Semifinite-gap problems of Whittaker-Hill equation and complex oscillation theory¹

Edmund Y. M. Chiang, a Xudan Luo b

^aHong Kong University of Science & Technology

^bUniversity at Buffalo (New York State Univ.)

The $7^{\rm th}$ International Conference on Nonlinear Mathematical Physics & The $14^{\rm th}$ National Workshop on Solitons and Integrable Systems

BISTU, 18-22 August, 2017

20 August, 2017

¹Research partially supported by Hong Kong Research Grant Council

Whittaker-Hill Eqn

Qualitative results

WH: Explicit general soln

Complex Oscillation theory

Stability intervals

Whittaker-Hill equation

- Schrödinger equations with potentials with period π .
- Mathieu equation (1868)

$$f''(z) + (A + B\cos 2z)f(z) = 0$$

(Separation of variables of 2D-Wave equation by elliptic cylindiical coordinates)

Whittaker-Hill equation (1907/1915)

$$f''(z) + (A + B\cos 2z + C\cos 4z)f(z) = 0.$$
 (1)

(Separation of variables of 3D-Helmholz equation by paraboloidal coordinates)

 Celestial machines, Quantum theory, Quantum chemistry, Integration of KdV with periodic BVP (Novikov), Quantum field theory, etc

Hill's equations

• Consider Hill's equation (1877)

$$\frac{d^2y}{dx^2} + Q(x)y(x) = 0, . (2)$$

which is a Schrödinger equation with periodic (even) potential

$$Q(x+\pi)=Q(x).$$

Hill's original treatment was to assume

$$Q(x) = \lambda + 2\sum_{k=1}^{\infty} \theta_k \cos 2kx$$

to converge on \mathbb{R} .

- How much do we know about the eigenvalues λ ?
- Do there exist any periodic solutions?
- Coexistence: Do there exist two linearly independent (LI) periodic solutions?



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Floquet (Bloch) Theory

- G. H. Hill (1886), G. Floquet (1883), A. M. Lyapunov (1907)
- L. Brillouin (1953) Wave propagation in periodic structures (Dover)
- Magnus & Winkler (1966): Hill's Equations (Dover)
- Arscott (1964): Periodic Differential Equations (Pergamon press)
- Eastham (1973): Spectral Theory of Periodic Differential Equations (Scottish Academic Press)
- Floquet theory: $\exists \rho \neq 0$ and non-trivial soln $\psi(x)$ of Eqn (2) such that

$$\psi(x+\pi) = \rho\psi(x).$$

- Similar to monodromy at a regular singular point (\mathbb{C}) .
 - $\rho = 1$ periodic soln;
 - $\rho = -1$ semi-periodic soln;
 - Since Q(x) is even, so the solutions of (2) could be even/odd solns.

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Floquet (Bloch) Theory (II)

• Suppose $\phi_1(x)$ and $\phi_2(x)$ are two linearly independent solutions with initial conditions

$$\phi_1(0) = 1$$
, $\phi_1'(0) = 0$, $\phi_2(0) = 0$, $\phi_2'(0) = 1$

• We observe \exists 2 × 2 matrix such that

$$\begin{pmatrix} \phi_1(x+\pi) \\ \phi_2(x+\pi) \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} \phi_1(x) \\ \phi_2(x) \end{pmatrix}$$

• It follows from the initial conditions on ϕ_1 , ϕ_2 above that

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = \begin{pmatrix} \phi_1(\pi) & \phi_1'(\pi) \\ \phi_2(\pi) & \phi_2'(\pi) \end{pmatrix}$$

$$\operatorname{tr}(A) = \phi_1(\pi) + \phi_2'(\pi), \quad \det(A) = \phi_1(\pi)\phi_2'(\pi) - \phi_1'(\pi)\phi_2(\pi).$$

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Floquet (Bloch) Theory (III)

• Suppose $\psi(x)$ is a solution such that $\psi(x+\pi)=\rho\psi(x)$ for certain ρ . Then $\psi(x)=c_1\phi_1(x)+c_2\phi_2(x)$ for some c_1, c_2

$$(A^T - \rho \operatorname{I}_2) \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{bmatrix} \begin{pmatrix} a_{11} & a_{21} \\ a_{12} & a_{22} \end{pmatrix} - \rho \operatorname{I}_2 \end{bmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

i.e.,

$$\begin{vmatrix} a_{11} - \rho & a_{21} \\ a_{12} & a_{22} - \rho \end{vmatrix} = 0$$

or just

$$\rho^2 - \operatorname{tr}(A) \rho + \det(A) = 0.$$

where $det(A) \neq 0$

• $\rho = \rho_1, \, \rho_2$ are called the characteristic (Floquet) multipliers and

$$D = \Delta(\lambda) = \operatorname{tr}(A) = \phi_1(\pi) + \phi_2'(\pi)$$

is called Hill's discriminant (Lyapunov fn) of the DE (1).

