Asymptotically exact solutions of Harper equation

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We present asymptotically exact solutions of an incommensurate Harper equation—one-dimensional Schrödinger equation of one particle on a lattice in a cosine potential. The wave functions can be written as an infinite product of string polynomials. The roots of these polynomials are solutions of Bethe equations. They are classified according to the string hypothesis. The string hypothesis gives asymptotically exact values of roots and reveals the hierarchical structure of the spectrum of the Harper equation.

PACS number(s): 05.45.+b, 71.23.Ft, 71.30.+h

1. Incommensurate quantum systems present a broad variety of complicated fractal objects and strange sets. The Harper equation (or almost Mathieu equation) is one of the most notable:

\[ \psi_n + \psi_{n-1} + 2\lambda \cos(\theta + 2\pi \eta) \psi_n = E \psi_n \]  

(1)

It has two competing periods \( \eta^{-1} \) and 1, and describes a particle on a one-dimensional lattice in a periodic potential. The same equation (1) also describes a particle on a two-dimensional square lattice in a uniform magnetic field \( \eta \) flux quanta per elementary plaquette (Azbel-Hofstadter problem). Then \( \lambda \) is an anisotropy of the square lattice and parameter \( \theta \) is a Bloch multiplier.

When \( \eta \) is an irrational number, i.e., the period of the potential is incommensurate with the period of the lattice, the spectrum and wave functions are known to have a rich hierarchical structure \( \vert \). The physics of the problem depends on the value of parameter \( \lambda \) and falls into three universality classes. For \( \lambda < 1 \) all wave functions are extended and the energy spectrum has a non-zero Lebesgue measure \( 4(1 - \lambda) \). For \( \lambda > 1 \) all wave functions are localized (in this letter we consider only “typical” irrational numbers which can not be approximated by rationals too well) and the energy spectrum has zero measure. At the most interesting “critical” point \( \lambda = 1 \) wave functions neither localized nor extended, but exhibit a power law scaling, while the spectrum is singular continuous (a set without isolated points but with zero Lebesgue measure).

Since the empirical observations of Hofstadter \( \vert \), the evidence has been mounting that these spectra are regular and universal rather than erratic or “chaotic”. Few years ago it has been shown \( \vert \vert \) that despite the complexity of the spectrum, the Harper equation at any rational \( \eta = P/Q \) is integrable and can be “solved” by means of the Bethe Ansatz (BA). This had opened the possibility of describing the complex behavior of an incommensurate system as a limit of a sequence of integrable models. In this letter we analyze the Bethe equations \( \vert \) for \( \lambda = 1 \) and show how the (BA) reveals the hierarchical structure of the spectrum. We show that (i) solutions of the BA equations (roots) fall into complexes—strings; (ii) the number of roots in a string (length of the string), known as Takahashi-Suzuki numbers \( \vert \) are intimately related to the Hall conductance of a state; (iii) strings provide an asymptotically exact wave functions for the entire spectrum.

To introduce the scaling concept let us consider an irrational \( \eta \) as the limit of rational approximants \( \eta_j = P_j/Q_j \). With rational number \( \eta \) instead of \( \eta \) the potential in (1) becomes commensurate with the lattice and the problem is reduced to diagonalization of a \( Q_j \times Q_j \) matrix. The spectrum consists of \( Q_j \) bands separated by \( Q_j - 1 \) gaps \( \vert \). In this letter we show that the wave function of the problem with rational \( \eta_j \) can be written approximately as a product of a wave function for the \( \eta_{j-1} \) (ancestor wave function) and some polynomial which roots form a so-called string. By recursion the wave function with irrational \( \eta \) appears as an infinite product of string polynomials. The multiplicative structure thus obtained is asymptotically exact (see eq.11). It resembles the multiplicative formulae conjectured in \( \vert \).

