\beta} \end{aligned}$$

and

$$S(\boldsymbol{\beta}) = \beta_N \boldsymbol{\alpha} + \beta_{N+1}\boldsymbol{\beta}.$$

Hence

$$S = \begin{pmatrix} \alpha_N & \beta_N \\ \alpha_{N+1} & \beta_{N+1} \end{pmatrix}.$$

From the characteristic equation we easily calculate

$$(\zeta_1 - \zeta_2)^2 = (\zeta_1 + \zeta_2)^2 - 4\zeta_1\zeta_2 \tag{24}$$

$$= (\operatorname{tr} S)^2 - 4\det S \tag{25}$$

$$= (\alpha_N + \beta_{N+1})^2 - 4. \tag{26}$$

The value of $\theta'(\omega)$ is slightly more complicated. The derivative of $\theta(\omega)$ can be obtained as a sum of determinants obtained from $\theta(\omega)$ by replacing one row by the corresponding row of derivatives. Each of these determinants is a pure tridiagonal determinant, a typical one being

$$\begin{vmatrix} \omega - a_1 & -b_1 & 0 & \cdot & \cdot & \cdot & 0 \\ -b_0 & \omega - a_1 & -b_1 & & & & \cdot \\ 0 & -b_1 & \cdot & \cdot & & & \cdot \\ \cdot & & \cdot & \cdot & \cdot & & \cdot \\ \cdot & & & \cdot & \cdot & \cdot & 0 \\ \cdot & & & & \cdot & \omega - a_{N-2} & -b_{N-2} \\ 0 & \cdot & \cdot & \cdot & 0 & -b_{N-2} & \omega - a_{N-1} \end{vmatrix}. \tag{27}$$

This determinant is readily seen to be β_N. The value of $\theta'(\omega)$ is then obtained as

$$\sum_{\sigma} \beta_N^{\sigma}$$

where summation is over all cyclic permutations of $\{0, \ldots, N-1\}$, and β^{σ} denotes the sequence β corresponding to this permutation of the parameters $\{a_0, \ldots, a_{N-1}\}$ and $\{b_0, \ldots, b_{N-1}\}$. We therefore can express $D(\omega)$ as

$$\sum_{\sigma} \frac{\beta_N^{\sigma}}{\sqrt{(\alpha_N + \beta_{N+1})^2 - 4}}.$$

The denominator, it is interesting to note, is symmetric with respect to σ. This is because the action of $S = E^N$ can also be expressed by

$$S = \begin{pmatrix} 0 & 1 \\ b_0 & a_0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ b_1 & a_1 \end{pmatrix} \cdots \begin{pmatrix} 0 & 1 \\ b_{N-1} & a_{N-1} \end{pmatrix} \tag{28}$$

so that permutation by σ merely yields a conjugate matrix. According to (18) and (25) the denominator is expressed by invariants to conjugation.

3.4. The polynomial $\theta(\omega)$

Let us have a closer look at the denominator of $D(\omega)$. We have

$$\theta^2(\omega) - 4 = \theta_{+1}(\omega)\theta_{-1}(\omega) \tag{29}$$

where each of $\theta(\omega), \theta_{+1}(\omega), \theta_{-1}(\omega)$ is the characteristic polynomial of a Hermitian matrix of degree N. Each is therefore a real polynomial of degree N with only real roots. By (14) $\theta_{+1}(\omega)$ and $\theta_{-1}(\omega)$ are just translates of $\theta(\omega)$ by a vertical offset of 2 and -2.

The extremal value of $\theta(\omega)$ between a pair of consecutive zeros therefore has a value of at least 2 (or at most -2). The whole range can therefore be split up [8]

$$-\infty < \omega_1' < \omega_1 \leq \omega_2' < \omega_2 \leq \cdots \leq \omega_N' < \omega_N$$

so that $\theta^2(\omega) - 4 \leq 0$ on the intervals $[\omega_i', \omega_i]$ and nowhere else.

On each of these intervals $[\omega_i', \omega_i]$ the density of states can be integrated in the form $\cos^{-1}(\theta(\omega)/2\Omega)$.

4. The degree of $\theta(\omega)$

The model as set in section 3 seems to be heavily dependent on the integer number N. Slight changes in Φ: for instance from $\frac{1}{3}$ to $\frac{11}{34}$ [9] lead to enormous changes in the value of N and in the form of the polynomial $\theta(\omega)$. However we will establish in this section that, although N and $\theta(\omega)$ may change violently, the physically significant quantities—the density of states, and its moments—vary in a reasonable way.

