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VLADIMIR BUSLAEV

ALEXANDER FEDOTOV

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# Spectral properties of the monodromy matrix for Harper equation

V.Buslaev, A.Fedotov\*

Departement of mathematical physics, St.Petersburg State University  
1, Uljanovskaja, St.Petersburg-Petrodvorets, 198904, Russia  
e-mail: buslaev@snoopy.niif.spb.su, fedotov@snoopy.niif.spb.su

## 1. Introduction

Harper equation is the following difference equation with a periodic coefficient:

$$\frac{1}{2}(\psi(x+h) + \psi(x-h)) + \cos x \psi(x) = E \psi(x), \quad (1.1)$$

where  $x \in \mathbb{R}$ ,  $\psi(x) \in \mathbb{C}$ ,  $h$  is fixed,  $0 < h < 2\pi$ ,  $E$  is the spectral parameter,  $E \in \mathbb{C}$ .

One encounters Harper equation in a series of problems of the solid state physics, in particular, it is a popular model for two-dimensional Bloch electrons in a weak magnetic field [H]. This equation is known also in the theory of operator algebras.

The spectrum of equation (1.1) in  $L_2(\mathbb{R})$  is rather complicated, see, for example, [BS], and it depends on the number theoretical properties of  $h/2\pi$ .

Our final aim is to give a detailed description of the geometry of the spectrum of Harper equation. However, the aim of this text is to describe properties of the solutions of (1.1) being entire analytic functions of  $x$ . These two problems are tightly related in view of the monodromization procedure, see [BF4, BF6], only briefly discussed here. The monodromization procedure forms a base for a systematic approach to the spectral theory of difference equations with periodic coefficients. It has many common points with the renormalization method suggested by B.Helffer and J.Sjöstrand [HS], but is independent of any semiclassical hypothesis on the number  $h$ . In our first works, the monodromization method was also developed under some semiclassical hypothesis [BF1, BF2, BF3, BF4]. Here we continue the work begun in [BF6] and complete the description of analytic properties of entire solutions of Harper equation without assuming that the parameter  $h$  is small.

The subject of the paper is in a certain sense very close to the subject of the classical analytic theory of differential equations.

The structure of the text is the following. Section 2 is devoted to the study of canonical solutions defined in a vicinity of the singular point of the equation

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\* The address up to the september 1996: Dept. de Mathématique, Faculté des Sciences et Technologie, Université Paris-XII Val de Marne

( $z = \infty$ ). There we construct also entire solutions, minimal in a certain sense, and introduce the main objects of the theory: the coefficients characterizing the asymptotic behaviour of minimal solutions in the vicinity of the singular point.

In Section 3, we construct of two minimal solutions a natural basis in the space of the entire solutions of (1.1). The choice of this two solutions reflects the symmetries of the equation. We introduce the monodromy matrix corresponding to this basis. Its elements are explicitly expressed in terms of the above coefficients characterizing the minimal solutions. Furthermore, we show that, in the case where  $h/2\pi$  is a Diophantine number, knowing these coefficients, one can reconstruct the minimal solution itself.

In section 4, we relate to the symbol of the operator corresponding to (1.1) two other operators  $H_0$  and  $H_1$  generated by this symbol on the lines  $i\mathbb{R}$  and  $\pi + i\mathbb{R}$ . These operators have simple discrete spectra  $\sigma_0$  and  $\sigma_1$ . The above asymptotic coefficients are explicitly described in terms of these two spectra. The proof of the corresponding representations is essentially based on the analysis of the behavior of these coefficients as  $E \rightarrow \infty$ .

The spectra  $\sigma_0$  and  $\sigma_1$  are not independent. The relations between these two spectra are discussed in Section 5. These relations lead to some analytic properties of the trace of the monodromy matrix. We discuss them in the end of the section. Note that, in the case where  $h$  is small, the trace of the monodromy matrix plays almost the same part in the spectral theory of (1.1) as the Lyapounov function does for the differential equations with periodic coefficients.

## 2. Minimal solutions

In this section, we reproduce results of [BF6] in a slightly modified form.

