A Simple Algorithm for Computing Stokes Multipliers

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Abstract

We propose a new simple algorithm to compute Stokes multipliers of the Schrödinger equation with a cubic potential. Our method gives a numerical solution of the direct monodromy problem for the first Painlevé equation.

1 Introduction

The aim of the present paper is to introduce a new algorithm for computing the Stokes multiplier of the following Schrödinger equation with a cubic potential (plus an apparent fuchsian singularity)

$$\frac{d^2\psi(\lambda)}{d\lambda^2} = Q(\lambda; y, y', z)\psi(\lambda) \,, \tag{1}$$

$$Q(\lambda; y, y', z) = 4\lambda^3 - 2\lambda z + 2zy - 4y^3 + y'^2 + \frac{\lambda}{\lambda - y} + \frac{3}{4(\lambda - y)^2} \,.$$

Remarkably, in the limit $y \to \infty, y'^2 - 4y^3 \to b, z \to a$, equation (1) becomes the cubic oscillator

$$\frac{d^2\psi(\lambda)}{d\lambda^2} = V(\lambda; a, b)\psi(\lambda) \,, \quad V(\lambda; a, b) = 4\lambda^3 - a\lambda - b \,. \tag{2}$$

Hence, for the rest of the paper we consider equation (2) as a particular case of equation (1).

The monodromy problem (i.e. the problem of computing Stokes multipliers) of the cubic anharmonic oscillator is a fundamental and rather interesting problem in itself and a large literature is devoted to it (see author's paper [Mas10c] for some bibliography).

Our study is however motivated by the relation of above linear equations with the Painlevé first equation

$$y'' = 6y^2 - z \,,\ z \in \mathbb{C} \quad , \tag{3}$$

which we briefly explain below.

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The relation goes as follows: any solution y of the Painlevé equation gives rise to an isomonodromic deformation of equation (1) (see [KT05] and [Mas10a]). In other words, if the parameters y, y' of the cubic potential evolve according to the Painlevé first equation, then the Stokes multipliers of equation (1) do not depend on z.

If z is a singular point of y then equation (1) is not well-defined. However, recently the author [Mas10a] (see also [Mas10b]) showed that if $\frac{a}{2}$ is a pole of a solution y of the Painlevé equation then, in the limit $z \to \frac{a}{2}$, equation (1) becomes equation (2). The parameter b in (2) corresponds to a particular coefficient of the Laurent expansion of y around the pole.

Our algorithm gives a numerical solution of the *direct monodromy problem* for the Painleve first equation: given the Cauchy data y, y', z of a particular solution of P-I we are able to compute the corresponding Stokes multipliers, even when z is a pole of that solution.

The paper is organized as follows. In Section 2 we introduce the Nevanlinna's theory of the cubic oscillator and the Schwarzian differential equation (5). Then we give a formula for computing the Stokes multipliers from any solution of the Schwarzian differential equation. Section 3 is devoted to the description of the algorithm. In Section 4 we test our algorithm against the WKB prediction and the Deformed TBA equations. For convenience of the reader, we explain the basic theory of cubic oscillators (Stokes sectors, Stokes multipliers, subdominant solutions, etc ...) in the Appendix.

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2 Schwarzian Differential Equation

The algorithm we propose for computing Stokes multipliers is based on Theorem 1 below, that gives a formula to compute Stokes multipliers from any solution of the Schwarzian differential equation (5).

Theorem 1 has its roots in the geometric theory of the Schrödinger equation, which was developed by Nevanlinna around 1920 [Nev70]. The author learned such a beautiful theory from the remarkable paper of Eremenko and Gabrielov [EG09]. In this section we follow quite closely [EG09] as well as author's recent paper [Mas10c]. Here and for the rest of the paper$\mathbb{Z}_5 = \{-2, \dots, 2\}$.

Remark. *Equation (1) has a fuchsian singularity at the pole* $\lambda = y$ *of the potential* $Q(\lambda; y, y', z)$. *However this is an apparent singularity*

[Mas10a]: the monodromy around the singularity of any solution of (1) is -1. As a consequence, the ratio of two solutions of (1) is a meromorphic function.

The main geometric object of Nevanlinna's theory is the Schwarzian derivative of a (non constant) meromorphic function $f(\lambda)$

$$\{f(\lambda),\lambda\} = \frac{f'''(\lambda)}{f'(\lambda)} - \frac{3}{2}\left(\frac{f''(\lambda)}{f'(\lambda)}\right)^2 . \tag{4}$$

The Schwarzian derivative is strictly related to the Schrödinger equation (2). Indeed, the following Lemma is true.