Our discussion of the variation caused by changes in Φ falls into three parts. First we show that our choice of a periodicity is effectively irrelevant with respect to the determination of the dimension of Z_ζ leaving it free to be determined by the choice of a resolution. Next we note the moments of the density of states must depend smoothly on Φ. Lastly we see how the various rational approximations can be used to describe the density of states in a general case.

4.1. Redundancy

Suppose that we mistakenly view an N-periodic system as a kN-periodic system. We shall then carry out the analysis of section 3, and find that the density of states is proportional to a sum of functions of the form

$$\frac{\beta_{kN}}{\sqrt{(\alpha_{kN}+\beta_{kN+1})^2-4}}.$$

Exactly as in (26) the denominator is given by

$$(\alpha_{kN}+\beta_{kN+1})^2-4=(\bar{\zeta}_1-\bar{\zeta}_2)^2 \tag{30}$$

where $\bar{\zeta}_1,\bar{\zeta}_2$ are the eigenvalues of E^{kN}. In terms of the eigenvalues of E^N, (that is of ζ_1,ζ_2) this yields

$$(\alpha_{kN}+\beta_{kN+1})^2-4=(\zeta_1^k-\zeta_2^k)^2. \tag{31}$$

To find β_{kN} we first diagonalize E^N on the space U:

$$H^{-1}E^NH=\begin{pmatrix}\zeta_1 & 0\\ 0 & \zeta_2\end{pmatrix} \tag{32}$$

where

$$H=\begin{pmatrix}\beta_N & \beta_N\\ \zeta_1-\alpha_N & \zeta_2-\alpha_N\end{pmatrix}$$

and

$$\det H=\beta_N(\zeta_2-\zeta_1).$$

Then

$$\begin{aligned}E^{kN}&=\begin{pmatrix}\alpha_{kN} & \beta_{kN}\\ \alpha_{kN+1} & \beta_{kN+1}\end{pmatrix}\\ &=\left[\frac{\begin{pmatrix}\beta_N & \beta_N\\ \zeta_1-\alpha_N & \zeta_2-\alpha_N\end{pmatrix}\begin{pmatrix}\zeta_1^k & 0\\ 0 & \zeta_2^k\end{pmatrix}\begin{pmatrix}\zeta_2-\alpha_N & -\beta_N\\ -(\zeta_1-\alpha_N) & \beta_N\end{pmatrix}}{\beta_N(\zeta_2-\zeta_1)}\right].\end{aligned} \tag{33}$$

The (1, 2)-entry of the right-hand side is easily calculated and yields

$$\beta_{kN} = \frac{\beta_N^2(\zeta_2^k - \zeta_1^k)}{\beta_N(\zeta_2 - \zeta_1)} = \beta_N \frac{(\zeta_2^k - \zeta_1^k)}{(\zeta_2 - \zeta_1)}. \tag{34}$$

From (31) and (34) we have

$$\frac{\beta_{kN}^2}{(\alpha_{kN} + \beta_{kN+1})^2 - 4} = \frac{\beta_N^2}{(\zeta_2 - \zeta_1)^2} = \frac{\beta_N^2}{(\alpha_N + \beta_{N+1})^2 - 4}. \tag{35}$$

The increased number of summands in the density of states cancels due to the normalization factor $1/2\pi kN$. As far as the density of states is concerned it makes no difference whether the periodicity is underestimated or not. In practice the cases $\Phi = \frac{1}{3}$, $\Phi = \frac{11}{34}$ can be viewed as the cases $\Phi = \frac{34}{102}$, $\Phi = \frac{33}{102}$ and discussed together.

4.2. The moments of the density of states

Following Lovesey [6] we shall now determine the moments of the density of states algebraically using the closure and orthogonality property of the eigenvectors f_α, where Greek letters label the frequency eigenvalue.

$$\sum_\gamma f_n(\gamma) f_m(\gamma) = \delta_{n,m} \tag{36}$$

$$\sum_n f_n(\gamma) f_n(\epsilon) = \delta_{\gamma,\epsilon}. \tag{37}$$

Labelling the cyclic permutations of the indices by their last elements m we can express the summands of $D(\omega)$ as [6]:

$$\frac{\beta_N^m}{\sqrt{(\alpha_N + \beta_{N+1})^2 - 4}} = \sum_\gamma |f_m(\gamma)|^2 \delta(\omega - \omega_\gamma). \tag{38}$$