### Space of analytic solutions.

Fix  $\alpha, \beta \in \mathbb{R}$ ,  $\alpha < \beta$ . Let  $S$  be the strip

$$S = \{z = x + iy \in \mathbb{C} : \alpha < y < \beta\}$$

and let  $\mathbb{M}_S$  be the set of the solutions of (1.1) analytic in this strip. Denote the ring of all  $h$ -periodic functions analytic in  $S$  by  $\mathbb{K}_S$ .

In the case of  $S = \mathbb{C}$ , we use the simplified notations:  $\mathbb{M} = \mathbb{M}_{\mathbb{C}}$  and  $\mathbb{K} = \mathbb{K}_{\mathbb{C}}$ .

The set  $\mathbb{M}_S$  is a two dimensional module over the ring  $\mathbb{K}_S$ . This means that there exists a basis of two solutions,  $\psi_1, \psi_2 \in \mathbb{M}_S$ , linearly independent over the ring  $\mathbb{K}_S$ . In other words, any solution  $\psi \in \mathbb{M}_S$  can be uniquely represented in the form

$$\psi = a\psi_1 + b\psi_2, \quad a, b \in \mathbb{K}_S.$$

For any two solutions  $\psi_1, \psi_2 \in \mathbb{M}_S$  the wronskian

$$\{\psi_1(z), \psi_2(z)\} = \psi_1(z)\psi_2(z-h) - \psi_1(z-h)\psi_2(z)$$

is an element of  $\mathbb{K}_S$ . The solutions  $\psi_1, \psi_2$  form a basis if  $\{\psi_1(z), \psi_2(z)\} \neq 0$ ,  $z \in S$ . The proof of the existence of such basis for  $S = \mathbb{C}$  (and thus, for any  $S$ ) was obtained in [BF1] for sufficiently small  $h$ , and in [BF6] for any  $h$ ,  $0 < h < 2\pi$ .

## Bloch solution $f$ .

To discuss the behavior of analytic solutions of (1.1) as  $z \rightarrow \pm i\infty$ , it is natural to change the variable  $z \mapsto \zeta$ ,  $\zeta = e^{iz}$ . This transforms the original equation to an equation with a rational coefficient having simple poles at  $\zeta = 0$  and  $\zeta = \infty$ . Thus, one can speak about Harper equation itself as about an equation with two singular "points"  $y = +\infty$  and  $y = -\infty$ . Here we are going to describe the simplest solutions living in certain vicinities of these points.

As  $y \rightarrow +\infty$ , Harper equation has the formal solution

$$f_D(z, E) = e^{\frac{i}{2h}(z-\pi)^2} e^{\frac{i}{2}z} \sum_{n \geq 0} f_n(E) e^{inz}, \quad f_0 = 1. \quad (2.1)$$

If  $h/2\pi$  is a Diophantine number, the series in (2.1) converges in the strip  $S_+ = \{z : y > \alpha > 0\}$ , where  $\alpha$  is a number depending on  $E$  and  $h$ , and gives a solution of (1.1) belonging to  $\mathbb{M}_{S_+}$ . This solution possesses the property

$$f_D(z + 2\pi, E) = -e^{i\frac{2\pi}{h}z} f_D(z, E) \quad (2.2)$$

which allows to call it a *Bloch solution*. The proof of the existence of this Bloch solution can be obtained by means of the techniques of [BF5].

For arbitrary  $h/2\pi$ , the series (2.1) does not converge and there is no natural way to fix a unique solution possessing a canonical behavior as  $y \rightarrow +\infty$ . Nevertheless, one can construct a solution  $f$  continuous in  $h$ , analytic in  $z$ ,  $f \in \mathbb{M}_{S_+}$ , and having the asymptotic representation:

$$f(z, E) = e^{\frac{i}{2h}(z-\pi)^2} e^{\frac{i}{2}z} (1 + o(e^{-y})), \quad y \rightarrow \infty, \quad (2.3)$$

For this solution the relation (2.2) is replaced by

$$f(z + 2\pi, E) = s(z, E) f(z, E), \quad (2.4)$$

where  $s$  is an  $h$ -periodic function,

$$s(z + h, E) = s(z, E), \quad (2.5)$$

having the property:

$$s(z, E) = -e^{i\frac{2\pi}{h}z} (1 + o(e^{-y})), \quad z \rightarrow +i\infty. \quad (2.6)$$

Note that the solution  $f$  is not uniquely defined. The methods of proof can be also borrowed from [BF5].

