Spectrum and bandwidth of an exactly soluble incommensurate model

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Abstract. The structure of the energy spectrum of the exactly soluble Maryland model is examined in detail for both incommensurate and commensurate modulations. The study is motivated by a formal similarity with Harper's equation describing crystal electrons in a uniform magnetic field. An exact expression is derived for the characteristic polynomial which determines the energy eigenvalues, allowing explicit verification of the transition from band structure, for commensurate modulations, to a point spectrum in the incommensurate limit. An application is the calculation of the total width of the bands. A semiclassical argument is used to assess the relevance of the results to models of physical interest.

1. Introduction

Physical systems in which two independent essential length scales are present display a number of novel properties (for reviews, see Sokoloff 1985 and Lovesey *et al* 1991). A frequently studied case is a tight-binding model of non-interacting electrons in a square lattice with an applied magnetic field. Unusual features of this system include extreme fragmentation and hierarchical structure of the energy spectrum and infinitely sensitive dependence on the magnetic field strength (Hofstadter 1976, Stinchcombe and Bell 1987), quantized Hall conductance (Thouless *et al* 1982), a transition between localized and extended wavefunctions (Aubry and André 1980), and scaling behaviour of the total width of energy bands (Thouless 1983, 1990, Watson 1991). Analogous effects occur in systems such as longitudinally modulated magnets (Lovesey 1988) and a model of the lattice dynamics of incommensurate crystals (Currat and Janssen 1988).

The systems mentioned possess an eigenvalue equation which is a second-order symmetric difference equation with periodically or quasi-periodically modulated coefficients. For the electron system, the amplitude u_n of a tight-binding wavefunction at site n satisfies Harper's equation,

$$u_{n-1} + u_{n+1} + 2\alpha \cos(2\pi n\phi + \Delta)u_n = Eu_n \tag{1.1}$$

where the incommensurability parameter ϕ is proportional to the magnetic field, α is unity for an isotropic lattice, and the phase Δ is the Bloch wavenumber along the perpendicular lattice axis.

One approach to the theoretical study of this class of eigenvalue problems has been the construction of exactly soluble models. Perhaps the most notable is the 'Maryland model' of Grempel *et al* (1982), described by the eigenvalue equation

$$u_{n-1} + u_{n+1} + 2\alpha \tan(\pi n\phi + \Delta)u_n = Eu_n. \tag{1.2}$$

Although the model was originally introduced in connection with a kicked oscillator system, our study is motivated largely by the formal similarity with (1.1). In both equations the modulation has period $1/\phi$. The tangent function, however, is unbounded; one consequence is that the small-α case cannot be regarded as a perturbation from $\alpha = 0$, since the modulated term takes on arbitrarily large values if ϕ is irrational. The formal similarity is more significant for commensurate modulations, ϕ rational, because then the waveform is sampled at only a finite number of points, avoiding the tangent's singularities.

In this paper, the energy (E) spectrum of the Maryland model is investigated in detail, using analytical techniques applied to an exact solution. New results include the Floquet wavenumber, which determines the location of energy band edges $\{E_i\}$ and the density of states, calculated in closed form for rational ϕ. A simple relationship is derived between commensurate and incommensurate modulations, by labelling bands with corresponding incommensurate eigenvalues. The results justify our hypothesis that a study of low-order periodicity modulations adequately characterizes these systems. Another result is the calculation of the total width of the bands in the limit of large periodicity. Finally, a semiclassical argument is used to assess the relevance of models with unbounded modulation to the electron system of physical interest.

2. Exact solution

The treatment presented here is a more direct version of that given by Grempel *et al* (1982). Multiplying (1.2) through by $\cos(\pi n\phi + \Delta)$ and defining the generating function,

$$v(\theta) = (E - 2\cos\theta - 2i\alpha) \sum_{n=-\infty}^{\infty} e^{in\theta} u_n \tag{2.1}$$

yields a first-order difference equation,

$$v(\theta) = e^{i[V(\theta)-2\Delta]}v(\theta - \tau) \tag{2.2}$$

where

$$V(\theta) = 2\tan^{-1}[\alpha^{-1}(E/2 - \cos\theta)] \tag{2.3}$$

and $\tau = 2\pi\phi$. Equation (2.2), together with the periodicity property, $v(\theta) = v(\theta - 2\pi)$, is equivalent to the eigenvalue equation (1.2).