Note that since the density of states is itself an even function of ω all odd moments vanish. Now we write down the first three even moments:

$$M_l = \int_{-\infty}^{\infty} d\omega\, \omega^l \sum_{m,\gamma} |f_m(\gamma)|^2 \delta(\omega - \omega_\gamma) \tag{39}$$

$$M_0 = \int_{-\infty}^{\infty} d\omega\, \omega^0 \sum_{m,\gamma} |f_m(\gamma)|^2 \delta(\omega - \omega_\gamma) \tag{40}$$

$$= \int_{\infty}^{-\infty} d\omega\, D(\omega) \tag{41}$$

$$= 1 \tag{42}$$

$$M_2 = \int_{-\infty}^{\infty} \mathrm{d}\omega\, \omega^2 \sum_{m,\gamma} |f_m(\gamma)|^2 \delta(\omega - \omega_\gamma) \tag{43}$$

$$= \int_{-\infty}^{\infty} \mathrm{d}\omega \sum_{m,\gamma} (b_{m-1} f_{m-1}(\gamma) + a_m f_m(\gamma) + b_m f_{m+1}(\gamma))^2 \delta(\omega - \omega_\gamma) \tag{44}$$

$$= \sum_m a_m^2 + b_m^2 + b_{m-1}^2 \tag{45}$$

$$= \sum_m a_m^2 + 2b_m^2 \tag{46}$$

$$M_4 = \sum_m 2b_{m-1}^2 b_{m-2}^2 + 2(b_{m-1}a_{m-1} + a_m b_{m-1})^2 + (a_m^2 + b_m^2 + b_{m-1}^2)^2$$

$$\vdots$$

It is due to the structure of the recurrence problem that the moments are composed of neighbour products of the coefficients. The depth of these products, i.e. the maximum difference of indices within one term is easily calculated to be $(l/2 - 1)$. The first K moments of a function are known to determine the Kth Padé approximant. This approximation scheme is via the continued fractions approach [6, 10] connected to the calculation of the determinant θ. Therefore we only need $\mathcal{N}$ moments for a desired resolution of $1/\mathcal{N}$ in Φ.

The structure of the moments of the density of states makes them smooth functions of Φ and the density of states is given via these moments as a Padé approximant.

4.3. Small rational variations

We now consider the effect of small rational variations in Φ which do not change the underlying periodicity. In each case the density of states is found by eliminating ζ from the equations

$$\theta(\omega) + \Omega(\zeta + \zeta^{-1}) = 0 \tag{47}$$

$$\zeta\theta'(\omega)\,\mathrm{d}\omega + \Omega(\zeta - \zeta^{-1})\,\mathrm{d}\zeta = 0. \tag{48}$$

Here the coefficients of $\theta(\omega)/\Omega$, but nothing else, depend on the parameter Φ.

Although values of Φ not of the form m/N may not lead to physically significant results, we can still, in principle, carry out the elimination and find what we may call $D_N(\omega)$. It is clear that in general the moments of $D_N(\omega)$ will depend smoothly on the coefficients of θ and on Ω, that is the a_n and the b_n. The density of states is itself problematic, as it shows square root singularities in ω.

In general, in problems where the a_n and b_n are sufficiently smoothly dependent on Φ, the moments will be smooth functions of this parameter.

4.4. Real values

The force of the previous subsection is that the moments of the density of states are (in general) smooth functions on the rationals. Because of the reality condition $4\Omega^2 \geq \theta^2(\omega)$ the effective range of interest is a compact set: $\theta(\omega) \pm 2\Omega$ are in fact $\theta_{\pm 1}(\omega)$ whose roots are real, and by Gershgorin's theorem are bounded by some function of the coefficients a_n and b_n.

It will therefore be possible (in general) to define the density of states for any real Φ by means of N-dimensional approximations. This accords with the physical requirements: the limits of the precision mean that a model differentiating rational and irrational values would be unacceptable.

5. Discussion

According to the plan sketched in the introduction, we have given a general solution for a modulated lattice problem for a rational modulation. We then proceeded to separate the modulation parameter from the dimensionality of the mathematical description. First we obtained that an underestimation of the periodicity by an integer number of periods gives no change in the physics. This enables us to investigate a range of different systems by founding the description on a common multiplier of the present denominators. The differences in the modulation now enter merely as variations of the coefficients of a polynomial of constant degree.

We further established a way to calculate approximations to a model with constant degree of $\theta(\omega)$, where the approximation becomes particularly good for high degrees. This finally decouples the dimensionality of the problem from its modulations. As indicated in the introduction the dimensionality can now be determined by other requirements, e.g. the correlation radius.

In this way physical systems become essentially finite and a description with finite dimensionality suffices. Modulations other than rational are accessible by allowing the numerator of Φ to take on real values.