**Canonical basis.**

Introduce the following basis in  $\mathbb{M}_{S_+}$ :

$$f_1(z, E) = f(z, E), \quad f_2(z, E) = e^{2\pi iz/h} \overline{f(-\bar{z}, \bar{E})},$$

where the bar denotes the complex conjugation. One can easily see that

$$\{f_1, f_2\} = 1 + O(e^{-y}), \quad y \rightarrow +\infty.$$

On the strip  $S_- = \overline{S_+} = -S_+$ , we shall consider the basis

$$g_1(z, E) = -f_1(2\pi - z, E), \quad g_2(z, E) = -f_2(2\pi - z, E).$$

**Minimal solution.**

Let  $\psi \in \mathbb{M}$ . Then one can write

$$\psi = A f_1 + B f_2, \quad A, B \in \mathbb{K}_{S_+}, \quad (2.7)$$

and

$$\psi = C g_1 + D g_2, \quad C, D \in \mathbb{K}_{S_-}.$$

**Theorem 2.1.** Let  $0 < h < 2\pi$ . Equation (1.1) possesses a solution  $\psi \in \mathbb{M}$ , such that the coefficients  $A$  and  $B$  from the corresponding representation (2.7) are bounded as  $y \rightarrow +\infty$ , the coefficients  $C$  and  $D$  are bounded as  $y \rightarrow -\infty$ , and

$$D(z) \rightarrow 0, \quad y \rightarrow -\infty.$$

This solution is unique up to a constant factor.

This theorem is proved in [BF6]<sup>1</sup>. The solution described in the theorem is called *minimal*.

The coefficients  $A$ ,  $B$ ,  $C$  and  $D$  can be represented in the form

$$A(z) = \sum_{n \geq 0} A_n(E) \zeta^n, \quad B(z) = \sum_{n \geq 0} B_n(E) \zeta^n,$$

$$C(z) = \sum_{n \geq 0} A_n(E) \zeta^{-n}, \quad D(z) = \zeta^{-1} \sum_{n \geq 0} A_n(E) \zeta^{-n},$$

where  $\zeta = e^{2\pi iz/h}$ . The series for  $A$  and  $B$  converge in  $\mathbb{K}_{S_+}$ , the series for  $C$  and  $D$  converge in  $\mathbb{K}_{S_-}$ . In the sequel, we are mostly interested in the coefficients  $A_0$ ,  $B_0$ ,  $C_0$  and  $D_0$ , and, in particular, in their dependence on  $E$ . The results we are going to discuss are proved in [BF6] and in [BF7].

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<sup>1</sup>For the case where the number  $h$  was sufficiently small, this theorem has been proved in [BF3].

### 3. Monodromy matrix

#### Basis of the module $\mathbb{M}$ .

Consider two solutions of (1.1):

$$\psi_1(z, E) = \psi(z, E), \quad \psi_2(z, E) = \psi(2\pi - z, E).$$

One can calculate their wronskian in terms of the coefficients  $B_0$  and  $C_0$ , see [BF6],

$$\{\psi_1, \psi_2\} = B_0 C_0.$$

Thus, for all  $E$  such that  $B_0 C_0 \neq 0$  the solutions  $\psi_1$  and  $\psi_2$  form a basis in  $\mathbb{M}$ . Note that since the product  $B_0 C_0$  is entire in  $E$  and is not identically zero, the set of its zeros is discrete. We describe this set later.

#### Monodromy matrix.

Together with  $\psi_1$  and  $\psi_2$  consider the functions  $\psi_1(z+2\pi, E)$  and  $\psi_2(z+2\pi, E)$ . They also form a basis in  $\mathbb{M}$ , and so one can write

$$\begin{pmatrix} \psi_1(z+2\pi, E) \\ \psi_2(z+2\pi, E) \end{pmatrix} = \mathcal{M}(z, E) \begin{pmatrix} \psi_1(z, E) \\ \psi_2(z, E) \end{pmatrix},$$

where  $\mathcal{M}$  is a matrix with coefficients belonging to the ring  $\mathbb{K}$ .

