Bethe ansatz for the Harper equation: Solution for a small commensurability parameter.

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Abstract. The Harper equation describes an electron on a 2D lattice in magnetic field and a particle on a 1D lattice in a periodic potential, in general, incommensurate with the lattice potential. We find the distribution of the roots of Bethe ansatz equations associated with the Harper equation in the limit as \( \alpha = 1/Q \to 0 \), where \( \alpha \) is the commensurability parameter (\( Q \) is integer). Using the knowledge of this distribution we calculate the higher and lower boundaries of the spectrum of the Harper equation for small \( \alpha \). The result is in agreement with the semiclassical argument, which can be used for small \( \alpha \).
1 Introduction

The Harper equation (see [1-5] and also [6,7,8] for recent reviews)

\[ \psi_{n-1} + 2 \cos(2\pi \alpha n + \theta) \psi_n + \psi_{n+1} = \varepsilon \psi_n, \quad n = \ldots, -1, 0, 1, \ldots, \quad \alpha, \theta \in \mathbb{R} \]

in \( l^2(\mathbb{Z}) \) describes a quantum particle on the line in two periodic potentials which are incommensurate if \( \alpha \) is irrational. It is also a model for an electron on a square lattice subject to a perpendicular uniform magnetic field (Azbel-Hofstadter). In the latter case \( \alpha \) is proportional to the value of the magnetic field and \( \theta \) is a quasi-momentum in the direction along one of the sides of the elementary square (see, e.g., [12]). The Harper equation has many deep connections to various fields of modern physics, e.g., quasicrystals, quantum Hall effect, and pure mathematics: number theory, functional analysis.

Equation (1) is the eigenvalue equation for a particular case of the almost Mathieu operator. The spectrum \( \sigma_M(\alpha, \theta) \) of the corresponding operator consists of \( Q \) intervals (bands) if \( \alpha = P/Q \), where \( P \) and \( Q \) are coprime integers.\(^1\) The spectrum \( \sigma_H(\alpha) \) of the Azbel-Hofstadter model is the union over all real \( \theta \) of \( \sigma_M(\alpha, \theta) \). At \( \alpha = P/Q \) the spectrum \( \sigma_H(P/Q) \) consists of \( Q \) bands. If \( \alpha \) is irrational, it is known that \( \sigma_M(\alpha, \theta) \) is independent of \( \theta \), and hence the spectrum \( \sigma_H(\alpha) = \sigma_M(\alpha, \theta) \). The plot of \( \sigma_H(\alpha) \) as a function of \( \alpha \) is the most interesting. There is a conjecture that the measure of the spectrum is zero for all irrational \( \alpha \)\(^2\). This and many other questions regarding the spectrum of the almost Mathieu operator at irrational \( \alpha \) are still unresolved (see [7,12,14] for a list of problems).

Recently a new approach to these problems has been proposed [12,13]. Let \( \alpha = P/Q \). First, it can be shown [12] that certain \( Q \) (one from each band) points of the spectrum\(^3\) are the solutions \( \varepsilon \) of the following eigenvalue equation:

\[ i(z^{-1} + qz)\Psi(qz) - i(z^{-1} + q^{-1}z)\Psi(q^{-1}z) = \varepsilon \Psi(z) \quad (2) \]

in the space of polynomials \( \Psi(z) = \prod_{k=1}^{Q-1} (z - z_k) \) of degree \( Q - 1 \). Here \( q = e^{i\gamma}, \gamma = \pi \alpha = \pi P/Q \). This equation is related to the algebra \( U_q(sl_2) \). One can obtain other difference equations similar to (2) with the same set of eigenvalues. Analogous equations are also available for other points of the spectrum \( \sigma_M(P/Q, \theta) \) [14,15].

\(^1\)That is they do not have a common divisor other than 1.
\(^2\) This is true both for \( \sigma_M(P/Q, \theta) \) and for \( \sigma_H(P/Q) \).
In the Appendix we present a simple derivation of (2) which is based on the fact that it can be regarded as an equation for the generating function of a finite system of orthogonal polynomials related to (1).

Now it is important to note [14] that the following set of relations can be obtained from (2) by substituting \( \Psi(z) = \prod_{k=1}^{Q-1} (z - z_k) \) and setting \( z = z_m, m = 1, \ldots, Q - 1 \):

\[
\frac{z_m^2 + q}{qz_m^2 + 1} = q^Q \prod_{k=1}^{Q-1} \frac{qz_m - z_k}{z_m - qz_k}, \quad m = 1, \ldots, Q - 1.
\]

(3)

Collecting the coefficients at \( z^{Q-1} \) in (2) gives the expression for the energy:

\[
\varepsilon = i q^Q (q - q^{-1}) \sum_{m=1}^{Q-1} z_m.
\]

(4)

Because of the analogy to one-dimensional integrable models, where a similar set of equations is obtained, expressions (3,4) are called Bethe ansatz equations. The Bethe ansatz equations for integrable models are solved in the limit of infinite system. In our case this limit corresponds to \( Q \to \infty \). Thus, we can hope to obtain from (3,4) information about the spectrum at irrational \( \alpha \).