The Fourier coefficients of $V(\theta)$, defined by

$$V(\theta) = \sum_{n=-\infty}^{\infty} e^{in\theta} V_n \tag{2.4}$$

are recorded here for future reference:

$$V_0 = \pi - 2\mu$$

$$V_n = V_{-n} = -2n^{-1}e^{-\gamma n}\sin(\mu n) \qquad n \geq 1 \tag{2.5}$$

where $\gamma > 0$ and $\mu \in [0, \pi]$ are defined by

$$\cosh\gamma\cos\mu = E/2 \qquad \sinh\gamma\sin\mu = \alpha. \tag{2.6}$$

2.1. Incommensurate modulation

An irrational value of ϕ describes the situation in which the two periods in the problem are not commensurate with each other. In that case, iterating (2.2) determines $v(\theta)$ at a dense set in $\theta \in [-\pi, \pi]$. Under conditions discussed below, $v(\theta)$ may be expanded as

$$v(\theta) = \exp\left[i\sum_{n=-\infty}^{\infty} e^{in\theta}f_n + \nu\theta\right] \tag{2.7}$$

where ν is an integer. The coefficients f_n are determined by substituting into (2.2), from which

$$f_n = (1 - e^{-in\tau})^{-1}V_n \qquad n \neq 0 \tag{2.8}$$

and

$$V_0 = 2(\pi\nu\phi + \Delta) \mod 2\pi. \tag{2.9}$$

Thus

$$\sum_{n=-\infty}^{\infty} e^{in\theta}f_n = \sum_{n=1}^{\infty} V_n\frac{\sin[n(\theta + \pi\phi)]}{\sin(\pi n\phi)} \tag{2.10}$$

determines the eigenfunction, while (2.9) is an implicit equation for the energy eigenvalues. The $n = 0$ term is absent from (2.10), since it contributes only an overall phase factor to $v(\theta)$. Combining (2.9) and (2.5) and eliminating γ from (2.6), we obtain

$$E_\nu = 2\tan(\pi\nu\phi + \Delta)\sqrt{\alpha^2 + \cos^2(\pi\nu\phi + \Delta)}. \tag{2.11}$$

The eigenvalues, labelled by the integer ν, form a countable set dense in the real line, in other words a pure point spectrum.

The solution presented here is valid only when ϕ is 'sufficiently irrational'. For special values of ϕ, the Liouville numbers, the series (2.10) fails to converge due to the presence of small denominators $\sin(\pi n\phi)$. In this case, analysed in detail by Prange *et al* (1983, 1984) and Simon (1985), the energy spectrum is singular continuous (not a countable union of points or line segments). This topic is not pursued here.

2.2. Commensurate modulation

When ϕ is a rational number, M/N (with M and N co-prime integers), general considerations applicable to periodic eigenvalue equations (Lovesey *et al* 1991) apply. The spectrum consists of N bands, in which the eigenvalue equation (1.2) admits solutions satisfying Floquet's theorem,

$$u_{n+N} = e^{iNk} u_n \qquad (2.12)$$

with real k. In the gaps separating stable bands, the Floquet wavenumber k is imaginary. The band edges are known to be the roots of

$$\theta_N(E) \equiv 2\cos(Nk) = \pm 2 \qquad (2.13)$$

which is a polynomial equation of degree N in E. The characteristic polynomial θ_N is readily generated for particular values of N; for instance,

$$\theta_1 = E - 2\alpha \tan \Delta$$

$$\theta_2 = E^2 + 4\alpha E \cot 2\Delta - 2(1 + 2\alpha^2) \qquad (2.14)$$

and

$$\theta_3 = E^3 - 6\alpha E^2 \tan 3\Delta - 3(1 + 4\alpha^2)E + 2\alpha(3 + 4\alpha^2) \tan 3\Delta.$$