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Stability intervals vs Gaps

Theorem

- If D = |tr(A)| > 2, then all non-trivial solutions of Eqn (2) are unbounded on \mathbb{R} (unstable),
- If D = |tr(A)| < 2, then all solutions of Eqn (2) are bounded on \mathbb{R} (stable)
- If D = |tr(A)| = 2, then there exists a non-trivial solution of Eqn (2) which is bounded on \mathbb{R} (conditionally stable)

Theorem

- The Eqn (2) has a non-trivial soln with period $\pi \iff D = 2$.
- The Eqn (2) has a non-trivial soln with semi-period $\pi \iff D = -2$ (i.e., $f(x + \pi) = -f(x)$)

Periodic boundary (eigenvalue) problem

• Periodic boundary value problem on $[0, \pi]$ (D = 2)

$$f(0) = f(\pi), \quad f'(0) = f'(\pi)$$

This is a self-adjoint problem and standard method of constructing Green's functions and defining compact symmetric linear opeartor with a suitable inner-product space on $[0,\pi]$ guarantees

• the existence of countably many orthogonal eigen-functions ψ_n and eigenvalues λ_n such that

$$\lambda_0 \leq \lambda_1 \leq \lambda_2, \cdots, \quad \lambda_n \to \infty$$

• Semi-periodic boundary value problem on $[0,\pi]$ (D=-2)

$$f(0) = -f(\pi), \quad f'(0) = -f'(\pi)$$

• corresponding eigenfunctions ϕ_n and eigenvalues λ'_n such that

$$\lambda_1' \leq \lambda_2', \cdots, \quad \lambda_n' \to \infty$$

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Bands and Gaps

Theorem

To every differential equation

$$y'' + [\lambda + Q(x)]y = 0, \quad Q(x + \pi) = Q(x), \quad \lambda \in \mathbb{R}$$
 (3)

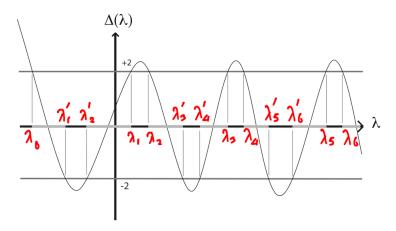
there exists two monotone sequences $(\lambda_n)_0^{\infty}$, $(\lambda'_n)_1^{\infty}$ such that

$$-\infty < \lambda_0 < \lambda_1' \le \lambda_2' < \lambda_1 \le \lambda_2 < \lambda_3' \le \lambda_4' < \lambda_3 \le \lambda_4 < \cdots,$$

for which

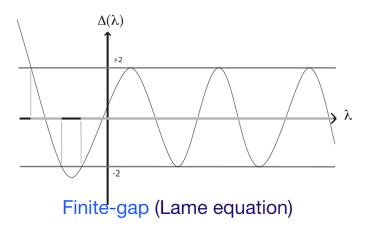
- stability intervals (bands): $(\lambda_0, \lambda_1'), (\lambda_2', \lambda_1), (\lambda_2, \lambda_3') \cdots$,
- instability intervals (gaps): $(\lambda_{2n+1}, \lambda_{2n+2})$, $(\lambda'_{2n+1}, \lambda'_{2n+2})$, \cdots , (simple point).
- Instability interval disappears (shrink to a point) so that $\lambda_{2n+1} = \lambda_{2n+2}$, or $\lambda'_{2n+1} = \lambda'_{2n+2}$, \cdots (stable double point).

Mathieu equation Ince (1922) infinitely many gaps

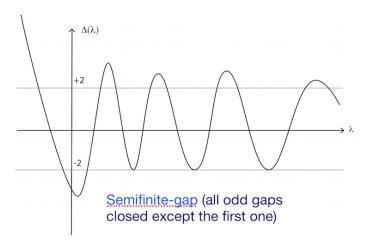




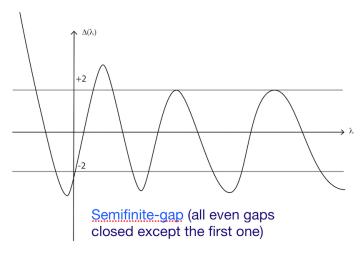
Finite-gaps or semi-finite gap potentials



Semi-finite gap (odd solutions)



Semi-finite gap (even solutions)





Semifinite-gap for WH-operator

Theorem (Djakov & Mityagin (2005))

Let

$$\nu(x) = -4\alpha t \cos 2x - 2\alpha^2 \cos 4x$$

be a potential of the Hill operator

$$\lambda f = Lf = -f'' + \nu(x)f, \quad 0 \le x \le \pi,$$

where both $(0 \neq) \alpha$ and t are real.