The analysis of (3,4) is only in its beginnings so far. The system (3,4) was investigated numerically (in the case of \( \varepsilon = 0 \) analytically) in [16]. An analytical approach based on the string hypothesis is proposed in [14].

In Section 2 we will obtain a solution (that is the distribution function of the roots \( z_k \)) in the limit as \( \alpha = 1/Q \to 0 \), thus explaining some numerical results of [16]. To obtain this solution, we will consider besides (3) another set of Bethe ansatz equations which follow from (2).

We find the solution under assumption that for \( \alpha = 1/Q \) the roots lie on the unit circle, and their limit distribution function \( \rho(\phi) \) depends piece-wise smoothly on the angle \( \phi \). The function \( \rho(\phi) \) satisfies an integral equation that follows from the Bethe ansatz equations. Besides \( \rho(\phi) \), another important function, \( \chi(\phi) \), naturally arises from the Bethe ansatz equations. It differs from unity only when \( \rho(\phi) = \text{const} = 1/\pi \) and describes in this case the changing with \( \phi \) exponentially small in \( Q \) correction to the constant distance between neighboring roots. Note that a nonconstant \( \rho(\phi) \) implies the increase of order \( 1/Q \) in this distance with \( \phi \).

As usual, \( Q\rho(\phi)d\phi \) is the number of roots in the interval \( d\phi \).
In Section 3, using the expressions for $\rho(\phi)$ and $\chi(\phi)$, we obtain the upper boundary $\varepsilon_{\text{max}}$ of the spectrum of (1) for small $\alpha$. The result is $\varepsilon_{\text{max}} = 4 - 2\pi/Q + o(1/Q)$. The value $2\pi (-2\pi)$ is the tangent of the lower (upper) boundary of the Hofstadter butterfly for small magnetic field. Alternatively, this result can be obtained using semiclassical considerations [17, 18]. Hopefully, the ideas introduced in the present work will be helpful in the cases where semiclassical techniques cannot be applied.

2 Distribution of the roots of the Bethe ansatz equations for $\alpha = 1/Q \to 0$

In order to obtain the results of this work, we will also need another set of Bethe ansatz equations which is derived from (2) by first replacing $z$ with $qz$ and then substituting $z = z_m$, $m = 1, \ldots, Q - 1$. We get

$$\varepsilon = \frac{Q-1}{i(q^{-1}z_m^{-1} + q^2z_m)} \prod_{k=1}^{Q-1} \frac{q^2 z_m - z_k}{q z_m - z_k}, \quad m = 1, \ldots, Q - 1. \quad (5)$$

Henceforth, we will be interested in the simplest case of the Harper equation when $\alpha = 1/Q \ (P = 1, \gamma = \pi/Q)$ and $Q$ is large. Numerical data [16] suggests that if $\alpha = 1/Q$ all the roots $z_k$ lie on the unit circle, they are simple, and their distribution becomes continuous as $Q \to \infty$. Let us therefore assume $z_k = e^{i\phi_k}$, $\phi_k \in \mathbb{R}$, substitute this expression into (3,4,5), and then try to find from these equations a piece-wise smooth distribution function $\rho(\phi)$, $\phi \in [-\pi, \pi]$ in the limit as $Q \to \infty$. After the substitution $z_k = e^{i\phi_k}$, the equations (3,4,5) take the form:

$$\cos(\phi_m - \gamma/2) \cos(\phi_m + \gamma/2) = - \prod_{k=1}^{Q-1} \frac{\sin\frac{1}{2}(\phi_m - \phi_k + \gamma)}{\sin\frac{1}{2}(\phi_m - \phi_k - \gamma)}, \quad (6)$$

$$-\varepsilon = \frac{2}{2 \cos(\phi_m + 3\gamma/2)} \prod_{k=1}^{Q-1} \frac{\sin\frac{1}{2}(\phi_k - \phi_m - 2\gamma)}{\sin\frac{1}{2}(\phi_k - \phi_m - \gamma)}. \quad (7)$$

We set $\phi_{k+1} - \phi_k = \delta_k$. According to our assumption $\delta_k$ is of order $1/Q$ so that $\rho(\phi_k) = 1/Q\delta_k$. Smoothness of the distribution function implies that $\phi_k - \phi_{k+p} = \mp p\delta_k$ for $p = 1, \ldots, N$ up to at most $O(N^2/Q^2)$ in the limit as $N, Q \to \infty$ in such a way that $N/Q \to 0$. Let us consider equations (6) in this
Figure 1: A few consecutive roots $z_k = e^{i\phi_k}$ of the Bethe ansatz equations near the point $k = m$ are shown as they lie with respect to each other for sufficiently large $Q$. The angles $\delta_m$, $\gamma$, $\Delta_{m,1}$ are, of course, increased.