In [BF1] for sufficiently small  $h$ , and in [BF6] for all  $h$  such that  $0 < h < 2\pi$  one has proved that the monodromy matrix has the following structure:

$$\mathcal{M}(z, E) = \begin{pmatrix} a(E) - 2 \cos(2\pi z/h) & s(E) + it(E) e^{-2\pi iz/h} \\ -s(E) - it(E) e^{2\pi iz/h} & d(E) \end{pmatrix},$$

where

$$d = ist, \quad ad = 1 - s^2 + t^2.$$

So,  $t$  and  $s$  can be considered as the only independent parameters of the monodromy matrix.

The functions  $s(E)$  and  $t(E)$  can be expressed in terms of the coefficients  $A_0$ ,  $B_0$ ,  $C_0$  and  $D_0$  of the minimal solution:

$$t = i \frac{A_0}{C_0}, \quad s = -\frac{D_0}{B_0}. \quad (3.1)$$

Let

$$\mathcal{E}(E) = \frac{a(E) + d(E)}{2} = \frac{1}{2i} \left( \frac{1}{s(E)} - s(E) \right) \left( \frac{1}{t(E)} + t(E) \right)$$

The role of this function in the spectral theory of (1.1) is as important as one of the Lyapounov function for the differential equations with periodic coefficients, see [BF4].

## Reconstruction of the minimal solution.

The coefficients  $A, B, C, D$  and the monodromy matrix  $\mathcal{M}$  are connected by the relation

$$\mathcal{M}(z, E) \Gamma(z, E) = -\Gamma(z + 2\pi, E) T(z, E), \quad (3.2)$$

where

$$\Gamma(z, E) = \begin{pmatrix} A(z, E) & B(z, E) \\ -C(2\pi - z, E) & -D(2\pi - z, E) \end{pmatrix},$$

$$T(z, E) = \begin{pmatrix} s(z, E) & 0 \\ 0 & s^{-1}(z, E) \end{pmatrix},$$

and  $s(z, E)$  is the coefficient characterizing the Bloch property of the solution  $f$ , see (2.4).

As we have remarked, if  $h/2\pi$  is a Diophantine number, then, instead of the solution  $f$ , one can construct the Bloch solution for which

$$s(z, E) = \exp\left(i \frac{2\pi}{h} z\right).$$

In this case the relation (3.2) allows to reconstruct explicitly the Fourier series for  $\Gamma$  (i.e. the Fourier series for  $A, B, C$  and  $D$ ) in terms of  $A_0, B_0, C_0$  and  $D_0$ . In result, knowing  $A_0, B_0, C_0$  and  $D_0$ , one can reconstruct the minimal solution  $\psi$ .

## 4. Analytic properties of the coefficients $A_0, B_0, C_0$ and $D_0$

### Operator $H_0$ .

The analytic properties of the coefficients  $A_0, B_0, C_0$  and  $D_0$ , and, therefore, the analytic properties of the functions  $s(E)$  and  $t(E)$  can be described in terms of the spectra of two operators  $H_0$  and  $H_1$  generated by the same symbol as Harper equation,

$$\cos p + \cos z,$$

but on the lines  $i\mathbb{R}$  and  $\pi + i\mathbb{R}$ .

The selfadjoint operator  $H_0$  is defined by the expression

$$H_0 = \text{ch } \hat{p} + \text{ch } y, \quad \hat{p} = \frac{h}{i} \frac{d}{dy},$$

on the natural domain in  $L_2(\mathbb{R})$ . Note the functions from this domain are analytic in the strip  $|\text{Im } y| < h$ . The operator  $H_0$  has simple discrete spectrum  $\sigma_0 = \{t_n\}_{n=1}^{\infty}$ ,

$$2 < t_1 < \dots < t_n < \dots, \quad t_n \rightarrow +\infty, \quad n \rightarrow \infty.$$

## Operator $H_1$ .

Let

$$H_1 = \text{ch } \hat{p} - \text{ch } y, \quad \hat{p} = \frac{h}{i} \frac{d}{dy}.$$

We say  $E$  is a point of the spectrum of the operator  $H_1$  if there is a solution of the equation  $H_1\phi = E\phi$  analytic in the strip  $|\text{Im } y| \leq h$  and having the asymptotics:

$$\phi(y) \sim \phi_{\pm} e^{\mp y/2} e^{-iy^2/(2h)}, \quad y \rightarrow \pm\infty.$$

The spectrum  $\sigma_1$  of the operator  $H_1$  consists of points  $\{is_n\}_{n=1}^{\infty}$  lying on the imaginary axis,

$$0 < s_1 < \dots < s_n < \dots, \quad s_n \rightarrow \infty, \quad n \rightarrow \infty.$$

Note that  $\sigma_1$  can also be described as the spectrum of a compact operator.