- 1. If t = 2p 1, $p \in \mathbb{N}$ with periodic boundary conditions, then the first 2p 1 eigenvalues are simple, and others are double.
- 2. If t = 2m, $m \in \mathbb{N}$ with semi-periodic boundary conditions, then the first 2m eigenvalues are simple and others are double.

Comments

 Compared with the Mathieu operator, the eigenvalues of Whittaker-Hill potential

$$\nu(x) = -(B\cos 2x + C\cos 4x)$$

may be simple or double both for periodic and semi-periodic boundary conditions.

• Djakov and Mityagin assumed that if $B = 4\alpha t$ and $C = 2\alpha^2$ for any real α and natural number t, i.e.,

$$B/(2\sqrt{2C})=t\in\mathbb{Z},$$

then they conclude that

- 1. all finitely many gaps exist
- 2. Semi-periodic BVP: t = 2m + 1, all the even gaps except the first m are closed,
- 3. Periodic BVP: t = 2m, the first m are closed.
- Djakov and Mityagin's argument is very elaborate and heavy in spectra analysis (and also long).



Riemann-Hilbert (21st) Problem

- Prove that there always exists a Fuchsian system (equation) with given singularities in \mathbb{CP}^1 and a given monodromy (representation).
- "Fuchsian" means the "coefficients" have at most poles at the given singularities.
- Solved by Plemelj (1908), Arnold (1988), Bolibruch (1989)
- Closely related to Riemann-Hilbert methods in integrable systems and Random matrices theory.
- Two singularities in \mathbb{CP}^1 :
 - E.g., Euler equation: $\{0, \infty\}$

$$x^2y'' + (1 - a - b)xy' + aby = 0$$

$$v = Ax^a + Bx^b$$

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2-3-4 Regular Singularties (I)

- Three singularities in CP¹:
 - E.g., Bessel equation: $\{0, \infty^2\}$

$$x^2y'' + xy' + (x^2 - \nu^2)y = 0.$$

$$y(x) = J_{\nu}(x) = \sum_{k=0}^{\infty} \frac{2^{\nu}}{2^{k} k! \Gamma(\nu + k)} x^{2k+\nu}$$

• E.g., Confluent hypergeometric equation: $\{0, \infty^2\}$

$$xy''(z) + (c - x)y'(x) - ay(x) = 0$$

$$_{1}F_{1}(a;c;x) = {}_{1}F_{1}\left(\begin{matrix} a \\ c \end{matrix};x\right) := \sum_{n=0}^{\infty} \frac{(a)_{n}}{n!(c)_{n}}x^{n}, \quad c \neq 0, -1, -2, \cdots,$$

where $(a)_k = a(a+1)\cdots(a+k-1)$ In particular, wher $a = -n = 0, -1, -2, \cdots, {}_1F_1(-n; c; x)$ is (the Laguerre) polynomial

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2-3-4 Regular Singularties (II)

- Four singularities in CP¹:
 - Rational form of the Mathieu Eqn., $(x = e^{2iz})$
 - Rational form of the Whittaker-Hill equation $(x = e^{2iz})$,
 - Rational form of Lamé equation $(x = \mathcal{P}(z))$
 - Rational form of Darboux-Trebibich-Verdier equation
- Painlevé equations (II-VI) arise as compatibility condition (Lax pairs) of Isomonodromy deformation of some of the DEs above (Fuchs (1905/07), Garnier (1912), Schlesinger (1912), Jimbo-Miwa-Ueno (1981)).

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WH-Eqn: General soln I

Theorem (C. & Luo) Suppose the coefficients A, B and C>0 of the WH-eqn

$$f''(z) + (A + B\cos 2z + C\cos 4z)f(z) = 0$$

are complex parameters, where $BC \neq 0$, then we have two linearly independent solutions

$$f_{1}(z) = (e^{2iz})^{\mp \frac{B}{4\sqrt{2C}} + \frac{1}{2}} \cdot e^{\pm \frac{\sqrt{2C}}{4}} e^{-2iz} \cdot e^{\mp \frac{\sqrt{2C}}{4}} e^{2iz}$$

$$\cdot \sum_{k=0}^{\infty} \frac{B_{k}^{\mp}}{\Gamma(k+2\mp \frac{B}{2\sqrt{2C}})} \cdot {}_{1}F_{1}\left(\frac{k+1}{k+2\mp \frac{B}{2\sqrt{2C}}} ; \pm \frac{\sqrt{2C}}{2} e^{2iz} \right)$$

and

$$f_{2}(z) = (e^{2iz})^{\pm \frac{B}{4\sqrt{2C}} + \frac{1}{2}} \cdot e^{\mp \frac{\sqrt{2C}}{4}e^{-2iz}} \cdot e^{\mp \frac{\sqrt{2C}}{4}e^{2iz}}$$
$$\cdot \sum_{k=0}^{\infty} \frac{\widehat{B}_{k}^{\pm}}{\Gamma(k+2\pm \frac{B}{2\sqrt{2C}})} \cdot {}_{1}F_{1}\left(\begin{matrix} k+1\pm \frac{B}{2\sqrt{2C}} \\ k+2\pm \frac{B}{2\sqrt{2C}} \end{matrix}\right); \pm \frac{\sqrt{2C}}{2}e^{2iz}\right).$$