A general solution is once again generated by iterating (2.2), beginning at $\theta = k$. After m iterations,

$$v(m\tau + k) = \exp\left(-2im\Delta + i\sum_{j=1}^{m} V(j\tau + k)\right) v(k) \qquad (2.15)$$

where the angular variables are taken modulo 2π. Since $N\tau = 0 \pmod{2\pi}$, $v(\theta)$ is determined at only N points in $[-\pi, \pi]$. Setting $m = N$, consistency requires

$$-2N\Delta + \sum_{j=1}^{N} V(j\tau + k) = 2\pi M \lambda \qquad (2.16)$$

for some integer λ. The resulting equation,

$$V_0 + 2\sum_{r=1}^{\infty} V_{rN} \cos(rNk) = 2(\pi\lambda\phi + \Delta) \qquad (2.17)$$

is the quantization condition, analogous to (2.9), for the commensurate case. It is an implicit equation for the energy eigenvalues as a function of the labels λ and k. The integer $\lambda = 0, 1, \ldots, N - 1$ labels the N bands while $k \in [-\pi/N, \pi/N]$ labels independent states within a band. Evaluating the sum in (2.17) explicitly we find

$$\theta_N/2 = \cos(Nk) = \cosh(N\gamma)\cos(N\mu) + \sinh(N\gamma)\sin(N\mu)\cot[N(\Delta + \pi/2)] \qquad (2.18)$$

from which the location of band edges may be calculated; the results (2.14) can be obtained from (2.18). The closed form expression (2.18) for the characteristic polynomial is a new result, whose consequences are developed in subsequent sections.

The analytic solution (2.18) is also convenient for numerical calculations of the spectrum. The results of such a calculation are plotted in figure 1, for selected values of the amplitude and phase parameters. The energy bands are shown as horizontal lines at each rational value of ϕ, ranging from 0 to 1 along the vertical axis. The figure corresponds to the well-known 'butterfly diagram' (Hofstadter 1976) for the electron system. Energy bands lying outside the range $-10 \leq E \leq 10$ are not shown.
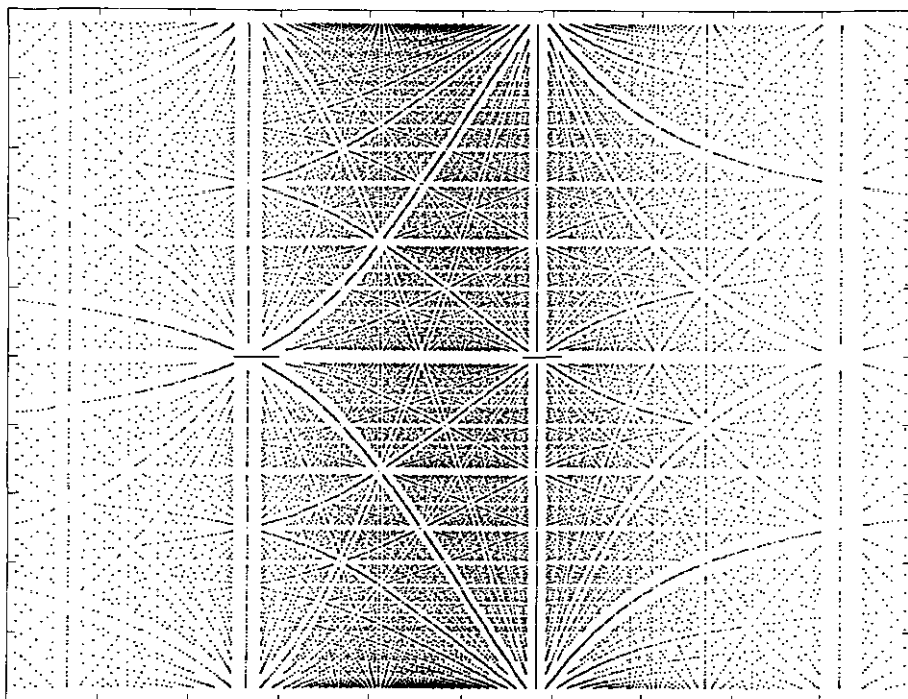
Figure 1. The energy spectrum for $\alpha = 1.2$ and $\Delta = 0.5$ is plotted horizontally as a function of the incommensurability parameter, taking rational values $\phi = M/N$ along the vertical axis with $N = 2, 3, \ldots, 50$. The horizontal energy scale ranges from -10 to 10.