2. The Bethe Ansatz. If \( \eta = P/Q \) is a rational number then the solution of (1) can be chosen as Bloch function \( \psi_n = e^{ik_{jx}n} \xi_n \) where \( \xi_n = \chi_{n+Q} \). Although the BA solution is known for arbitrary values of Bloch multipliers \( k_x \) and \( k_y \equiv \theta \), below we consider only the points of Brillouin zone \( (k_x, k_y) \) which correspond to edges and centers of bands. At these (rational) points the BA solution is particularly simple \( \vert \). BA solution can be obtained in two steps. The first step is the isospectral transformation:

\[ \psi_n = \sum_{m=0}^{M} c_{nm} \Psi(-ipq^m) \]  

(2)

to the difference equation:
\[\mu \kappa z E \Psi(z) = i q (z + i \tau \kappa q^{-\frac{1}{2}})(z - i \kappa q^{-\frac{1}{2}}) \Psi(qz) - \frac{i q^{-1}(z - i \kappa q^{\frac{1}{2}})(z + i \kappa q^{\frac{1}{2}}) \Psi(qz^{-1})}{1 - i \kappa q^{1/2}}, \quad (3)\]

where \(\rho = \exp(i \frac{k}{2} \kappa \pi P)\), \(M = 2Q - 1\) if \(P\) is odd and \(M = Q - 1\) if \(P\) is even; \(q = e^{i \pi \eta}\). The choice of \(\tau = \pm 1\) yields either levels at the center or at the edges of bands respectively. The rational points are degenerate and are labeled by discrete parameters \(\kappa, \mu = \pm 1\). The coefficients in (3) are given by “quantum dilogarithms”

\[c_{nm} = \prod_{j=0}^{m-1} \left( e^{ik_s q^{2j+1/2} (1 + i \tau \kappa q^{-1} q^{-j/2})/1 - i \kappa q^{1/2}} \right). \quad (4)\]

The second step is based on the integrability of eq. (3): \(Q\) its (regular) solutions are polynomials of \(z\) of the degree \(Q - 1\):

\[\Psi(z) = \prod_{i=0}^{Q-1} (z - z_i). \quad (5)\]

The roots \(\{z_i\}\) satisfy the system of Bethe equations:

\[q^Q \prod_{k=1}^{Q-1} q z_i - z_k = \frac{(z_i - i \tau \kappa q^{\frac{1}{2}})(z_i + i \kappa q^{\frac{1}{2}})}{(q^{\frac{1}{2}} z_i + i \tau \kappa)(q^{\frac{1}{2}} z_i - i \kappa)} \quad (6)\]

Solutions of the BA equations give the wave functions of the Harper equation at band’s edges and centers. Their energy is given by

\[E = i \mu q^Q (q - q^{-1}) \left[ \kappa \sum_{i=1}^{Q-1} z_i - i \frac{1 - \tau}{q^{1/2} - q^{-1/2}} \right]. \quad (7)\]

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At first glance, the BA equations (6) look even more complicated than the original Harper equation. However, the BA equations (6) provide a better description of the problem in the most interesting, incommensurate, limit \(Q \to \infty\). In a sense, the incommensurate limit plays the role of the thermodynamic limit, with \(Q\) being the size of the system.

3. **String hypothesis.** Below we formulate the string hypothesis which allows us to obtain the approximate solutions of the BA equations. The hypothesis is based on the analysis of singularities of the BA, and is supported by extensive numerics. We present a detailed analysis of singularities in a more extended publication [15]. Here we just formulate the string hypothesis and present some immediate consequences. First, we need the notion of strings, a Hall conductance, a hierarchical spectral flow and a hierarchical tree.

a) A string of spin \(l\), parity \(v = \pm 1\) and center \(x\) is a set of \(2l + 1\) complex numbers:

\[\psi(x) = \{ q_1^{-\frac{l}{2}} , q_1^{-\frac{l+1}{2}} , \ldots , q_1^{\frac{l+1}{2}} \}, \quad (8)\]

where \(x\) is a real positive number and \(q_1^{2l+1} = \pm 1\).

b) The Hall conductance \(\sigma(k)\) of the band \(k = 1, \ldots , Q\) is the Chern class of the band, i.e., the number of zeros of the wave function as a function of \(k_x, k_y\) in the Brillouin zone. We will also need the Hall conductance of \(k\) filled bands: \(\sigma_k\). The latter is assigned to the \(k\)-th gap, so that \(\sigma(k) = \sigma_k - \sigma_{k-1}\). They are determined by the Diophantine equation \([14, 13]\)

\[P \sigma_k = k \text{ (mod } Q\text{)} \quad (9)\]

restricted to the range \(-Q/2 < \sigma_k < Q/2\).

c) **Hierarchical spectral flow.** We refer to the band \(k\) of the problem with parameter \(\eta = P/Q\), as to the parent band of the parent generation corresponding to the daughter band \(k\) of the daughter generation \(\eta = P/Q\) if:

(i) the Hall conductance of the band \(k\) is the ratio between the difference of the number of states of parent and daughter bands and the difference between the periods of generations

\[\frac{1}{Q} - \frac{1}{Q'} = \sigma(k)(\frac{P}{Q} - \frac{P'}{Q'}), \quad (10)\]

(ii) \(\eta'\) and \(\eta\) are closest rationals with \(Q' \leq Q\), and \((k' - 1)/Q' < (k - 1)/Q < k'/Q'\). These conditions may be viewed as the integrated Streda formula (see Ref. [15]), which determines the spectral flow while varying the period from \(\eta'\) to \(\eta\). Starting from some particular band \(k\) of the generation \(\eta\) one can obtain from Eq. (10) the sequence of “ancestor” bands belonging to generations \(\eta_j \equiv \frac{P_j}{Q_j}\)—subsequent rational approximants to \(\eta\).

The bands belonging to different periods \(\eta_j\) together with parent-daughter relations the hierarchical tree. Let us notice that the sequence \(\eta_j\) differs from the approximants obtained by truncating the continued fraction expansion of \(\eta\). Instead, it consists of intermediate fractions [19]. Let us also notice, that parents of states of a given generation do not necessarily belong to the same generation.

Now we are ready to formulate the string hypothesis. At large \(Q\) each solution of the BA consists of strings, so that each state can be labeled by spins \(\{l_j, l_{j-1}, \ldots \}\) and parities \(\{v_j, v_{j-1}, \ldots \}\) of strings, such that the total number of roots \(\sum_{i=1}^{k} (2l_i + 1) = Q - 1\). We refer to the set of lengths and parities of strings constituting the solution for a given energy level as to a string content of this level. The length of the longest string in a string content of a given energy level is the Hall conductance of the corresponding energy band: \(2l + 1 = \sigma(k)\). The “period” of this string \(q_1 = e^{i \pi \eta_i}\) is uniquely determined by the requirement that \(\eta_i = \frac{P_i}{Q_i}\) is the best approximant for the period \(\eta\) of the state. The parity of the longest string is \(v_i = -i q_1^{l_i + 1/2} = (-1)^{l_i} \kappa\). The remaining roots are given by the solution of the BA equation for the parent state of the parent generation. In other words

\[\psi^{\text{daughter}}(z) \approx \psi^{\text{parent}}(z) \prod_{m=-l}^{l} (z - x v_i q_1^m), \quad (11)\]
The accuracy of eq. (11) is determined by the accuracy of approximation of \( \eta \) by \( \eta' \) and \( \eta'' \) which is of the order of \( 1/l^2 \) (\( \eta, \eta' \) and \( \eta'' \) are all rational approximants of some “typical” irrational number). Thus the formula (11) is asymptotically exact. It gives the roots of the largest string of the length \( 2l + 1 \) with the accuracy \( 1/l^2 \) which gets higher along the hierarchical tree when \( \eta \to \text{irrational} \).

The complete string composition of a given state can be obtained by means of the iterative procedure. Starting from a state of the generation \( \eta \), first we find the branch of the hierarchical tree that this state belong to. Then we determine the Hall conductances of all states of the branch down to the origin. This determines the lengths, periods and parities of strings.

The strings hierarchy has been obtained through the analysis of singularities of BA (see [15]). As it was expected a set of possible lengths of strings is a set of Takahashi-Suzuki numbers (dimensions of irreducible representations of \( U_1(SL_2) \) with definite parity \( [21] \)). Eq. (8) provides a relation between them and Hall conductances.

The iterative procedure provides an algorithm for writing down the wave functions of all states for any rational \( \eta \). The only unknowns are the centers of strings. They, however approach 1 with accuracy \( O(1/l) \). The accuracy of the recursive eq. (11) is \( O(l^{-2}) \). The string content of a state (i.e., lengths and parities of strings) is a topological characteristics, while the centers of strings are not.

To illustrate the iterative procedure let us consider the bottom edges of the lowest band of the spectrum and choose \( \eta = \sqrt{5/2} \) to be the golden mean. The sequence of rational approximants is given by ratios of subsequent Fibonacci numbers \( \eta_k = \frac{F_{k+1}}{F_k} \), where the \( F_i \) are Fibonacci numbers (\( F_1 = F_{-2} + F_{-1} \) and \( F_0 = F_1 = 1 \)). The set of Hall conductances is Takahashi-Suzuki numbers = allowed lengths of strings are again Fibonacci numbers: \( Q_k = F_k \). The considered branch of hierarchical tree connects edges (\( \tau = -1, \kappa = 1, \mu = 1 \)) of the lowest bands of generations \( \eta_{3k} = F_{3k-1} / F_{3k} \). Their string content consists of pairs of strings with lengths \( 2l_n + 1 = F_{3n+1} \), \( n = 0, 1, \ldots, k-1 \), parities \( v_{sn} = +1 \) and inverted centers \( x_{ln} \) and \( x_{ln}^{-1} \). According to the string hypothesis the wave function of this state is