WH-Eqn: General soln II

where the coefficients B_k^{\mp} and \widehat{B}_k^{\pm} satisfy the following three-term recurrence relations (infinite determinants)

$$-\frac{C}{2}(k+1)B_{k}^{\mp} + \left[(k+1)\left(k+2 \mp \frac{B}{2\sqrt{2C}}\right) + \frac{C-A+1}{4} \frac{B^{2}}{32C} \mp \frac{B}{4\sqrt{2C}} \right] B_{k+1}^{\mp} - (k+2)B_{k+2}^{\mp} = 0$$

and

$$\frac{C}{2} \left(k + 1 \pm \frac{B}{2\sqrt{2C}} \right) \cdot \widehat{B}_{k}^{\pm} + \left[(k+1) \left(k + 2 \pm \frac{B}{2\sqrt{2C}} \right) \right] \\
\pm \frac{B}{4\sqrt{2C}} + \frac{B^{2}}{32C} + \frac{-A - C + 1}{4} \right] \cdot \widehat{B}_{k+1}^{\pm} - (k+2) \cdot \widehat{B}_{k+2}^{\pm} = 0$$

respectively.



WH-Eqn: General soln III

Theorem (C. & Luo) In particular, if $\pm \frac{B}{2\sqrt{2C}} = -n - 1 \in \mathbb{Z}_{<0}$ and the tri-diagonal determinate $|\widehat{D}_{n+1}^{\pm}| = 0$, where $\widehat{D}_{n+1}^{\pm} = \{\widehat{b}_{ki}\}_{1 \le k, i \le n+1}$ is defined as

$$\widehat{b}_{k,k-1} = \frac{C}{2} \left(k - 1 \pm \frac{B}{2\sqrt{2C}} \right),$$

$$\hat{b}_{kk} = (k-1)\left(k \pm \frac{B}{2\sqrt{2C}}\right) \pm \frac{B}{4\sqrt{2C}} + \frac{B^2}{32C} + \frac{-A-C+1}{4},$$

$$\hat{b}_{k,k+1} = -k$$

and $\hat{\mathbf{b}}_{kj} = \mathbf{0}$ for other \mathbf{j} , then

$$f_{2}(z) = (e^{2iz})^{-\frac{n}{2}} \cdot e^{\mp \frac{\sqrt{2C}}{4}e^{-2iz}} \cdot e^{\mp \frac{\sqrt{2C}}{4}e^{2iz}} \cdot \sum_{k=0}^{n} \widehat{B}_{k}^{\pm} \cdot \frac{(-n-k)_{n-k}}{(n-k)!} \cdot \left(\pm \frac{\sqrt{2C}}{2}e^{2iz}\right)^{n-k}.$$

Idea of proof I

• The WH-eqn in a rational form $(x = e^{2iz})$ looks like:

$$x^{2}y''(x) + \left[-\frac{\sqrt{2C}}{2}x^{2} + \left(2 - \frac{B}{2\sqrt{2C}}\right)x - \frac{\sqrt{2C}}{2} \right]y'(x) + \left(-\frac{\sqrt{2C}}{2}x + \frac{C - A + 1}{4} + \frac{B^{2}}{32C} - \frac{B}{4\sqrt{2C}} \right)y(x) = 0.$$
(4)

when divide x on both sides yields

$$xy''(x) + \left[-\frac{\sqrt{2C}}{2}x + \left(2 - \frac{B}{2\sqrt{2C}}\right) + O(1/x)\right]y'(x) + \left(-\frac{\sqrt{2C}}{2} + O(1/x)\right)y(x) = 0.$$

$$(5)$$

which is asymptotically like the confluent hypergeometric Eqn.

- Recursion and asymptotic fomrulae of ₁F₁
- Three-term recursion: *Poincaré's theorem* and *Perron's* theorems.



Complex Oscillation: Philosophy

- Liouville theorem (1840's): If f is a bounded entire function, then $f \equiv \text{const.}$ (i.e., f misses most of \mathbb{C})
- Little Picard theorem (1879-80) states that if an entire function f on $\mathbb C$ misses two values in $\mathbb C$, then $f \equiv const.$
- The number "2" is best possible: (e.g. $f(x) = e^x \neq 0$)
- Little Picard theorem says that entire functions are quite rigid.

