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LETTER TO THE EDITOR

Hierarchical band clustering and fractal spectra in incommensurate systems

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Abstract. An analytic derivation is given of rules exactly describing the hierarchical band clustering in the spectrum of Harper's equation for various incommensurate systems. These rules, involving transformations of the incommensurability parameter ϕ, are shown to apply exactly for arbitrary coupling strength. The approach also provides energy scale factors and hence the fractal dimension D_f ($=0.50\pm0.01$) of the self-similar spectrum occurring when ϕ takes a fixed point value ϕ_g (the golden mean).

There is mounting numerical evidence that the empirically discovered Hofstadter rules [1] describe the hierarchical subdivision of the spectra for large classes of incommensurate [1-4] and quasicrystal systems [5-7]. These rules are proved analytically in this letter. The calculation of energy band scaling factors and of a resulting spectrum fractal dimension [8] are also briefly described to illustrate further applications of the analytic method.

Though a wide variety of incommensurate and quasicrystal systems may be similarly treated, those discussed here are the incommensurate systems described by Harper's equation [2-4, 9-11]

$$2a_n\lambda^{1/2}\cos 2\pi n\phi + \lambda^{-1/2}(a_{n+1}+a_{n-1}) = \varepsilon a_n. \tag{1}$$

This equation was first given as a one-dimensional reformulation of the eigenvalue problem for electrons in a two-dimensional crystal in a magnetic field. The basic incommensurability parameter ϕ is there the (fractional part of the) number of flux quanta through a unit cell. Harper's equation also provides the tight-binding description of electrons in the presence of a charge density wave [12]. It also arises in connection with phonons in modulated structures [13] or in other situations described by the Frenkel-Kontorova model [14, 15] and also in special problems such as superconducting networks [16, 17], etc. In all these cases ϕ controls the structure of the spectrum.

Numerical investigations of Harper's equation [1] (in relation to Bloch electrons in a field), for the special case $\lambda = 1$, provided the well known 'butterfly' spectral diagram giving the allowed energies ε against ϕ. It was noticed that, for any given ϕ, the spectrum is separated by two principal gaps into a 'centre' band and two outer ('side') bands; each of these contains gaps of smaller size and is like a reduced version of the full band at a transformed value of ϕ equal to $R(\phi)$ for each side band and to $S(\phi)$ for the centre band, where [1]

$$R(\phi) \equiv \{1/\phi\} \qquad \phi < \tfrac{1}{2} \qquad R(\phi) = R(1-\phi) \tag{2}$$

$$S(\phi) \equiv \{\phi/(1-2\phi)\} \qquad \phi < \tfrac{1}{2} \qquad S(\phi) = S(1-\phi) \tag{3}$$

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where $\{x\}$ denotes the fractional part of x. These 'clustering rules' imply the hierarchical nature of the 'butterfly' diagram. Hierarchical band splittings had previously been suggested [18] to arise from the continued fraction representation of ϕ. However, the resulting clustering is not quantitatively consistent with (2) and (3), which seem to correctly describe the spectrum. Using existing numerical data [5] the clustering rules can be observed to also apply to the spectrum of a quasicrystal model.

Our main aim is to show how the hierarchical spectrum develops and to derive the fundamental rules (2) and (3) for Harper's equation. The essential steps in the development are very general: it transpires that (2) and (3) describe the clustering for any λ (not just $\lambda = 1$); moreover, the approach applies to any system with two basic periodicities and also to quasicrystal models [19]. It can also provide analytic estimates of energy band and gap scaling factors, which are in agreement with our [13, 19] and previous [2, 3] numerical work, and also of fractal dimensions associated with the spectrum.

The approach is based on the treatment of (1) by a degenerate perturbation method similar to that in nearly free electron band theory, but to arbitrary order in λ. A dual transformation [10], related to a gauge change in the Bloch electron-in-field problem, takes (1) into an identical equation with $\lambda \to \lambda^{-1}$. So the perturbation theory applies, and gives related results, in both limits of λ small and λ large. Moreover, in the k space cataloguing of the sequence of gaps used here, the gap positions and all the successive results leading to (2) and (3) are independent of λ, so the description is not limited to λ small or λ large. This conclusion can be supported by periodicity arguments of the type used in Bloch's theorem in simple lattice systems.