## Infinite products.

The properties of the functions  $A_0$ ,  $B_0$ ,  $C_0$  and  $D_0$  depend on the normalization of the minimal solution (which is defined only up to an independent of  $z$  factor). The coefficients of the monodromy matrix  $s$  and  $t$  are independent of the normalization of the minimal solution  $\psi$ . One has

**Theorem 4.1.** The minimal solution  $\psi$  can be normalized so that the coefficients  $A_0$ ,  $B_0$ ,  $C_0$  and  $D_0$  could be represented by the infinite products

$$A_0(E) = -i \prod_{n \geq 1} (1 - E/t_n), \quad (4.1)$$

$$B_0(E) = -\sqrt{2} e^{i\pi/4 - ih/8} \prod_{n \geq 1} (1 + iE/s_n), \quad (4.2)$$

$$C_0(E) = \prod_{n \geq 1} (1 + E/t_n), \quad (4.3)$$

$$D_0(E) = \sqrt{2} e^{\pi^2 i/h - i\pi/4 - ih/8} \prod_{n \geq 1} (1 - iE/s_n) \quad (4.4)$$

which converge uniformly in  $E \in \mathbb{C}$ .

Note that to prove this theorem, one has to investigate the behavior of the minimal solutions as  $E \rightarrow \infty$ . This is done in [BF7].

Theorem 4.1 and formulae (3.1) imply that

$$t(E) = \prod_{n \geq 1} \frac{1 - E/t_n}{1 + E/t_n}, \quad (4.5)$$



$$s(E) = -i e^{i\pi^2/h} \prod_{n \geq 1} \frac{1 - iE/s_n}{1 + iE/s_n}. \quad (4.6)$$

### Symmetries of Harper equation.

Note that the representations (4.1) – (4.4) lead to the formulae

$$\overline{A_0(\overline{E})} = -A_0(E), \quad (4.7)$$

$$A_0(-E) = -i C_0(E), \quad (4.8)$$

$$\overline{B_0(\overline{E})} = -e^{ih/4 - \pi^2 i/h} D_0(E), \quad (4.9)$$

$$B_0(-E) = -i e^{-i\pi^2/h} D_0(E). \quad (4.10)$$

These formulae, being an immediate consequence of theorem 4.1, reflect the the main symmetries of Harper equation: the invariance with respect to the complex conjugation,  $\psi(z, E) \rightarrow \psi(\overline{z}, \overline{E})$ , the invariance wrt the reflections  $\psi(z, E) \rightarrow \psi(-z, E)$  and  $\psi(z, E) \rightarrow \psi(2\pi - z, E)$ , the invariance wrt the Fourier transform, and the invariance wrt the transformation  $\psi(z, E) \rightarrow e^{\pi iz/h} \psi(\pi - z, E)$ . Formulae of the type (4.7) – (4.10) can be obtained directly, without representations (4.1) – (4.4), and moreover, in fact, such formulae were used to prove the theorem 4.1. The full list of the formulae following from the invariance properties of Harper equation includes also

$$B_0(E) \overline{B_0(\overline{E})} = C_0^2(E) - A_0^2(E), \quad E \in \mathbb{R},$$

which follows from the invariance with respect to the complex conjugation. In fact, this formula is an explicit relation between the spectra  $\sigma_0$  and  $\sigma_1$ :

$$\prod_{n \geq 1}^2 (1 - E/t_n) + \prod_{n \geq 1}^2 (1 + E/t_n) = 2 \prod_{n \geq 1} (1 + iE/s_n) \prod_{n \geq 1} (1 - iE/s_n). \quad (4.11)$$

We shall discuss it in the next section.