3. Labelling theorem

We now investigate the relationship between the point spectrum and the band spectrum occurring in the generic irrational and rational cases, respectively. First, note that when ϕ is rational, the incommensurate energy formula (2.11) generates only N distinct eigenvalues rather than a countable dense set. That these correspond to the N bands in the commensurate problem may be verified as follows: when (2.9) is satisfied, we have

$$\cot(N\mu) = -\cot[N(\Delta + \pi/2)] \tag{3.1}$$

and hence

$$|\theta_N(E_\nu)/2| = e^{-N\gamma}|\cos(N\mu)| \leq 1 \tag{3.2}$$

implying that E_ν lies within a stable band. It can be shown that exactly one E_ν lies in each band. Thus each of the N values of E_ν marks the approximate positions of a band, and the index ν labels the bands for commensurate modulations.

It will be shown in the next section that the width of a single band decreases extremely rapidly with increasing N, namely as $N^{-1}e^{-N\gamma}$. Hence for large N the bands are very closely concentrated about the labelling points E_ν. In fact, a plot of

the points E_ν against rational values of ϕ is indistinguishable from figure 1, on the scale used, for all but the smallest values of N.

The labelling of bands in the periodic problem via the corresponding incommensurate eigenvalues (2.11) thus provides a valuable picture of the correspondence between the two extreme cases. A rational value of ϕ may be approached by a sequence of rationals with increasing denominators. As the denominator increases, the bands become narrower and increase in number. In the (generic) incommensurate limit, the number of bands becomes infinite, each of them reducing to a single point.

It has been suggested by Lovesey (1989) that, from an experimental standpoint, examination of small-N cases is sufficient to characterize the behaviour of these systems. The band labelling result proved here justifies this belief that the essential physics is contained in low-periodicity cases, for this particular model. Similar considerations are likely to apply to the electron model, and other systems of physical interest, although the details may be complicated by the possibility of a singular continuous spectrum in the generic incommensurate case.

4. Total bandwidth

As an application of the band labelling result, we calculate the total width W of the energy spectrum for the Maryland model. Of interest in itself as a characterization of the spectrum for large periodicity, the bandwidth may also be compared with the corresponding quantity for the Harper model (1.1). This has an interesting scaling behaviour near its self-dual point $\alpha = 1$, and the product NW appears to approach a universal large-N limit independent of M (Thouless 1983, 1990, Watson 1991).

The bandwidth here is different from that normally calculated for Harper's equation: we define W as the total width for a fixed value of the phase Δ, rather than the union over all Δ. This is an essential step, since the union of eigenvalues for all Δ is the entire real line. The exact solutions (2.11) and (2.18) do not depend on M, so we may set $M = 1$ for convenience.

It has been shown that a single band, for ϕ rational, is an interval of the energy axis over which the characteristic polynomial, given by (2.18), varies from -2 to 2. Hence the width of the band is given, to first order, by

$$W_\nu \simeq 4 \left| \frac{\mathrm{d}\theta_N}{\mathrm{d}E} \right|_{E_\nu}^{-1} \tag{4.1}$$

where the derivative is evaluated at $E = E_\nu$ in accordance with the labelling theorem of the previous section. The terms neglected vanish in the large-N limit, so this
and hence

$$|\theta_N(E_\nu)/2| = \mathrm{e}^{-N\gamma} |\cos(N\mu)| \leq 1 \tag{3.2}$$

implying that E_ν lies within a stable band. It can be shown that exactly one E_ν lies in each band. Thus each of the N values of E_ν marks the approximate positions of a band, and the index ν labels the bands for commensurate modulations.

It will be shown in the next section that the width of a single band decreases extremely rapidly with increasing N, namely as $N^{-1}\mathrm{e}^{-N\gamma}$. Hence for large N the bands are very closely concentrated about the labelling points E_ν. In fact, a plot of

Evaluating the derivative using (2.6) and summing contributions from individual bands, the total width of the energy spectrum for large N is given by

$$W = 8N^{-1}|\sin[N(\Delta + \pi/2)]| \sum_{\nu=0}^{N-1} e^{-N\gamma} \left(\frac{\sinh^2 \gamma + \sin^2 \mu}{\cosh \gamma \sin \mu} \right)\bigg|_{E_\nu}. \quad (4.4)$$