The unperturbed ('hopping') term from (1) is diagonal in k space and the associated unperturbed energy is $\varepsilon_0(k) = 2\lambda^{-1/2} \cos k$; the perturbation provided by the first term then links states with wavevectors differing by $2\pi\phi$. A gap occurs in leading order by virtue of the coupling of the degenerate states $k = \pm\pi\phi$ or $k = \pm\pi(1-\phi)$, where a reduced zone description is being employed. This 'principal gap' (leading order in perturbation theory) separates the upper side band (the k space interval $(-\pi\phi, \pi\phi)$), the centre band (interval $(-\pi(1-\phi), -\pi\phi)$ and $(\pi\phi, \pi(1-\phi))$) and the lower side band (the remainder of the reduced zone). For the present we take the case $\phi < \frac{1}{2}$: the case $\frac{1}{2} < \phi < 1$ is similar with ϕ everywhere replaced by $(1-\phi)$.

To obtain the gap sequence, higher-order degenerate perturbation theory is now required. In mth order, the perturbation link states whose k vectors differ by $2l\pi\phi$, where $l \leqslant m$. Only the case $l = m$ provides new splittings not already present in lower order, and the associated degenerate states linked by the perturbation, and hence also the new gaps, are in mth order at

$$k = \pm\pi\{m\pi\}, \pm\pi(1-\{m\phi\}) \tag{4}$$

in the reduced zone. The k labels (4) of the degenerate states linked in mth order can be obtained by 'walking' m steps of length $\pi\phi$ to left or right from the points $n\pi$ about which the unperturbed energy is symmetric, where n is any integer such that one arrives in the reduced zone. Since m gives the order of the perturbation theory in which these splittings arise, the gaps decrease with increasing m. The mth-order gap is at values $\pm 2\lambda^{-1/2} \cos \pi m\phi$ of the unperturbed energy, which gives a family (members labelled by m) of curves of energy plotted against ϕ. Non-degenerate perturbation theory shifts (e.g. from the Brillouin-Wigner method used later here to obtain energy scale factors and hence the fractal dimension of the spectrum) will distort the family, keeping for each value of ϕ the energy ordering of the different members. Such a distortion is

enough to produce curves $m = 1, 2, \ldots$, following the principal gap, the next largest gap, and so on, in the butterfly diagram, showing that the approach contains the essential features of the gap ordering.

To discuss the hierarchical relationship of gaps, we consider the subgaps which occur in the side and centre bands, using the 'walk' procedure described above. These gaps occur in the upper side band in mth-order ($m \geqslant 2$) degenerate perturbation theory if m steps of $\pi\phi$ to right or left from $\mp n\pi$ (for some non-negative integer n related to m) arrive at $k = \pm(m\pi\phi - n\pi)$ lying in the interval $(-\pi\phi, \pi\phi)$ corresponding to the upper side band, i.e. when the integers m and n satisfy

$$n/\phi - 1 < m < n/\phi + 1. \tag{5}$$

The corresponding equation for the subgaps in the lower side band has n shifted by 1, while that for the centre band is

$$N(n)/\phi + 1 < m < (N(n)+1)/\phi - 1 \tag{6}$$

where $N(n) = n$ or $n-1$. These equations are of a type occurring in number theory in connection with Diophantine approximations [20]. Using the variable

$$x = \phi/1(1-2\phi) \tag{7}$$

and denoting the integer $m - 2N - 1$ by p, (6) becomes

$$N < px < N + 1. \tag{8}$$

If $[y]$ denotes the integer part of y, the solution of (8) is clearly $N = [px]$. It follows that (6) is solved by

$$m = p + 2[px] + 1 \tag{9}$$

where p can be any non-negative integer. Hence the gaps in the centre subband occur at