We find that in this approach incommensurability anomalities are absent, as it has to be in the presence of a finite resolution. This leads to a satisfying physical picture.

Appendix 1. Further properties of $\theta(\omega)$

In this appendix we give more detailed results mainly for the case of Harper's equation. These illustrate more clearly the mathematical structure of θ especially in this particularly symmetric case of the general problem and indeed are of value in making explicit calculations.

A1.1. Harper's equation

Harper's equation, to which we restrict our attention here, arises in the case of the system

$$(\omega - 2\cos(k_y + n2\pi\Phi))f_n = \mathrm{e}^{\mathrm{i}k_x} f_{n+1} + \mathrm{e}^{-\mathrm{i}k_x} f_{n-1}. \tag{49}$$

Let

$$\xi := \mathrm{e}^{\mathrm{i}k_x} \tag{50}$$

$$\eta := \mathrm{e}^{\mathrm{i}k_y} \tag{51}$$

$$\varpi := \mathrm{e}^{\mathrm{i}2\pi\Phi} \tag{52}$$

then our finite matrix is given by

$$Z = \begin{pmatrix} a_1 & \xi & 0 & \cdot & \cdot & \cdot & \xi^{-1} \\ \xi^{-1} & a_2 & \xi & & & & \cdot \\ 0 & \xi^{-1} & \cdot & \cdot & & & \cdot \\ \cdot & & \cdot & \cdot & \cdot & & \cdot \\ \cdot & & & \cdot & \cdot & \cdot & 0 \\ \cdot & & & & \cdot & a_{N-1} & \xi \\ \xi & \cdot & \cdot & \cdot & 0 & \xi^{-1} & a_N \end{pmatrix}. \tag{53}$$

Now let

$$X = \begin{pmatrix} 0 & 1 & 0 & \cdot & \cdot & 0 \\ 0 & 0 & 1 & & & \cdot \\ 0 & 0 & \cdot & \cdot & & \cdot \\ \cdot & & & \cdot & \cdot & 0 \\ \cdot & & & & 0 & 1 \\ 1 & \cdot & \cdot & \cdot & 0 & 0 \end{pmatrix} \tag{54}$$

and

$$Y = \begin{pmatrix} 1 & & & \\ & \varpi & & \\ & & \varpi^2 & \\ & & & \ddots \end{pmatrix}. \tag{55}$$

For our present purpose we can most conveniently treat Z by the decomposition:

$$Z = \xi X + \xi^{-1}X^{-1} + \eta Y + \eta^{-1}Y^{-1} \tag{56}$$

A1.2. Cylindrical symmetry

Suppose now that $\Phi = M/N$ in lowest terms. Let Ξ be the matrix whose (n, l)th entry is ϖ^{nl}. As ϖ is of multiplicative order N we have that Ξ—which is in fact an ordinary character table for the cyclic group of order N—is non-singular, and has inverse Ξ^*. Moreover Ξ satisfies

$$X\Xi = \Xi Y \tag{57}$$

$$Y\Xi = \Xi X^{-1} \tag{58}$$

so that Ξ conjugates X to Y and Y to X^{-1}.

Hence

$$\Xi^{-1}Z\Xi = \xi Y + \xi^{-1}Y^{-1} + \eta X^{-1} + \eta^{-1}X. \tag{59}$$

The characteristic polynomial is unaltered by this conjugation. Hence ξ and η^{-1} enter into the characteristic polynomial in exactly the same way.

We know, however, in general the way ξ enters. An easy conjugation transforms all off-diagonal entries of Z (except the corner elements) to 1, the corner elements to

ξ^N and ξ^{-N}. From equation (14) we have that ξ enters the characteristic equation only in the form $(\xi^N + \xi^{-N})$ appearing in the constant term. Hence we have that

$$\theta_{\zeta,\eta}(\omega) := \det(\omega I - Z) = \theta(\omega) + (\xi^N + \xi^{-N} + \eta^N + \eta^{-N}) \tag{60}$$

or

$$\theta_{\xi,\eta}(\omega) = \theta(\omega) + 2\cos Nk_x + 2\cos Nk_y. \tag{61}$$

Here $\theta(\omega)$ can be taken as a suitable $\theta_{\xi,\eta}(\omega)$.

It should be noted that this result only holds when M/N is in lowest terms. In general Ξ becomes singular, X and Y are not conjugate, and in special cases the ηs may be detected in higher coefficients. Our general result on the irrelevancy of the exact period could not hold if this were not so.