The sum in this expression may be evaluated asymptotically using a standard technique analogous to Laplace's method for integrals (Bender and Orszag 1978). The only appreciable contribution to the sum is concentrated in a small region near the point

$$\mu_0 = \pi/2 \qquad \gamma_0 = \sinh^{-1} \alpha \qquad\qquad (4.5)$$

at which $e^{-N\gamma}$ attains an extremely sharp maximum. Expanding the exponent in a power series yields

$$W = 8N^{-1}|\sin[N(\Delta + \pi/2)]| \cosh \gamma_0 \, e^{-N\gamma_0} \sum_{\nu'} \exp(-\alpha\pi\nu'^2/2 \cosh \gamma_0) \qquad (4.6)$$

where the sum is over all integers ν'. The remaining sum is readily approximated by its corresponding Riemann integral, and we obtain the result

$$W = 16|\sin[N(\Delta + \pi/2)]| \, (2\pi N \tanh \gamma_0)^{-1/2} \cosh \gamma_0 \, e^{-N\gamma_0} \qquad (4.7)$$

giving the total width of the energy spectrum, for a particular phase Δ, in the large-N limit.

The Maryland model does not have a self-dual point, and the behaviour of W is clearly dominated by the singularity at $\alpha = 0$, arising from the property, mentioned earlier, that $\alpha \approx 0$ does not correspond to a small modulation. An interesting feature of (4.7) is that if α decreases so that $N\alpha$ remains constant, W tends, apart from the Δ-dependent prefactor, to a finite limit.

5. WKB picture

Some properties of the Maryland model differ considerably from those of Harper's equation: the generic incommensurate spectrum is a countable set of points with no hierarchical clustering, all the states are localized in the lattice, and the bandwidth diverges for $\alpha = 0$ and is exponentially small for $\alpha > 0$. The differences are readily understood in terms of a WKB analysis applicable to discrete eigenvalue equations (Watson 1991, and references therein). The essential feature is the unbounded nature of the tangent modulation.

The qualitative picture is as follows. For large N we imagine a quantum particle moving in an series of one-dimensional potential wells, with classical momentum

$$p(x) = \cos^{-1}[E/2 - \alpha \tan(\pi x)]. \qquad (5.1)$$

To a leading approximation, the eigenfunctions will be bound states, localized in a particular well. The eigenvalues, determined by a Bohr–Sommerfeld quantization condition of the type

$$N \oint p(x)\mathrm{d}x = 2\pi(n + \Gamma) \qquad (5.2)$$

where the integral is around a closed classical orbit and Γ depends on the phase Δ, form a set of N discrete points. In the $N \rightarrow \infty$ limit these yield the countable spectrum of the generic incommensurate. There are no other possibilities since the classical trajectories are closed for any energy. Broadening of the bands for finite N, arising as a higher order effect of tunnelling between adjacent potential wells, is exponentially small. These features are to be expected for any modulated system in which the diagonal coefficient is unbounded.

For Harper's equation, by contrast, the potential wells are of finite depth and there are some regions, near the classical separatrix, in which the effect of tunnelling remains appreciable for large N. Roughly speaking, these bands are broad enough for the spectrum to remain uncountable even as $N \rightarrow \infty$, resulting in a Cantor set structure. Clearly both localized and extended states are possible, depending on α.

6. Conclusions

Our study of the Maryland model has been motivated by the formal similarity of its eigenvalue equation with the Harper equation describing an electron in a lattice subject to a uniform magnetic field. The characteristic polynomial, which generates the band edges, for the latter model can be determined exactly only in the asymptotic limit of large periodicity (Watson 1991). Subtle features of the spectrum, such as hierarchical structure, are not resolved at the level of approximation used. The Maryland model, however, is exactly soluble for any periodicity. We have derived an exact expression for the characteristic polynomial, equation (2.18), which displays explicitly the transition from band structure to point spectrum as incommensurability is approached. A similar transition is imagined to occur for the Harper model, but has not been directly confirmed. It implies that studies of low-order periodicity cases are adequate for comparison with experiment, in which the resolution of spectral structure is necessarily limited.

Significant differences between the two models, such as the behaviour of the total bandwidth calculated in section 4, and the absence of a transition from localized to extended wavefunctions in the Maryland model, have been explained by a WKB argument, sketched in section 5. An alternative explanation of the dominance of localization in the Maryland model is the presence of inherently long-range interactions in its dual problem (Stephen and Akkermans 1986).

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