Consider

$$y''(x) + A(x)y(x) = 0$$

where A(x) is an entire potential

• Suppose a solution f(x) omits x = 0. Then what can we say about the solution f(x)

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Measuring zeros of Entire Functions

We first review some complex analytic theory.

• Suppose f(z) has zeros. We define

$$n(r) :=$$
 numbers of zeros of f in $\{|z| < r\}$,

and define the exponent of convergence of the zeros of f(z):

$$\lambda(f) = \limsup_{r \to +\infty} \frac{\log n(r)}{\log r}$$

• Relation between order and exponent of convergence of f(z):

$$\limsup_{r\to +\infty} \frac{\log n(r)}{\log r} = \lambda(f) \le \limsup_{r\to +\infty} \frac{\log \log M(r, f)}{\log r} = \sigma(f).$$

Essentially just Poisson-Jensen formula.



Bank-Laine's Complex Oscillation (Nevanlinna) Theory

Theorem (Bank & Laine (1983))

Let $f \not\equiv 0$ be a solution of

$$f''(z) + A(z) f(z) = 0$$

where

$$A(z) = B(e^z) = \sum_{j=-k}^{\ell} K_j e^{jz},$$

such that $\lambda(f) < +\infty (= \sigma(f))$. Moreover, we have

$$f(z) = \begin{cases} \psi(e^{z/2}) \exp\left(\sum_{j=0}^{\ell} d_j e^{jz/2} + dz\right), & \ell \text{ is odd and } k = 0; \\ \psi(e^z) \exp\left(\sum_{j=-k/2}^{\ell/2} d_j e^{jz} + dz\right), & \ell \text{ is even.} \end{cases}$$

$\frac{1}{16}$ – theorem

Theorem

(Bank, Laine, Langley (1986), C. & Ismail (2006)) Let $K \in \mathbb{C}$. Then the equation

$$f'' + (e^z - K)f = 0. (6)$$

admits linearly independent solutions

$$y_{\pm}(z) = A_{\pm} J_{2\sqrt{K}}(\pm 2e^{z/2}) + B_{\pm} Y_{2\sqrt{K}}(\pm 2e^{z/2}).$$
 (7)

Each of the solutions of (6) has $\lambda(f) < \infty$ if and only if

$$K = (n+1)^2/16, \quad n \in \mathbb{N} \cup \{0\}$$
 (8)

$$y_{\pm}(z) = \theta_n \left(\pm 2ie^{z/2} \right) \exp\left(\mp 2ie^{z/2} + dz \right), \tag{9}$$

where $\theta_n(x)$ is the reversed Bessel polynomial of degree n.



Complex oscillation of WH-Eqn

Theorem (C & Luo) Suppose the Whittaker-Hill Eqn admits a non-trivial solution f with $\lambda(f) < \infty$, where $BC \neq 0$. Then,

$$\pm B/(2\sqrt{2C}) = -n-1.$$

Moreover, if the tri-diagonal determinant $|\widehat{D}_{n+1}^{\pm}| = 0$, where the tri-diagonal matrix $\widehat{D}_{n+1}^{\pm} = \{\widehat{b}_{kj}\}_{1 \leq k, j \leq n+1}$ is defined as

$$\widehat{b}_{k,k-1} = \frac{C}{2} \left(k - n - 2 \right), \quad \widehat{b}_{k,k+1} = -k$$

$$\hat{b}_{kk} = (k-1)(k-n-1) + n^2 - A - C/4,$$

and $\hat{b}_{kj} = 0$ for other j, then this solution can be represented by

$$f(z) = (e^{2iz})^{-\frac{n}{2}} \cdot e^{\mp \frac{\sqrt{2C}}{4}e^{-2iz}} \cdot e^{\mp \frac{\sqrt{2C}}{4}e^{2iz}}$$
$$\cdot \sum_{k=0}^{n} \frac{\widehat{B}_{k}^{\pm}}{\Gamma(-n+k+1)} \cdot {}_{1}F_{1} \begin{pmatrix} -n+k \\ -n+k+1 \end{pmatrix}; \pm \frac{\sqrt{2C}}{2}e^{2iz}$$

Complex oscillation of WH-Eqn

where the coefficients \widehat{B}_k satisfy the following three-term recurrence relation

$$\frac{C}{2}(k-n)\widehat{B}_{k}^{\pm} + \left[(k+1)(k-n+1) + \frac{n^{2}-A-C}{4}\right]\widehat{B}_{k+1}^{\pm} - (k+2)\widehat{B}_{k+2}^{\pm} = 0.$$

(1) New explicit solutions

Theorem

Suppose the coefficients ${\color{red}B}$ and ${\color{gray}C}$ of the Whittaker-Hill equation

$$f''(x) + (A + B\cos 2x + C\cos 4x)f(x) = 0$$

are real, and $BC \neq 0$, $0 \leq x \leq \pi$. Then it admits two linearly independent solutions of periodic or semi-periodic π if and only if $\frac{B}{2\sqrt{2C}} \in \mathbb{Z} \dots$