A1.3. General representations of M/N

We turn now to the relationship between the cases $\Phi = M/N$ and $\Phi = kM/kN$ of Harper's equation. We continue to suppose that M, N are coprime. For convenience set $\chi(\omega) := \theta_{\xi,\eta}(\omega)$ as previously calculated from the value $\Phi = M/N$.

For $\Phi = kM/kN$ we let ϖ now denote $e^{i2\pi(M/kN)}$; we then have (in kN dimensions) the expression

$$Z = \xi X + \xi^{-1}X^{-1} + \eta Y^k + \eta^{-1}Y^{-k}. \tag{62}$$

Conjugation by Ξ now yields

$$\Xi Z \Xi^{-1} = \xi Y + \xi^{-1}Y^{-1} + \eta X^{-k} + \eta^{-1}X^k. \tag{63}$$

The matrix X represents the cyclic permutation of the row vectors; hence X^k permutes these in k blocks of size N. In fact the whole of $\Xi^{-1}Z\Xi$ decomposes into a direct sum of Harper matrices, The parameters (ξ, η) being replaced by $(\eta^{-1}, \xi\varpi^l), l = 0, \ldots, k-1$. In an obvious notation

$$\chi_k(\omega) = \prod_{r=0}^{k-1} (\theta(\omega) + \eta^N + \eta^{-N} + \xi^N\tau^r + \xi^{-N}\tau^{-r}) \tag{64}$$

where $\tau = e^{i2\pi/k}$.

The polynomial for the k-fold system is merely a product of k vertical translates of the polynomial for the single system. This allows us to form a fairly clear picture of $\chi_k(\omega)$.

A1.4. In the general case

In the case when the parameter Φ is given by kM/kN, we found that the denominator of the density of states reads

$$(\zeta_2 - \zeta_1)(\zeta_1^k - \zeta_2^k). \tag{65}$$

Therefore

$$\theta_k^2(\omega) - 4 = (\zeta - \zeta^*)^2(\zeta^k - (\zeta^*)^k)^2 \tag{66}$$

$$= (\theta^2(\omega) - 4)\prod_{l=1}^{k}(\zeta - \mathrm{e}^{\mathrm{i}2\pi l/k}\zeta^*)^2. \tag{67}$$

($\theta_k(\omega)$ denotes the polynomial $\theta(\omega)$ in the redundant case.)

$$\zeta - \zeta^* = \sqrt{\theta^2(\omega) - 4} \tag{68}$$

$$= 2\sin Nq \tag{69}$$

say, where q is the wavevector as defined by Bloch's theorem. Now (67) reads

$$\theta_k^2(\omega) - 4 = 16\sin^2 Nq \sin^2 kNq \tag{70}$$

$$\sqrt{\theta_k^2(\omega) - 4} = 4\sin^2 Nq \sin kNq / \sin Nq \tag{71}$$

$$= 4\sin^2 Nq T_{k+1}(2\cos Nq). \tag{72}$$

Here T_k denotes the kth Chebyshev polynomial. The argument $2\cos Nq$ is twice the real part of ζ, which is nothing other than $\theta(\omega)$.

The Chebyshev polynomials are defined by the recurrence relation:

$$T_k(x) = xT_{k-1} - T_{k-2} \tag{73}$$

$$T_0 = 0 \tag{74}$$

$$T_1 = 1 \tag{75}$$

or in case of $x = 2\cos\alpha$

$$\sin k\alpha = 2\cos\alpha \sin(k-1)\alpha - \sin(k-2)\alpha.$$

A1.5. Symmetry in ω

As

$$Z = \xi X + \xi^{-1}X^{-1} + \eta Y + \eta^{-1}Y^{-1} \tag{76}$$

we have

$$-Z = (-\xi)X + (-\xi)^{-1}X^{-1} + (-\eta)Y + (-\eta)^{-1}Y^{-1}. \tag{77}$$

Now the characteristic polynomial is both $\theta_{\xi,\eta}(\omega)(-1)^N$ on general grounds, and $\theta_{-\xi,-\eta}(\omega)$ in view of (77). So we have

$$\theta(\omega) + (-\xi)^N + (-\xi)^{-N} + (-\eta)^N + (-\eta)^{-N} = (-1)^N[\theta(-\omega) + \xi^N + \xi^{-N} + \eta^N + \eta^{-N}]. \tag{78}$$

Hence

$$\theta(\omega) = (-1)^N\theta(-\omega). \tag{79}$$

That is the polynomial $\theta(\omega)$ is even or odd with N.

In another case with $a_n = 0$ and b_n arbitrary, we find the same property as the b_n enter only in squares in the α and β [10].

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