The product is separated into three distinct parts. First, the contribution of the two possible points $\phi_{m+n}$ and $\phi_{m+2n}$ such that $\phi_{m+n} - \phi_m - \gamma = o(1/Q)$ and $\phi_{m+2n} - \phi_m - 2\gamma = o(1/Q)$, where $n$ is a certain integer which is the same in the region of angles $\phi_k$ from $k = m - N$ to $k = m + N$. Define $\Delta_{m,i} = \phi_{m+i} - \phi_m - \gamma$ (See Figure 1). Then $\phi_{m+2n} - \phi_m - 2\gamma = \Delta_{m+n,n} + \Delta_{m,n}$. Note that if to the main order in $1/Q$ the distance $\delta_m \neq \gamma, \gamma/2, \gamma/3, \ldots$, then, whatever $i$, both $\Delta_{m,i} = O(1/Q)$ and $\Delta_{m+i,i} = \Delta_{m,i} + o(1/Q)$. In this case the ratio $\sin \frac{1}{2}(\phi_{m+2n} - \phi_m - 2\gamma)/\sin \frac{1}{2}(\phi_{m+n} - \phi_m - \gamma)$ is always equal to 2 in the limit and, as we shall see, is not necessary to distinguish it as a separate contribution. However, when $\delta_m = \gamma, \gamma/2, \gamma/3, \ldots$ up to $o(1/Q)$, this ratio is an unknown and should be treated separately. Below only the case $\delta_m = \gamma = \pi/Q$ will be relevant because in the solution we obtain, $\delta_m \geq \pi/Q$ for any $\phi_m$.

The second contribution to the product comes from the rest of the points $\phi_{m\pm p}$, where $p = 1, \ldots, N$. All the points not included into these two groups give
the third contribution.

Thus, in the limit $N, Q \to \infty$, $N/Q \to 0$, which we denote just “lim”, we can write (7) as follows (denoting $\phi = \lim \phi_m$, $\phi \in [-\pi, \pi]$):

$$\frac{-\varepsilon}{2 \cos \phi} = \lim ABC.$$  

Here $A$ stands for the contribution of the points with the indices $k = m + n$ and $k = m + 2n$. Expanding the sinus in $1/Q$, we can write:

$$A = \left(1 + \frac{\Delta_{m+n,n}}{\Delta_{m,n}}\right) \frac{n\delta_m - 2\gamma}{2n\delta_m - \gamma} \sin \frac{1}{2} \left(n\delta_m - 2\gamma\right) \sin \frac{1}{2} \left(n\delta_m + \gamma\right) \sim \prod_{p=1 \atop p \neq n, 2n}^N \frac{1 - (2\gamma/p\delta_m)^2}{1 - (\gamma/p\delta_m)^2}.$$  

The factor $B$ denotes the contribution of the points with the indices $k = m$, $k = m - n$, $k = m - 2n$, and also $k = m \pm p$, $p = 1, \ldots, N$, $p \neq n, 2n$:

$$B = 2 \sin \frac{1}{2} \left(n\delta_m + 2\gamma\right) \sin \frac{1}{2} \left(2n\delta_m + 2\gamma\right) \prod_{p=1 \atop p \neq n, 2n}^N \frac{1 - (2\gamma/p\delta_m)^2}{1 - (\gamma/p\delta_m)^2}.$$

Thus

$$AB \sim \left(1 + \frac{\Delta_{m+2n-1}}{\Delta_{m+n-1}}\right) \prod_{p=1 \atop p \neq n, 2n}^N \frac{1 - (2\gamma/p\delta_m)^2}{1 - (\gamma/p\delta_m)^2} \sim \left(1 + \frac{\Delta_{m+2n-1}}{\Delta_{m+n-1}}\right) \prod_{p=1 \atop p \neq n, 2n}^N \frac{1 - (2\gamma/p\delta_m)^2}{1 - (\gamma/p\delta_m)^2}.$$  

where we used the formula $\cos(\pi a/2) = \prod_{k=0}^\infty (1 - a^2/(2k + 1)^2)$. Finally, $C$ in (8) is the contribution of the points with the indices $k$ outside the range $m - N, \ldots, m + N$. We denote the latter restriction by primes at the sums and products:

$$C = \prod_k \sin \frac{1}{2} \left(\phi_m - \phi_k + 2\gamma\right) \sin \frac{1}{2} \left(\phi_m - \phi_k + \gamma\right) \sim \prod_k \frac{1 + \gamma \cot \frac{1}{2} (\phi_m - \phi_k)}{1 + \frac{2}{\gamma} \cot \frac{1}{2} (\phi_m - \phi_k)} \sim \exp \left(\frac{\gamma}{2} \sum_k \cot \frac{1}{2} (\phi_m - \phi_k)\right),$$  