• (1) If $\frac{B}{4\sqrt{2C}} = -n - \frac{1}{2}$ $n \ge 0$, and the solutions satisfy the periodic boundary conditions, then the first 2n + 1 eigenvalues are simple $(\lambda(f) < \infty)$, and others are double $(\lambda(f) = \infty)$:

$$A_0^+ < A_2^- < A_2^+ < A_4^- < A_4^+ < \dots < A_{2n}^- < A_{2n}^+ < A_{2n+2}^- < A_{2n+4}^- = A_{2n+4}^+ < \dots,$$

where A_{2j}^+ and A_{2j}^- are the eigenvalues corresponding to non-trivial odd and even solutions with period π respectively.



(1) Even, Odd (stable) solutions

• Moreover, (i) when $A = A_{2k}^-$, $1 \le k \le n$,

$$f_{odd}^{\pi}(x) = e^{-\sqrt{\frac{C}{2}} \cdot \cos 2x} \cdot \sin 2x$$

$$\cdot \sum_{k=0}^{n-1} A_k^{-(1)} \cdot {}_1F_1\left(\frac{-n+1+k}{k+3}; \sqrt{2C}(\cos 2x - 1)\right);$$

when $A = A_{2k}^+$, $0 \le k \le n$,

$$f_{\text{even}}^{\pi}(x) = e^{-\sqrt{\frac{C}{2}} \cdot \cos 2x}$$

$$\cdot \sum_{k=0}^{n} A_{k}^{-(2)} \cdot {}_{1}F_{1} \begin{pmatrix} -n+k \\ k+1 \end{pmatrix}; \sqrt{2C}(\cos 2x - 1);$$

(1) Coexistence solutions

• (ii) when $A=A_{2k}^-=A_{2k}^+$, k>n, then the two linearly independent solutions of the Whittaker-Hill differential equation are given by

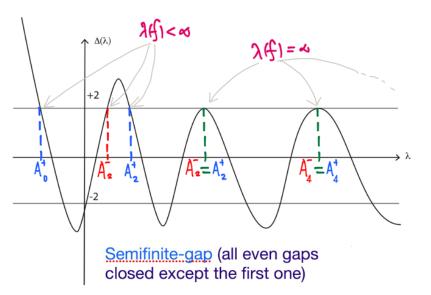
$$f_{odd}^{\pi}(x) = e^{-\sqrt{\frac{c}{2}} \cdot \cos 2x} \cdot \sin 2x$$
$$\cdot \sum_{k=0}^{\infty} A_k^{-(1)} \cdot {}_1F_1\left(\frac{-n+1+k}{k+3}; \sqrt{2C}(\cos 2x - 1)\right)$$

and

$$f_{\text{even}}^{\pi}(x) = e^{-\sqrt{\frac{c}{2}} \cdot \cos 2x}$$

$$\cdot \sum_{k=0}^{\infty} A_k^{-(2)} \cdot {}_1F_1\left(\frac{-n+k}{k+1}; \sqrt{2C}(\cos 2x - 1)\right).$$

Even gaps closed



(2) New explicit solutions

• (2) If $\frac{B}{4\sqrt{2C}} = -n - 1$, $n \in \mathbb{N}^+ \cup \{0\}$, and the solutions satisfy the semi-periodic boundary conditions, then the first 2n + 2 eigenvalues are *simple*, and others are *double*, i.e.,

$$A_1^+ < A_1^- < A_3^+ < A_3^- < \dots < A_{2n+1}^+ < A_{2n+1}^- < A_{2n+1}^+ < A_{2n+5}^- < \dots,$$

where A_{2j-1}^+ and A_{2j-1}^- are the eigenvalues corresponding to non-trivial odd and even solutions with semi-period π respectively.

Remark This appears to be the case that Djakov & Mityagin (2005) missed.

(2) Even, Odd (stable) solutions

• Moreover, (i) when $A = A_{2k-1}^-$, $1 \le k \le n+1$,

$$f_{odd}^{2\pi}(x) = \sin x \cdot e^{-\sqrt{\frac{C}{2}} \cdot \cos 2x}$$

$$\cdot \sum_{k=0}^{n} A_{k}^{-(3)} \cdot {}_{1}F_{1}\left(\frac{-n+k}{k+2}; \sqrt{2C}(\cos 2x - 1)\right);$$

when $A = A_{2k-1}^+$, $1 \le k \le n+1$,

$$f_{even}^{2\pi}(x) = \cos x \cdot e^{-\sqrt{\frac{C}{2}} \cdot \cos 2x}$$

$$\cdot \sum_{k=0}^{n} A_k^{-(4)} \cdot {}_1F_1\left(\frac{-n+k}{k+2}; \sqrt{2C}(\cos 2x - 1)\right);$$