Representations (4.5) – (4.6) lead to the formulae

$$s(-E) = -\frac{e^{2i\pi^2/h}}{s(E)}, \quad t(-E) = \frac{1}{t(E)} \quad (4.12)$$

and

$$t(0) = 1, \quad s(0) = -i e^{i\pi^2/h}, \quad (4.13)$$

and to the relations

$$t(E) \in \mathbb{R}, \quad |s(E)| = 1, \quad E \in \mathbb{R}. \quad (4.14)$$

The last ones imply that  $\mathcal{E}(E) \in \mathbb{R}$  if  $E \in \mathbb{R}$ . This is the property of the monodromy matrix which was very important for the spectral analysis of Harper equation in the case of small  $h$ , see [BF4]. In that paper, we have found that

the spectrum of Harper equation can be considered as the Julia set of a certain dynamical system, and the relations (4.14) themselves were important to describe the phase space of this system.

### Asymptotic formulae.

In [BF7] we have investigated the minimal solution as  $|E| \rightarrow \infty$  and have described the asymptotics of the coefficients  $A_0$ ,  $B_0$ ,  $C_0$  and  $D_0$ . For the functions  $t(E)$  and  $s(E)$  this has implied

**Theorem 4.2.** Fix  $\epsilon$ ,  $0 < \epsilon < \pi$ . If  $-\pi + \epsilon < \arg E < \pi - \epsilon$ , then

$$t(E) = 2e^{-2\pi\lambda/h + o(1)} \cos(2\lambda^2/h + o(1)),$$

$$\lambda = \ln(2E), \quad E \rightarrow \infty;$$

if  $-3\pi/2 + \epsilon < \arg E < \pi/2 - \epsilon$ , then

$$s(E) = -2ie^{-2\pi\lambda/h + o(1)} \cos(2\lambda^2/h + 2\pi i\lambda/h + o(1)),$$

$$\lambda = \ln(2E), \quad E \rightarrow \infty.$$

The asymptotic formulae for  $t$  and  $s$  on the complements of the described sectors of the complex plane, can be obtained by means of the formulae (4.12).

The asymptotic formulae described in the theorem 4.2 characterize, in particular, the asymptotics of  $t_n$  and  $s_n$ :

$$t_n \sim e^{\sqrt{\pi hn/2}}, \quad s_n \sim e^{\sqrt{\pi hn/2}}, \quad n \rightarrow \infty.$$

## 5. Relations between the spectra $\sigma_0$ and $\sigma_1$

### Direct relation.

Knowing the spectra  $\sigma_0$  and  $\sigma_1$  of the operators  $H_0$  and  $H_1$  one can explicitly describe  $s$  and  $t$ . However, these two spectra are not independent, see (4.11). In principle, one can reconstruct  $\sigma_1$  in terms of  $\sigma_0$ .

Formula (4.11) and the representation (4.5) imply that

$$t(s_n) = (-1)^{(n+1)} i, \quad t(-s_n) = (-1)^n i. \quad (5.1)$$

This allows to split (4.11) into two relations:

$$\prod_{n \geq 1} (1 - E/t_n) \pm i \prod_{n \geq 1} (1 + E/t_n) = (1 \pm i) \prod_{n \geq 1} (1 \mp i(-1)^n E/s_n). \quad (5.2)$$

### Additional relation and the trace of the monodromy matrix.

We have seen before that the pair  $\psi_1, \psi_2$  exists and forms a basis in  $\mathbb{M}$  if  $B_0 C_0 \neq 0$ . Now we can say that this pair is a basis if  $E \notin (-\sigma_0) \cap (-\sigma_1)$ .

Note that if  $E \in \sigma_0$  then  $t(E) = 0$ . This implies that

$$\mathcal{M}(E) = \begin{pmatrix} a(E) - 2 \cos(2\pi z/h) & s(E) \\ -s(E) & 0 \end{pmatrix},$$

where  $a(E)$  is a finite number. Since  $\det \mathcal{M} \equiv 1$  this implies that  $s(t_n) = \pm 1$ . In fact, one can get more precise relation:

$$s(t_n) = (-1)^n.$$

This formula is independent of (5.1), it complements formulae (5.2).

The last result allows to get the following representation for the function  $\mathcal{E}(E)$

$$\mathcal{E}(E) = 2 \cos(\pi^2/h) \prod_{n \geq 1} \frac{1 - E/r_n}{1 - E/t_n},$$

where  $r_n$  are real numbers,

$$2 > r_1 > r_2 > \dots, \quad r_n \rightarrow -\infty, \quad n \rightarrow \infty,$$

satisfying the equation:

$$s^2(r) = 1, \quad r < 2.$$

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