(12)
where the last product was replaced by the exponent of its logarithm. The small-parameter expansion of the logarithm is valid here because in this range of \( k \) the quantity \( \gamma \cot \frac{1}{2}(\phi_m - \phi_k) \) is of order \( 1/N \) or less. Note that because we take the limit \( N, Q \to \infty \) in such a way that \( N/Q \to 0 \), the factor (12) includes the contribution of all roots of the Bethe ansatz equations except for those lying in the infinitesimally small neighborhood of \( z_m = e^{i\phi_m} \). Replacing the sum in (12) by the integral and inserting (11), (12) into (8), we obtain:

\[
-\varepsilon \frac{2}{\cos \phi} = \left( 1 + \lim_{\Delta m,n} \frac{\Delta_{m+n,n}}{\Delta_{m,n}} \right) \cos(\pi^2 \rho(\phi)) \times \exp \left( \frac{\pi V.p.}{2} \int_{-\pi}^{\pi} \cot \frac{1}{2}(\phi - \omega) \rho(\omega) d\omega \right).
\]

(13)

A similar analysis of (6) yields the result:

\[
1 = \lim \left[ \frac{\Delta_{m,n}}{\Delta_{m-n,n}} \right] \exp \left( \pi V.p. \int_{-\pi}^{\pi} \cot \frac{1}{2}(\phi - \omega) \rho(\omega) d\omega \right).
\]

(14)

We see that the function \( \chi(\phi) \equiv \lim(\Delta_{m,n}/\Delta_{m-n,n}) \) is continuous. Hence, we can substitute \( \lim(\Delta_{m+n,n}/\Delta_{m,n}) = \chi(\phi) \), which is expressed from (14), in (13). Thus,

\[
-\varepsilon \frac{4}{\cos \phi} = \cosh \left( \frac{\pi V.p.}{2} \int_{-\pi}^{\pi} \cot \frac{1}{2}(\phi - \omega) \rho(\omega) d\omega \right) \cos(\pi^2 \rho(\phi)).
\]

(15)

Substituting here the energy

\[
\varepsilon = 2\pi \int_{-\pi}^{\pi} e^{i\omega} \rho(\omega) d\omega,
\]

(16)

we obtain an integral equation for the distribution function \( \rho(\phi) \). It is not the only possible form of the integral equation for \( \rho(\phi) \) we can obtain. We can derive others by considering other sets of Bethe ansatz equations which follow from (2) in a similar manner as (3).

Equation (15) reflects the well-known symmetry of the roots \( \{z_m\} \). They lie symmetrically with respect to the real axis. So \( \rho(-\phi) = \rho(\phi) \).

Note that the function \( \rho(\phi) \) must also satisfy the normalization condition

\[
\int_{-\pi}^{\pi} \rho(\phi) d\phi = 1.
\]

(17)

\[\text{We omit the index } n \text{ of } \chi(\phi) \text{ because in the solution we will obtain, it is always } n = 1.\]
Eliminating the exponents from (13) and (14) we get a simple relation between $\chi(\phi)$ and $\rho(\phi)$:

$$-\varepsilon\sqrt{\chi(\phi)} = 2 \cos \phi \cos(\pi^2 \rho(\phi))(1 + \chi(\phi)).$$

(18)

We can guess the form of the solution $\rho(\phi)$ using the following argument. Since $\rho(\phi)$ is even, it follows from (14) that $\chi(0) = \chi(\pi) = 1$. Thus, in some neighborhood of the points $\phi = 0, \pi$ equation (18) simplifies to the form $\varepsilon = -4 \cos \phi \cos(\pi^2 \rho(\phi))$.

This can hold only in the range $|\cos \phi| \geq \varepsilon/4$. Outside of it, $\chi(\phi)$ can no longer be 1, which means that $\rho(\phi)$ can be only a piece-wise constant function there taking some of the values $1/\pi, 2/\pi, ...$ or zero. A precise form of $\rho(\phi)$ is given by the following

**Statement.**

$\rho(\phi) = \frac{1}{\pi} \arccos \frac{\varepsilon}{-4 \cos \phi}$ if $\phi \in [-\psi, \psi] \cup [\pi - \psi, \pi] \cup [-\pi, -\pi + \psi],$

where $\psi = \arccos \frac{\varepsilon}{4}, 0 \leq \arccos(x) \leq \pi; \varepsilon \in [0, 4].$

$\rho(\phi) = 1/\pi$ if $\phi \in [\psi, \pi/2) \cup (\pi/2, -\psi];$

$\rho(\phi) = 0$ if $\phi \in [\pi/2, \pi - \psi] \cup [-\pi + \psi, -\pi/2].$ (See Figure 2)