(2) Coexistence solutions

• (ii) when $A = A_{2k-1}^- = A_{2k-1}^+$, k > n+1, then the two linearly independent solutions of the Whittaker-Hill differential equation are

$$f_{odd}^{2\pi}(x) = \sin x \cdot e^{-\sqrt{\frac{C}{2}} \cdot \cos 2x}$$

$$\cdot \sum_{k=0}^{\infty} A_k^{-(3)} \cdot {}_1F_1\left(\frac{-n+k}{k+2}; \sqrt{2C}(\cos 2x - 1)\right)$$

and

$$f_{\text{even}}^{2\pi}(x) = \cos x \cdot e^{-\sqrt{\frac{c}{2}} \cdot \cos 2x}$$
$$\cdot \sum_{k=0}^{\infty} A_k^{-(4)} \cdot {}_1F_1\left(\frac{-n+k}{k+2}; \sqrt{2C}(\cos 2x - 1)\right).$$

The remaining two cases

• (3) If
$$-\frac{B}{4\sqrt{2C}} = -n - \frac{1}{2}$$
, $n \in \mathbb{N}^+ \cup \{0\}$,

• (4) If
$$-\frac{B}{4\sqrt{2C}} = -n - 1$$
, $n \in \mathbb{N}^+ \cup \{0\}$,

• We skip the details.

Complex oscillation and semifinite-gaps

Theorem (C. & Luo) Suppose the WH-Eqn admits a solution f with $\lambda(f) < \infty$. Then $B/(2\sqrt{2C}) \in \mathbb{Z}$ holds. Moreover, if f satisfies the normalised initial condition, then we can express f in explicit non-oscillatory-soln form:

- 1. the odd and even solutions $f_{\text{odd}}^{\pi}(x)$ and $f_{\text{even}}^{\pi}(x)$ in cases (I) and (III) of the last Theorem corresponding to the periodic boundary condition and for the eigenvalues $A = A_{2k}^- (1 \le k \le n)$ and $A = A_{2k}^+ (1 \le k \le n)$;
- 2. the odd and even solutions $f_{\text{odd}}^{2\pi}(x)$ and $f_{\text{even}}^{2\pi}(x)$ in cases (II) and (IV) of the last Theorem corresponding to the semi-periodic boundary condition and for the eigenvalues $A = A_{2k-1}^ (1 \le k \le n+1)$ and $A = A_{2k-1}^+$ $(1 \le k \le n+1)$.

Moreover, the eigenvalues $A = A_{2k}^ (1 \le k \le n)$, $A = A_{2k}^+$ $(1 \le k \le n)$, $A = A_{2k-1}^ (1 \le k \le n+1)$ and $A = A_{2k-1}^+$ $(1 \le k \le n+1)$ are solutions of certain determinants $|D_n(j)| = 0$ (j = 1, 2, 3, 4) respective, whose respective entries are suitably defined.

hittaker-Hill Eqn Qualitative results WH: Explicit general soln Complex Oscillation theory Stability interval

E. T. Whittaker (1873-1956)



Figure: (MathTutor, 1915)

• Supervisor: A. R. Forsyth

• Students: G. H. Hardy, W. Hodge, G. N. Watson, A. Eddington



E. L. Ince (FRSE: 1891-1941)



Figure: (MathTutor, 1923)

Instability intervals (gaps) of the Hill operator I

In the case of specific potentials, like the Mathieu potential

$$\nu(x) = -B\cos 2x,$$

where $0 \neq B$ is real, or more general trigonometric polynomials

$$\nu(x) = \sum_{-N}^{N} c_k e^{ikx}, \quad c_k = \overline{c_{-k}}, \quad 0 \le k \le N < \infty,$$

one comes to two category of questions:

- 1. (Notation change) The left-end point λ_n^- and right-end points
- 2. Is the n-th intervals of instability *closed*, i.e.,

$$\gamma_n = \lambda_n^+ - \lambda_n^- = 0,$$

or, equivalently, is the multiplicity of λ_n^+ double?

3. If $\gamma_n \neq 0$, what could we say about $\gamma_n = \gamma_n(\nu) \rightarrow ?$ as $n \rightarrow \infty$?

Instability intervals (gaps) of the Mathieu operator II

- Ince (1922) answered in a negative way for question (1) the Mathieu-operator has only simple eigenvalues both for periodic and semi-periodic boundary conditions, i.e., infinitely many gaps.
- Harrell (1981), Avron & Simon (1981) gave

$$\gamma_n = \lambda_n^+ - \lambda_n^- = \frac{8}{[(n-1)!]^2} \cdot \left(\frac{|B|}{8}\right)^n \left(1 + o\left(\frac{1}{n^2}\right)\right).$$

as $n \to \infty$ which was improved by Anahtarci & Djakov (2012). ($[1 - \pi^2/4n^3 + O(1/n^4))$.