Lemma 1. *The (non constant) meromorphic function $f:\mathbb{C}\to\overline{\mathbb{C}}$ solves the Schwarzian differential equation*

$$\{f(\lambda),\lambda\} = -2V(\lambda;a,b) . \tag{5}$$

iff $f(\lambda)=\frac{\phi(\lambda)}{\chi(\lambda)}$ where $\phi(\lambda)$ and $\chi(\lambda)$ are two linearly independent solutions of the Schrödinger equation (2). Hence, the first derivative of any (non constant) solution of (5) vanishes only at the pole $\lambda=y$ of the potential.

We define the Asymptotic Stokes Sector S_k as

$$S_k = \left\{\lambda : \left|\arg\lambda - \frac{2\pi k}{5}\right| < \frac{\pi}{5}\right\}, k\in\mathbb{Z}_5 . \tag{6}$$

Every solution of the Schwarzian equation (5) has limit for $\lambda\to\infty$, $\lambda\in S_k$. More precisely we have the following

Lemma 2 (Nevanlinna)**.** *(i) Let $f(\lambda)=\frac{\phi(\lambda)}{\chi(\lambda)}$ be a solution of (5) then for all $k\in\mathbb{Z}_5$ the following limit exists*

$$w_k(f) = \lim_{\lambda\ \to\infty\ \lambda\in S_k} f(\lambda)\in\mathbb{C}\cup\infty , \tag{7}$$

provided the limit is taken along a curve non-tangential to the boundary of S_k.

(ii) $w_{k+1}(f)\neq w_k(f)$, $\forall k\in\mathbb{Z}_5$.

(iii) Let $g(\lambda)=\frac{af(\lambda)+b}{cf(\lambda)+d}=\frac{a\phi(\lambda)+b\chi(\lambda)}{c\phi(\lambda)+d\chi(\lambda)}$, $\begin{pmatrix} a & b\\ c & d\end{pmatrix}\in Gl(2,\mathbb{C})$. *Then*

$$w_k(g) = \frac{a\,w_k(f)+b}{c\,w_k(f)+d} . \tag{8}$$

(iv) If the function f is evaluated along a ray contained in S_k, the convergence to $w_k(f)$ is super-exponential.

Proof. (i-iii) Let ψ_k be the solution of equation (2) subdominant in S_k and ψ_{k+1} be the one subdominant in S_{k+1} (see the Appendix for their definitions). From the WKB theory , we know that ψ_k and ψ_{k+1} are linearly independent: ψ_k is dominant is S_{k+1} and ψ_{k+1}

is dominant is S_k. Hence, we have that $f(\lambda) = \frac{\alpha\psi_k(\lambda)+\beta\psi_{k+1}(\lambda)}{\gamma\psi_k(\lambda)+\delta\psi_{k+1}(\lambda)}$, for some $\begin{pmatrix}\alpha & \beta \\ \gamma & \delta\end{pmatrix} \in Gl(2,\mathbb{C})$. Hence $w_k(f) = \frac{\beta}{\delta}$ if $\delta \neq 0$, $w_k(f) = \infty$ if $\delta = 0$. Similarly $w_{k+1}(f) = \frac{\alpha}{\gamma}$. Since $\begin{pmatrix}\alpha & \beta \\ \gamma & \delta\end{pmatrix} \in Gl(2,\mathbb{C})$ then $w_k(f) \neq w_{k+1}(f)$

(iv) From WKB estimates (see the Appendix) we know that inside S_k,

$$\left|\frac{\psi_k(\lambda)}{\psi_{k+1}(\lambda)}\right| \sim e^{-Re\left(\frac{8}{5}\lambda^{\frac{5}{2}} - a\lambda^{\frac{1}{2}}\right)} ,$$

where the branch of $\lambda^{\frac{1}{2}}$ is chosen such that the exponential is decaying.