The same but reflected with respect to the imaginary axis distribution corresponds to the interval $\varepsilon \in [-4, 0].$

Henceforth, we always assume $\varepsilon \in [0, 4].$

We verify the statement substituting this expression for $\rho(\phi)$ in (15), (16), (17) and integrating. For (16) we have:

$$2\pi \int_{-\pi}^{\pi} e^{i\omega} \rho(\omega) d\omega =$$

$$2 \left( \int_{\psi}^{\pi/2} + \int_{-\pi/2}^{-\psi} \right) e^{i\omega} d\omega + \left( \int_{-\psi}^{\psi} + \int_{\pi-\psi}^{\pi+\psi} \right) \frac{1}{\pi} e^{i\omega} \arccos \frac{\varepsilon}{-4 \cos \omega} d\omega =$$

$$4 - \frac{8}{\pi} \int_{0}^{\psi} \cos \omega \arccos \frac{\varepsilon}{4 \cos \omega} d\omega =$$

$$4 - \frac{2\varepsilon}{\pi} \int_{0}^{\nu} \arctan x \frac{x dx}{\sqrt{\nu^2 - x^2}} = 4 - \frac{2\varepsilon \nu}{\pi} \int_{\nu}^{\infty} \frac{\sqrt{u^2 - \nu^2} du}{u(1 + u^2)} = \varepsilon,$$

where $\nu = \sqrt{(4/\varepsilon)^2 - 1}$. Henceforth, we take $\sqrt{x} > 0$ if $x > 0.$

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5 Comparing this with (13) we see that only the points lying in the infinitesimally small neighborhood of $z_m$, whose contribution is described by (11), influence $\rho(\phi_m)$. 

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Figure 2: Distribution of the roots of the Bethe ansatz equations in the limit as $\alpha = 1/Q \to 0$. In the upper figure, the regions on the unit circle are shown where the roots lie with the density $\rho(\phi)$, where $\phi$ is the angle. In the lower figure, $\rho(\phi)$ for some $\varepsilon$ is plotted as a function of the angle.
Figure 3: The contour in the complex plane used to evaluate the integral (20). The thick lines denote cuts. There are two simple poles at the points \( \mu \) and \( -\mu \).

Since \( \rho(\phi) \) is an even function, it is sufficient to verify expression (15) only for \( \phi \in [0, \pi] \). There are three distinct cases: \( \phi \in [0, \psi] \), \( \phi \in [\psi, \pi/2] \), \( \phi \in [\pi - \psi, \pi] \). Most of the relevant integrals are easy to evaluate. Perhaps only the calculation of the following one is somewhat less straightforward:

\[
V.p. \frac{1}{2} \int_{-\psi}^{\psi} \left\{ \cot \frac{1}{2}(\phi - \omega) + \tan \frac{1}{2}(\phi - \omega) \right\} \arccos \frac{\varepsilon}{4 \cos \omega} d\omega = \]

\[
V.p. \int_{-\psi}^{\psi} \arccos \left\{ \frac{\varepsilon}{4 \cos \omega} \right\} \frac{d\omega}{\sin(\phi - \omega)} = 8 \sin \phi \frac{\varepsilon}{\varepsilon} V.p. \int_{0}^{\nu} \frac{x \arctan x}{(x^2 - \mu^2) \sqrt{\nu^2 - x^2}} dx = \]

\[
\frac{\pi}{2} \ln \frac{1 + \sin \phi}{1 - \sin \phi},
\]

where \( \nu = \sqrt{(4/\varepsilon)^2 - 1} \), \( \mu = \sqrt{(4 \cos \phi/\varepsilon)^2 - 1} \), \( \cos \phi > \varepsilon/4 \). The contour used for evaluation of the last integral in (20) is shown in Figure 3.

From (13) we obtain the expression for \( \chi(\phi) \) on the set \( \phi \in [\psi, \pi/2] \cup (-\pi/2, -\psi] \) where \( \rho(\phi) = 1/\pi \) (note that \( \chi(\phi) = 1 \) if \( \phi \in [-\psi, \psi] \cup [\pi - \psi, \pi] \cup \)
Thus, in the region $\phi \in (\psi, \pi/2)$ we have $\Delta_{m-1+k,1} = \chi(\phi)^{(k/Q)} \Delta_{m-1,1}$, $0 < \chi(\phi) < 1$, which means that as $\phi$ increases from $\psi$, the distance between the roots $\phi_m$ approaches the constant value $\pi/Q$ exponentially fast. We shall use the function $\chi(\phi)$ in the next section to determine the finite $Q$ correction to the boundary $\varepsilon = 4$ of the spectrum.