$$\begin{aligned} k &= \pm\pi(p\phi + 2\phi[px] + \phi - [px]), \pm\pi(p\phi + 2\phi[px] + \phi - [px] - 1) \\ &= \pm\pi(\phi + (1-2\phi)\{p\{x\}\}), \pm\pi(\phi - 1 + (1-2\phi)\{p\{x\}\}) \end{aligned} \tag{10}$$

using (9), (7) and the identities (valid for any integer p and any x)

$$\{x\} = x - [x] \tag{11a}$$

$$\{p\{x\}\} = \{p(x - [x])\} = \{px\}. \tag{11b}$$

Similarly the solution of (5) is clearly $m = [n/\phi], [n/\phi] + 1$, where n is any integer, so the resulting gaps in the upper side band occur at

$$k = \pm(m\pi\phi - n\pi) = \pm\pi\phi\{n\{1/\phi\}\}, \pm\pi\phi(1 - \{n\{1/\phi\}\}) \tag{12}$$

using (11*a*, *b*).

We now carry out rescalings to take the k space region occupied by a given subband into the region spanned by the full band. For the upper side band this involves division of k by ϕ to obtain k where (using (12))

$$k \equiv k/\phi = \pm\pi\{n\{1/\phi\}\}, \pm\pi(1 - \{n\{1/\phi\}\}). \tag{13}$$

The rescaling of k for the centre band is a shift of $k_0 = \pm\pi\phi$ to bring the left and right sections of this subband together and division by $(1-2\phi)$ to dilate the composite band into an equivalent full band. The centre band gaps then occur (using (10)) at

$$k \equiv (k-k_0)/(1-2\phi) = \pm\pi\{p\{x\}\}, \pm\pi(1-\{p\{x\}\}) \tag{14}$$

in the equivalent full band.

In the rescaled side and centre bands the gaps occur, comparing (13) and (14) with (4), at places corresponding to equivalent full bands with ϕ replaced by ϕ', ϕ'', respectively, where

$$\phi' = R(\phi) = \{1/\phi\} \tag{15}$$

$$\phi'' = S(\phi) = \{x\} = \{\phi/(1-2\phi)\} \tag{16}$$

($\phi < \frac{1}{2}$) and the gaps associated with (13) and (14) decrease with increasing n, p (which like m in (4) can be any positive integer) because (see, e.g., (9)) increasing n or p implies increasing order (m) in perturbation theory. Hence, for the upper side and central subbands at any $\phi < \frac{1}{2}$ the gap sequence and position in k space are the same as in rescaled full bands at transformed values $R(\phi)$, $S(\phi)$ of ϕ. All the steps from (5)-(16) generalise to $\frac{1}{2} < \phi < 1$ by replacing ϕ by $1-\phi$ and in an obvious way to the lower side band. This establishes the Hofstadter clustering rules (2) and (3) for the principal subbands.

We have shown that the full band at ϕ is composed of (upper and lower) side and centre bands whose gap sequences are the same as those in full bands at $\phi' = R(\phi)$, $\phi'' = S(\phi)$, respectively. The same arguments can then be applied to the full bands at ϕ', ϕ'' and so on indefinitely. This completes the proof of the Hofstadter clustering rules (a more detailed account will be published in [19]).

The formulation can be further exploited to arrive at quantitative analytically derived results for energy scaling factors and hence for the fractal dimension of the spectrum at the self-dual point [2] $\lambda = 1$ at ϕ values for which it is self-similar. To illustrate the procedure [19] we consider the special value ϕ_g ($=(\sqrt{5}-1)/2 =$ golden mean). This is one of the (four) fixed points ϕ^* of the joint scaling equations: $\phi^* = R(\phi^*) = S(\phi^*)$. At ϕ_g the full band is composed of side and centre bands which have the same gap sequence as the full band itself at ϕ_g and so on for the hierarchy of subbands, so the spectrum at the fixed point $\lambda = 1$, $\phi = \phi_g$ (or any other ϕ^*) is self-similar (a Cantor set), as illustrated in figure 1. If α and β are the (asymptotic) ratios of the widths (maximum energy less minimum energy) of a subband to, respectively, the widths of the side and central bands of which it is composed, the fractal dimension D_f of the spectrum is given by

$$M(L) = 2M(L/\alpha) + M(L/\beta) \qquad M(L) \propto L^{D_f} \tag{17}$$

where $M(L)$ is the measure of the spectrum.