• Levy & Keller (1963) gave the asymptotics of $\gamma_n = \gamma_n(B)$, i.e., for fixed n and real $B \neq 0$, when $B \rightarrow 0$,

$$\gamma_n = \lambda_n^+ - \lambda_n^- = \frac{8}{[(n-1)!]^2} \cdot \left(\frac{|B|}{8}\right)^n (1 + O(B)).$$

• Djakov & Mityagin (2007): WH Eqn contains modular forms studied by Kac & Wakimoto, Milne and Zagier in 1990's.

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Summary

- We have introduced (semi)finite-gap problems for Hill's equations.
- We have reviewed some classical and recent results for Mathieu and Whittaker-Hill operators
- We have found exact solutions in terms of ₁F₁ as basis.
 (N. Katz's rigid local systems theory can offer a deeper monodromy/geometric insight: on going project)
- We relate complex oscillatory and non-oscillatory solutions to those semi-finite gap solutions (Picard-type viewpoint).
- Very little is known about the real nature of the eigenvalues $\lambda = A$ with respect to B and C.

International J. Quantum Chemistry (2010)

Whittaker–Hill Equation, Ince Polynomials, and Molecular Torsional Modes

LUIZ F. RONCARATTI, VINCENZO AOUILANTI

Dipartimento di Chimica, Università di Perugia, 06123 Perugia, Italy

Received 23 December 2008; accepted 11 March 2009 Published online 26 August 2009 in Wiley InterScience (www.interscience.wiley.com). DOI 10.1002/qua.22255

Figure: (Wiley)

Roncaratti and Aquilanti ($H_2O_2: \lambda(B, C)$)

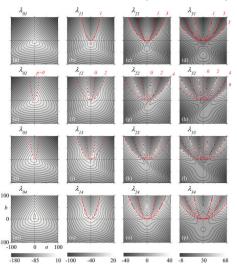


FIGURE 2. Surfaces λ_m (a, b) where λ's are the eigenvalues of Whittaker-Hill equation; n and τ are quantum numbers, a and b are the torsional potential parameters. Valley bottoms and ridges follow parabolic curves defined by the parameter p (see text). Each color bar describes the color scale for the pictures in the column above it. [Color figure can be viewed in the online issue, which is available at www.interscience.wilev.com.]

Ince's contour plot

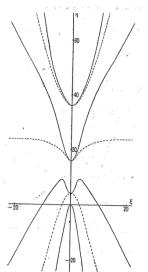


Figure: Proc. Lond. Math Soc. (1923)



References

- 1. F. M. Arscott, Periodic differential equations, Pergamon press, 1964
- S. Bank, & I. Laine, Representations of solutions of periodic second order linear differential equations, J. Reine Angew. Math. 344 (1983), 1-21
- Y. M. Chiang, & M. Ismail, On value distribution theory of second order periodic ODES, special functions and orthogonal polynomials, Canad. J. Math. 58 (2006) 726–767.
- Y. M. Chiang & Xudan Luo, Explicit determination of complex oscillatory and semifinite-gap solutions of the Whittaker-Hill equation, (In preparation).
- P. Djakov and B. Mityagin, Simple and double eigenvalues of the Hill operator with a two-term potential, J. Approx. Thy. 135 (2005), 70-104.
- P. Djakov and B. Mityagin, Asymptotics of instability zones of the Hill operator with a two term potential, Journal of Functional Analysis 242 (2007), 157?194.
- A. D. Hemery & A. P. Veselov, Whittaker-Hill equation and semifinite-gap Schrödinger operator, J. Math Phys. 51 no. 7, 17 pp.
- 8. E. L. Ince, *A linear differential equation with periodic coefficients*, Proc. London Math. Soc., **23** (1923), 56-74.
- 9. E. T. Whittaker, On a class of differential equations whose solutions satisfy integral equations, Proc. Edinburgh Math. Soc. 33 (1915), 14–33.



/hittaker-Hill Eqn Qualitative results WH: Explicit general soln Complex Oscillation theory Stability intervals

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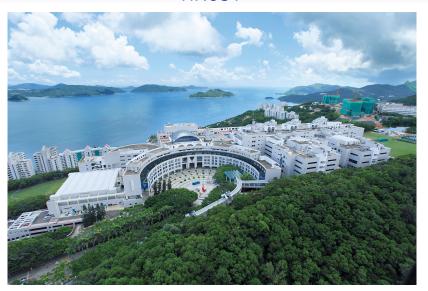


Figure: Clear Water Bay, Hong Kong Thank you for your attention !!