Because of the mentioned symmetry of the Bethe ansatz equations, it is sufficient to write the expressions for $\chi(\phi)$ only for $\phi \in [0, \pi]$. This symmetry implies $\chi(-\phi) = \chi(\phi)^{-1}$.

## 3 The boundaries of the spectrum of the Harper equation for small $\alpha$.

Consider now the simplest case $\varepsilon = 4$ in more detail. In this case $\rho(\phi) = 1/\pi$ if $\phi \in (-\pi/2, \pi/2)$ and zero otherwise. Equation (21) takes the form

$$
\chi(\phi) = \frac{1 - \sin \phi}{1 + \sin \phi}, \quad \phi \in [0, \pi/2].
$$

We shall calculate the largest finite $Q$ correction to the energy $\varepsilon = 4$. It turns out that the shift (from the uniform distribution defined below) of the roots of the Bethe ansatz equations described by (22) is responsible for this correction. Since according to (22), $\Delta_{m,1}$ decreases exponentially as $\phi_m$ moves away from the point $\phi = 0$, only an infinitesimally small neighborhood of $\phi = 0$ gives considerable contribution to the shift. Let us assume the following distribution of the roots $\phi_0 = 0, \phi_m = m\pi/Q + \sum_{i=0}^{m-1} \Delta_{i,1}$, $m = 1, \ldots, Q/2-1, \phi_{-m} = -\phi_m$ (we set $Q$ even for definiteness). The mentioned property of $\Delta_{i,1}$ implies that if $\phi_m \to \phi \neq 1$ as $Q \to \infty$, then with an exponential accuracy $\phi_m = m\pi/Q + (m/|m|)s/Q^\delta$, where $s/Q^\delta = \sum_{i=0}^{\infty} \Delta_{i,1}$. The quantities $s$ and $\delta$ are to be found from the Bethe ansatz equations. Henceforth, we assume $m > 0$. Further, set

$$
\frac{\sin(\Delta_{m,1}/2)}{\sin(\Delta_{m-1,1}/2)} = \chi \left( \frac{\pi m}{Q} \right) \left\{ 1 + \frac{r_m}{Q^\delta} + o \left( \frac{1}{Q^\delta} \right) \right\}.
$$

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Retaining now in equations (6) not only the largest in 1/Q quantities (of order 1) as before, but also the next largest (that is of the order of 1/Q, 1/Q^β, 1/Q^δ), we obtain with this accuracy the following expression for the logarithm of (6)

\[
\frac{\pi}{Q} \tan \frac{\pi m}{Q} = \ln \chi \left(\frac{\pi m}{Q}\right) + \frac{r_m}{Q^\beta} - 2s \left\{ \frac{\pi}{2Q} \sum_{k=-(Q/2-1)}^{0} \sin^{-2} \frac{\pi (m-k)}{2Q} \right\} + \frac{\pi}{Q} \sum_k \cot \frac{\pi (m-k)}{2Q}.
\]

(24)

Replacing the first sum over \(k\) in (24) by the integral gives

\[
\frac{\pi}{2Q} \sum_{k=-(Q/2-1)}^{0} \sin^{-2} \frac{\pi (m-k)}{2Q} \sim \int_{-\pi/2}^{0} \sin^{-2} \frac{\pi m - x}{2} \frac{dx}{2} = \frac{2}{1 - \cos \frac{\pi m}{Q} + \sin \frac{\pi m}{Q}}.
\]

(25)

As to the second sum over \(k\) in (24), we need to evaluate it up to 1/Q. Using the Poisson summation formula, we have

\[
\frac{\pi}{Q} \sum_k \cot \frac{\pi (m-k)}{2Q} = \frac{\pi}{Q} \sum_{k=-(Q/2-1)}^{0} \cot \frac{\pi (m-k)}{2Q} =
\]

\[
\frac{\pi}{Q} \int_{-\frac{\pi}{2}+\frac{\pi m}{Q}}^{\frac{\pi}{2}+\frac{\pi m}{Q}} \cot \frac{\pi m}{Q} - x \frac{2}{\cos(2Qkx)} \cot \frac{\pi m}{Q} - x \frac{2}{2} \cos(2Qkx) dx =
\]

\[
\ln \frac{1 + \sin \frac{\pi m}{Q}}{1 - \sin \frac{\pi m}{Q}} + \frac{\pi}{Q} \tan \frac{\pi m}{Q} + O(1/Q^2).
\]

(26)

Here the value of the last sum over \(k\) is estimated by integration by parts. It is of order 1/Q^2. Thus, (24) reduces to

\[
\frac{r_m}{Q^\beta} - \frac{4s}{Q^\delta} = 0.
\]

(27)

A similar analysis of (7) gives the result

\[
-\frac{\pi}{2Q \cos \frac{\pi m}{Q}} = \frac{s}{Q^\delta} \left( 1 - \tan \frac{\pi m}{Q} + \frac{2}{1 - \cos \frac{\pi m}{Q} + \sin \frac{\pi m}{Q}} \right) + \frac{r_m \cos^2 \frac{\pi m}{Q}}{2Q^\delta (1 + \sin \frac{\pi m}{Q})}.
\]

(28)
From (27,28) we get $\delta = \beta = 1, s = \pi/2$. The equation for the energy reads $\varepsilon = 4(1 - s/Q) + o(1/Q) = 4 - 2\pi/Q + o(1/Q)$. (Correspondingly, the lower boundary of the spectrum is $\varepsilon = -4 + 2\pi/Q + o(1/Q)$.) The same correction $2\pi/Q$ can be obtained from semiclassical considerations [18].