Accurate values of α, β are found by applying Brillouin-Wigner perturbation theory to obtain the spectrum $\varepsilon(k)$. The gap edges at $k = \pi\phi$ are dominated by the terms coming from the coupling of k to $k - 2\pi\phi$ which, working to order λ^2, gives $\varepsilon = 0.201$, 1.841 for the gap edges for $(\phi, \lambda) = (\phi_g, 1)$. For the upper band edge $\varepsilon(k=0)$ the couplings of k to $k \pm 2\pi\phi$ contribute comparable terms, but it is sufficient to work to order λ, resulting in $\varepsilon(k=0) = 5.01$. The resulting scale factors and consequent fractal dimension (using (17)) are $\alpha = 7.57$, $\beta = 12.46$, $D_f = 0.51$ ($\phi = \phi_g$, $\lambda = 1$). The results are in good agreement with our numerical work on the Hofstadter spectrum, which gives $\alpha = 7.59$, $\beta = 13.73$, $D_f = 0.496$, and with a separate analytic argument [19]

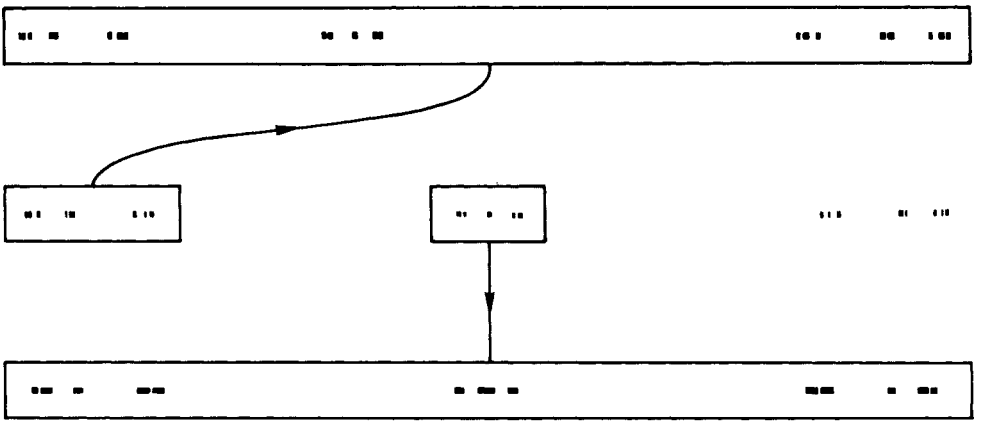

Figure 1. An approximation to the self-similar spectrum of Harper's equation occurring when ϕ is the golden mean, ϕ_g. Expanded versions of side and central bands are shown above and below the original full band, for $\phi = \frac{34}{55}$ (an accurate rational approximant to ϕ_g).

suggesting $D_f = \frac{1}{2}$, for the same ϕ, λ. It is possible to investigate in similar ways the self-similar spectrum at other fixed point values ϕ^* (e.g. $\sqrt{2}-1$) of the clustering rules [19].

The approach given above, and in particular the derivation of the clustering rules, is not limited to $\lambda = 1$ nor to the Harper equation. A separate numerical investigation of the Harper spectrum has been performed [19] to confirm the applicability of the clustering rules for $\lambda \neq 1$. Our treatment has yielded the exact transformation of ϕ (the Hofstadter rules) and of k (equations (13) and (14)). The latter provide, in Brillouin-Wigner perturbation theory, an approximate energy scaling sufficient to obtain the Cantor set nature of the self-similar spectrum and its fractal dimension, etc. The scaling of the parameter λ is the remaining ingredient for a full renormalisation group transformation of the system [19] from which wavefunction scaling properties and the localisation transition can, in principle, also be obtained [11]. Finally, a related derivation of clustering rules for other incommensurate systems and quasicrystal models will be presented elsewhere [19].

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