□

Definition 1. *Let $f(\lambda)$ be a solution of the Schwarzian equation (5) and $w_k(f)$ be defined as in (7). We call $w_k(f)$ the k-th asymptotic value of f.*

The author noticed in a previous paper [Mas10c] that the Stokes multipliers of the Schrödinger equation are rational functions of the asymptotic values $w_k(f)$:

Theorem 1. *[Mas10c] Denote σ_k the k-th Stokes multiplier of the Schrödinger equation (2) (for its precise definition, see equation (14) in the Appendix). Let f be any solution of the Schwarzian equation (5). Then*

$$\sigma_k = i\left(w_{1+k}(f), w_{-2+k}(f); w_{-1+k}(f), w_{2+k}(f)\right) \ , \forall k \in \mathbb{Z}_5 \ , \qquad (9)$$

where $(a,b;c,d) = \frac{(a-c)(b-d)}{(a-d)(b-c)}$ is the cross ratio of four point on the sphere.

Proof. Due to equation (8) all the asymptotic values of two different solutions of (5) are related by the same fractional linear transformation. As it is well-known, the cross ratios of four points of the sphere is invariant if all the points are transformed by the same fractional linear transformation. Hence the right-hand side of (9) does not depend on the choice of the solution of the Schwarzian equation.

Let ψ_{k+1} be the solution of (2) subdominant in S_{k+1} and ψ_{k+2} be the one subdominant in S_{k+2} (see the Appendix for the precise definition). By choosing $f(\lambda) = \frac{\psi_{k+1}(\lambda)}{\psi_{k+2}(\lambda)}$, one verifies easily that the identity (9) is satisfied. □

Remark. *The same construction presented here holds for anharmonic oscillators with polynomial potentials of any degree. For any degree, there are formulas similar to (9) for expressing Stokes multipliers in terms of cross ratios of asymptotic values. The general formula will be given in a subsequent publication.*

2.1 Singularities

Since the Schwarzian differential equation is linearized (see Lemma 1) by the Schrödinger equation, any solution is a meromorphic function and has an infinite number of poles [Nev70]. The poles, however, are localized near the boundaries of the Stokes sectors $S_k, k \in \mathbb{Z}_5$. Indeed, using the complex WKB theory one can prove the following

Lemma 3. *Let $f(\lambda)$ be any solution of the Schwarzian equation (5). Fix $\varepsilon > 0$ and define $\tilde{S}_k = \left\{\lambda : \left|\arg\lambda - \frac{2\pi k}{5}\right| \leq \frac{\pi}{5} - \varepsilon\right\}, k \in \mathbb{Z}_5$. Then $f(\lambda)$ ha a finite number of poles inside $\tilde{S}_k$. Hence, there are a finite number of rays inside $\tilde{S}_k$ on which $f(\lambda)$ has a singularity.*

3 The Algorithm

In the previous section we have proved the following remarkable facts

- Inside the Stokes Sector S_k, any solution to the Schwarzian differential equation (1) f converges super-exponentially to the asymptotic value $w_k(f)$. See Lemma 2 (iv).
- The Stokes multipliers of the Schrödinger equation (1) are cross ratios of the asymptotic values $w_k(f)$. See equation (9).
- Inside any closed subsector of S_k, f has a finite number of poles. See Lemma 3.

Hence the Simple Algorithm for Computing Stokes Multipliers goes as follows:

1. Set k=-2.
2. Fix arbitrary Cauchy data of f: $f(\lambda^*), f'(\lambda^*), f''(\lambda^*)$, with the conditions $\lambda^* \neq y$, $f'(\lambda^*) \neq 0$.
3. Choose an angle α inside S_k, such that the singular point $\lambda = y$ does not belong to the corresponding ray, i.e. $\alpha \neq \arg y$. Define $t : \mathbb{R}^+ \cup 0 \to \mathbb{C}$, $t(x) = f(e^{i\alpha}x + \lambda^*)$. The function t satisfies the following Cauchy problem

$$\begin{cases} \{t(x), x\} = e^{2i\alpha} Q(e^{i\alpha}x + \lambda^*; y, y', z), \\ t(0) = f(\lambda^*), t'(0) = e^{i\alpha} f'(\lambda^*),\ t''(0) = e^{2i\alpha} f''(\lambda^*)\ . \end{cases} \tag{10}$$

4. Integrate equation (10) either directly [1] or by linearization (see Remark below), and compute $w_k(f)$ with the desired accuracy and precision.
5. If $k < 2, k++$, return to point 3.
6. Compute σ_l using formula (9) for all $l \in \mathbb{Z}_5$.

[1] Integrating equation (10) directly, one can hit a singularity $x*$ of y. To continue the solution past the pole, starting from $x^* - \varepsilon$ one can integrate the function $\tilde{y} = \frac{1}{y}$, which satisfies the same Schwarzian differential equation.