4 Conclusions

In this work we have studied the distribution of the roots $z_k$ of the Bethe ansatz equations for the Harper equation in the limit as $Q \to \infty$ while the commensurability parameter $\alpha = P/Q$, $P = 1$. We considered two related sets of the Bethe ansatz equations to the main order as $1/Q \to 0$ and obtained functions $\rho(\phi)$ and $\chi(\phi)$ that characterize the distribution. It is a continuous distribution of the roots on the unit circle.

Considering the Bethe ansatz equations to the next (smaller) order in $1/Q$ we calculated the small $\alpha$ correction to the upper and lower boundaries of the spectrum of the Harper equation.

One more step further could be to extend our treatment to the case of any fixed $P$, while $Q \to \infty$. Numerical data suggests that in this case the roots $z_k$ for the largest eigenvalue $\varepsilon_{\max}$ become continuously distributed on $P$ smooth curves.

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6 Appendix

Here we derive the $q$-difference equation (3).

Assume $\alpha = P/Q$ with coprime integers $P, Q$. Then (1) is the eigenvalue equation for a periodic tridiagonal matrix (denote this matrix $M$) with the period $Q$ (that is the matrix elements $M_{ik} = M_{i+Q,k+Q}$). The approach to the spectral problem for such a matrix is well known [e.g., 19]. We look for solutions to (1) in the form $\psi_{j+Qk} = e^{i\omega k}\mu_j, j = 0, 1, \ldots, Q-1$, where $\omega$ is an arbitrary real number.
This reduces (2) to the following eigenvalue equation
\[
\mu_{n-1} + (q^{2n} e^{i\theta} + q^{-2n} e^{-i\theta}) \mu_n + \mu_{n+1} = \varepsilon \mu_n, \\
n = 0, 1, \ldots, Q - 1; \quad q = e^{i\pi\alpha}; \quad \mu_0 = e^{i\omega} \mu_0, \quad \mu_Q = e^{i\omega} \mu_0.
\] (29)
for a \(Q \times Q\) matrix (denote it \(L\)). It is easy to show that \(\det(L - \varepsilon I) = (-1)^Q(S_Q(\varepsilon; \alpha, \theta) - 2 \cos \omega)\), where \(S_Q(\varepsilon; \alpha, \theta)\) is a polynomial of degree \(Q\) in \(\varepsilon\), which is called the discriminant of \(M\). The spectrum of \(M\) is obviously given by the equation \(S_Q(\varepsilon; \alpha, \theta) = 2 \cos \omega, \omega \in [0, \pi]\). As is known, the spectrum consists of exactly \(Q\) intervals, the image of \([-2, 2]\) under the inverse of the transform \(S_Q(\varepsilon; \alpha, \theta) = \lambda\) (see Figure 1). Hence, all the extremal points of \(S_Q(\varepsilon; \alpha, \theta)\) are maxima and minima; moreover, at all maxima points \(S_Q(x_{\text{max}}; \alpha, \theta) \geq 2\) and at all minima points \(S_Q(x_{\text{min}}; \alpha, \theta) \leq -2\).

As we mentioned in the introduction, the spectrum \(\sigma_H(\alpha)\) of the Azbel-Hofstadter problem is the union over all real \(\theta\) of the spectra of \(M\). The Chambers formula [20] says that the polynomial \(\Sigma_Q(\varepsilon; \alpha) = S_Q(\varepsilon; \alpha, \theta) + 2 \cos \theta Q\) does not depend on \(\theta\), which implies that \(\sigma_H(\alpha)\) is the image of \([-4, 4]\) under the inverse of the transform \(\Sigma_Q(\varepsilon; \alpha) = \lambda\). Considering the Chambers formula at \(\theta = 0\) and \(\theta = \pi/Q\), we see that \(\Sigma_Q(x_{\text{max}}; \alpha) \geq 4\) and \(\Sigma_Q(x_{\text{min}}; \alpha) \leq -4\) at all its extremal points. So that \(\sigma_H(\alpha)\) also consists of \(Q\) intervals (see Figure 1).