\[
\Psi(z|\eta_{3k}) \approx \prod_{n=0}^{k-1} \left( \prod_{j=-l_n}^{l_n} (z - x_{ln} q_{jn}^{-1}) (z - x_{ln}^{-1} q_{jn}^{-1}) \right). \tag{12}
\]

FIG. 1. Shown in the figure are the roots of the lowest rational state of the Harper equation at \( \eta = 34/55 \). The roots are organized in strings: two of the length 1(+) and two of the length 5(×) and two of the length 21(*). These roots can be approximated by ansatz (12) and are plotted in the Figure as boxes(□). Roots tend to repel each other. This “splitting” is of the order of \( O(1/l) \).

As an another example, let us consider a branch of the hierarchical tree for the golden mean, which goes through levels \( r_{2k} = \frac{2F_{2k} - F_{2k-1}}{5} + \frac{5 + (-1)^k}{10} \) of generations \( \eta_{2k} = F_{2k-1} / F_{2k} \). Here \( k = 1, 2, \ldots, \) and \( r_{2k} \) is the number of the level counted from the bottom of the spectrum. This branch leads to the point of the spectrum characterized by an irrational number (filling factor) \( \zeta \equiv \lim_{k \to \infty} r_{2k}/F_{2k} = (5 - \sqrt{5})/10 \). Each state along the branch consists of strings of lengths \( 2s_n + 1 = F_{2n+1} \) and parities \( v_{sn} = (-1)^{3(n/3)} \), where \( n = 0, 1, \ldots, k-1 \) and \( \{ \cdot \} \) denotes fractional part. The wave function along the branch is

\[
\Psi(z|\eta_{2k}) \approx \prod_{n=0}^{k-1} \prod_{j=-s_n}^{s_n} (z - v_{sn} q_{jn}). \tag{13}
\]

The iterative procedure allows one to generate the string content and wave functions out of two irrational numbers: a period \( \eta \) and a filling factor \( \zeta \).

4. Numerical evidence for the string hypothesis. We now present a fragment of an extensive numerical analysis that we have performed in order to check the string hypothesis. Let us consider the bottom edge of the lowest energy band for \( \eta_9 = 34/55 \) from the golden mean sequence. According to (12) the string content of this level consists of strings of lengths \( 1, 1, 5, 5, 21, 21 \). All string parities in this example are +1. The actual numerically calculated roots are shown in Fig. 1. One notices immediately that the roots organize themselves into distinct groups whose members have roughly the same radius: two groups with 1 root(+), two with 5 roots(×), and two groups with 21 roots(*). The centers of strings are \( x_{ln} = 2.10, 1.23, 0.81, 1.05, \approx 1 + 1.14/F_{3n+1} \). The roots
produced by eq.(12) on Fig.[1] are in a good agreement with the numerical results. In fact one can prove that their accuracy of each root of the string of the length $2l+1$ is $O(1/l^2)$.

The overlap between the asymptotic ansatz wave function $|\psi_{\text{ansatz}}\rangle$ and the direct numerical solution of the eq.(3) for $\eta_{15} = 6/60$ is $\langle \psi_{\text{direct}} | \psi_{\text{ansatz}} \rangle \approx 0.99475$. To see how the accuracy of ansatz $|\psi_{\text{ansatz}}\rangle$ is increasing with the length of the string we replace all roots of ansatz wave function $\psi_{\text{ansatz}}$ except for the ones belonging to two largest strings of the length 377 by numerically obtained roots. The new wave function $\psi_{\text{interm}}$ is in some sense intermediate between pure ansatz $\psi_{\text{ansatz}}$ and numerical $\psi_{\text{direct}}$ wave functions. The overlap $\langle \psi_{\text{direct}} | \psi_{\text{interm}} \rangle \approx 0.999435$. This increase of an accuracy of approximation is due to a higher accuracy of the long strings of the length 377 with respect to the shorter ones.