Let us now turn to the derivation of (2). Set \(\omega = 0\). Substituting \(\mu_n = \sum_{k=0}^{Q-1} U_{nk} e^{i\theta k} \phi_k\), where \(U_{nk} = q^{2nk}\), \(n, k = 0, 1, \ldots, Q - 1\) in (29), we have
\[
\phi_{k-1} + (q^{2k} + q^{-2k}) \phi_k + \phi_{k+1} = \varepsilon \phi_k, \\
k = 0, 1, \ldots, Q - 1; \quad \phi_{-1} = e^{iQ\theta} \phi_{Q-1}; \quad \phi_Q = e^{-iQ\theta} \phi_0.
\] (30)

By the nondegenerate transformation
\[
\phi_k = \sum_{n=0}^{Q-1} q^{(k+1/2)^2+2kn} \zeta_n
\] (31)
we get rid of the middle term in (30):
\[
(1 + q^{2n}) \zeta_{n-1} + (1 + q^{-2(n+1)}) \zeta_{n+1} = \varepsilon \zeta_n, \\
n = 0, 1, \ldots, Q - 1; \quad \zeta_{-1} = \zeta_{Q-1}; \quad \zeta_Q = \zeta_0.
\] (32)

One can prove this by showing that \(S_Q(M; \alpha, \theta) = E\), where the matrix elements of \(E\) are \(E_{ij} = 1\) if \(|i - j| = Q\) and zero otherwise. The spectrum of \(E\) is obviously \(2Q\)-degenerate, while the spectrum of the tridiagonal matrix \(M\) can be at most doubly degenerate.

The matrix \(U\) is nondegenerate. \(\det U \neq 0\) because \(UU^* = QI\).
Figure 4: The plot of $S_Q(\varepsilon; \alpha, \theta)$ and $\Sigma_Q(\varepsilon; \alpha)$ for $Q = 4$ and some fixed $\theta$. (For $Q = 4$ the curves do not depend on $P$: $P = 1$ or $P = 3$.) The thickest lines on the axis $\varepsilon$ are the intervals of the spectrum $\sigma_M(\alpha, \theta)$ of $M$. The less thick lines are the intervals of the spectrum $\sigma_H(\alpha)$. Two of the latter intervals touch at $\varepsilon = 0$. The curves shown are not the actual ones but qualitatively similar.
In order to obtain (32) we had to assume the following condition: for $Q$ even $Q\theta = \pi (\text{mod } 2\pi)$; for $Q$ odd $Q\theta = 0 (\text{mod } 2\pi)$. If $Q$ is even, we can make the shift $\zeta_{n+Q/2} = \zeta_n$, so that we get the equations

$$
(1 - q^{2n})\zeta_{n-1} + (1 - q^{-2(n+1)})\zeta_{n+1} = \varepsilon \zeta_n,
$$

$$
n = 0, 1, \ldots, Q - 1
$$

with zero boundary conditions ($\xi_{-1}$ and $\xi_Q$ may be arbitrary, e.g., zero). Further transformation $\xi_n = p_n i^n q^{n(n+1)/2}$ gives

$$
i(q^n - q^{-n})p_{n-1} + i(q^{n+1} - q^{-(n+1)})p_{n+1} = \varepsilon p_n,
$$

$$
n = 0, 1, \ldots, Q - 1.
$$

(34)

Now multiplying (34) by $z^n$ and then taking the sum over $n$ from $n = 0$ to $Q - 1$, we get

$$
i(z^{-1} + qz)\Psi(qz) - i(z^{-1} + q^{-1}z)\Psi(q^{-1}z) = \varepsilon \Psi(z),
$$

(35)

which is equation (2). Here $\Psi(z) = \sum_{n=0}^{Q-1} z^n p_n$. We derived (33) on condition that $\omega = 0$, $Q\theta = \pi (\text{mod } 2\pi)$, and $Q$ is even (hence, $P$ is odd). It is easy to derive the same equation (33) for the two other possible cases (that is $P$ even, $Q$ odd, and $P$ odd, $Q$ odd) using slightly different from (31) transformations. In all cases we have the same restriction $\omega = 0$, $Q\theta = \pi (\text{mod } 2\pi)$. This implies that the solutions $\varepsilon$ of (2) are the points satisfying $\Sigma_Q(\varepsilon; \alpha) = 0$, so they lie inside the bands of the spectrum $\sigma_H(\alpha)$ of the Azbel-Hofstadter problem. As follows from the Chambers formula, they also lie in the bands of $\sigma_M(\alpha, \theta)$ for any $\theta$. Take any band of $\sigma_M(\alpha, \theta)$. It has a single point in it which is a solution of (2). As $\theta$ changes from $\theta = 0$ to $\theta = \pi/Q$ the band moves through this point from one boundary where $S_Q(\varepsilon; \alpha, 0) = -2$ to the other where $S_Q(\varepsilon; \alpha, \pi/Q) = 2$.

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