5. Gaps. A direct application of the string hypothesis is the calculation of the gap distribution $\rho(D)$, i.e., the number of gaps with magnitude between $D$ and $D+dD$. To find the gap distribution we estimate the size of the smallest gap in the spectrum of Harper equation with $\eta = P/Q$. Let us, first, consider an arbitrary gap of a generation with $P$-even and trace the genealogy of lower and upper edges ($\tau = -1$) of the gap along two paths $J_{-}$ and $J_{+}$ of the tree, until we find the nearest common ancestor at the generation with denominator $Q'$. The minimal gap would correspond to the shortest paths $J_{\pm}$, i.e., when $Q'$ is the denominator of the generation which is parent of $P/Q$. The string decompositions of the two edges have a common part consisting of strings of length smaller than $Q'$ (they correspond to the common path from the origin of the tree to the parent generation $Q'$) and different strings with lengths bigger than $Q'$ belonging to the paths $J_{\pm}$. Then according to (2), the width of the gap is the difference between energies of strings with length greater than $Q'$ along the path $J_{-}$ and the energies of strings along $J_{+}$. The energy of a string with a spin $l$ which connects the center of the band ($\tau = +1$) with the edge of the band ($\tau = -1$) is

$$\varepsilon_l = 2i(q - \frac{1}{q}) \sum_{k=-l}^{l} x_l \eta q^k + 4(q^{1/2} + \frac{1}{q^{1/2}}) \sim \frac{1}{Ql}$$ (14)

For a typical $\eta$ the length of the largest string $2l+1$ scales as $Q$ along the sequence of rational approximants, which gives an estimate $\varepsilon_l \sim 1/Q^2$. The difference of energies of strings (i.e., the width of the minimal gap) is of the same order. This gives the size of the minimal gap $D_{\text{min}} \sim 1/Q^2$.

While moving along the tree new gaps appear, while older gaps stay approximately the same. There is no overlap between bands—all gaps are open (except for $\eta$ having even denominators and $E = 0$ where bands touch) [2]. Therefore the full set of gaps in the spectrum for irrational $\eta_{\text{irr}}$ consists of $Q-1$ gaps which has been opened at the period $\eta = P/Q$ plus the smaller gaps which open at rational approximants to $\eta_{\text{irr}}$ with denominators higher than $Q$. One can write

$$\rho(D) dD = \int_{D_{\text{min}}}^{\infty} \rho(D) dD = Q-1 \sim Q.$$ Assuming smooth power law gap distribution $\rho(D) \sim D^{-\gamma}$ one obtains $\gamma = -3/2$ and the gap distribution function: $\rho(D) \sim D^{-3/2}$. This confirms numerical analysis of Ref. [21].

6. Stating the problem: scaling hypothesis. The string hypothesis solves the Bethe Ansatz equations with an accuracy $O(Q^{-2})$ for roots belonging to the largest strings. This gives asymptotically exact results for the “evolution” along the hierarchical tree in the incommensurate limit $Q \to \infty$ (see eq.(11)). However, the most interesting quantitative characteristics of the spectrum are actually in the finite size corrections of the order of $Q^{-2}$ to the bare value of strings. Among them are the anomalous dimensions of the spectrum. Let us choose a branch $J$ of the hierarchical tree and consider energies of the states along the branch $E_j(J)$. The scaling hypothesis states that they converge to a point of the spectrum $E(J)$ such that $Q^{-\gamma} |E_j(J) - E(J)|$ is bounded but does not converge to zero. The numbers $\epsilon_J$ are anomalous exponents. They depend on the branch (signature of multifractality) and on $\eta$ (according to ref. [22] for $\eta = \sqrt{\frac{5}{3}}$). One can write $\epsilon_J$ vary between 0.171 and −0.374. Can anomalous dimensions be found analytically? They are determined by the finite size corrections to the strings which, we believe, can be obtained via a more detailed study of the BA equations. This is a technically involved but a fascinating problem. Its solution may suggest the conformal field theory approach, which has been proven to be effective for finding the finite size corrections of integrable systems, without the actual solving the Bethe Ansatz.

7. We would like to thank J. Bellissard, who suggested that the noninteracting strings determine the gap distribution function and pointed out the Ref. [21], and Y. Hatsugai for inspiring numerics during the initial stages of this project. We acknowledge useful discussions with Y. Avron, G. Huber, S. Jitomirskaya, M. Kohmoto, Y. Last, R. Seiler and A. Zabrodin. AGA was supported by MRSEC NSF Grant DMR 9400379. PBW was supported under NSF Grant DMR 9509533.

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