Remark. *As was shown in Lemma 1, any solution f of the Schwarzian equation is the ratio of two solutions of the Schrödinger equation. Hence, one can solve the nonlinear Cauchy problem (10) by solving two linear Cauchy problems.*

Whether the linearization is more efficient than the direct integration of (10) will not be investigated in the present paper.

4 A Test

We have implemented our algorithm using MATHEMATICA's ODE solver NDSOLVE integrating equation (10) with steps of length 0.1. We decided the integrator to stop at step n if

$$\begin{aligned} |t(0.1n) - t(0.1(n-1))| &< 10^{-13} \text{ and} \\ \left| \frac{t(0.1n) - t(0.1(n-1))}{t(0.1n)} \right| &< 10^{-13} \,. \end{aligned}$$

To test our algorithm we computed the Stokes multiplier $\sigma_0(b)$ of the equation

$$\frac{d^2\psi(\lambda)}{d\lambda^2} = (4\lambda^3 - b)\psi(\lambda) \,. \tag{11}$$

According to the WKB analysis (see [Sib75], [Mas10a]) the Stokes multiplier $\sigma_0(b)$ has the following asymptotics

$$\sigma_0(b) \sim \begin{cases} -ie^{\frac{\sqrt{\frac{\pi}{3}}\Gamma(1/3)}{2^{2/3}\Gamma(11/6)} b^{\frac{5}{6}}} \,, & \text{if } b > 0 \\ -2ie^{-\frac{\sqrt{\pi}\Gamma(1/3)}{2^{\frac{5}{3}}\Gamma(11/6)}(-b)^{\frac{5}{6}}} \cos\left(\frac{\sqrt{\frac{\pi}{3}}\Gamma(1/3)}{2^{5/3}\Gamma(11/6)}(-b)^{\frac{5}{6}} \right), & \text{if } b < 0 \,. \end{cases} \tag{12}$$

Our computations (see Figure 1 and 2 below) shows clearly that the WKB approximation is very efficient also for small value of the parameter b.

We also tested our results against the numerical solution (due to A. Moro) of the Deformed Thermodynamic Bethe Ansatz equations (Deformed TBA), which has been recently introduced by the author [Mas10c], developing the seminal work of Dorey and Tateo [DT99]. The Deformed TBA equations are a set of nonlinear integral equations which describe the exact correction to the WKB asymptotics. The numerical solution of the Deformed TBA equations enable to a-priori set the relative error in the evaluation of the Stokes multiplier $\sigma_0(b)$ rescaled with respect to the WKB exponentials (12). Hence, in the range of $-20 \leq b \leq 20$ we could verify that we had computed the rescaled $\sigma_0(b)$ with a relative error less than 10^{-8}.

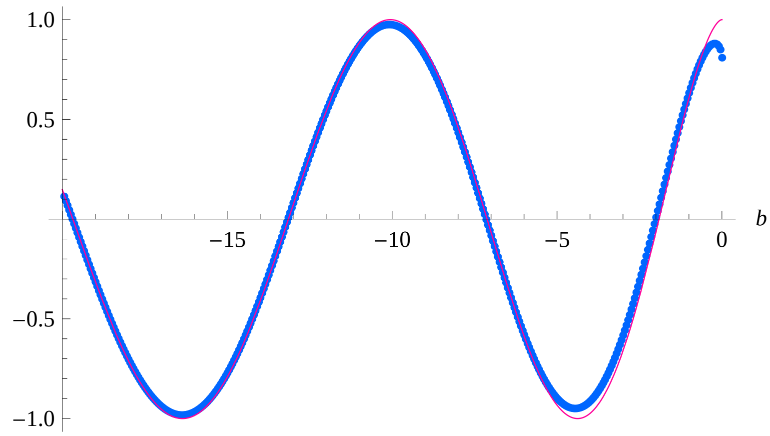

Figure 1: Thick dotted line: the rescaled Stokes multiplier $\frac{i}{2} e^{-\frac{\sqrt{\pi}\Gamma(1/3)}{2^{\frac{5}{3}}\Gamma(11/6)}(-b)^{\frac{5}{6}}} \sigma_0(b)$ evaluated with our algorithm; thin continuous line: $\cos\left(\frac{\sqrt{\frac{\pi}{3}}\Gamma(1/3)}{2^{5/3}\Gamma(11/6)}(-b)^{\frac{5}{6}}\right)$, i.e. the WKB prediction for the rescaled Stokes multiplier.

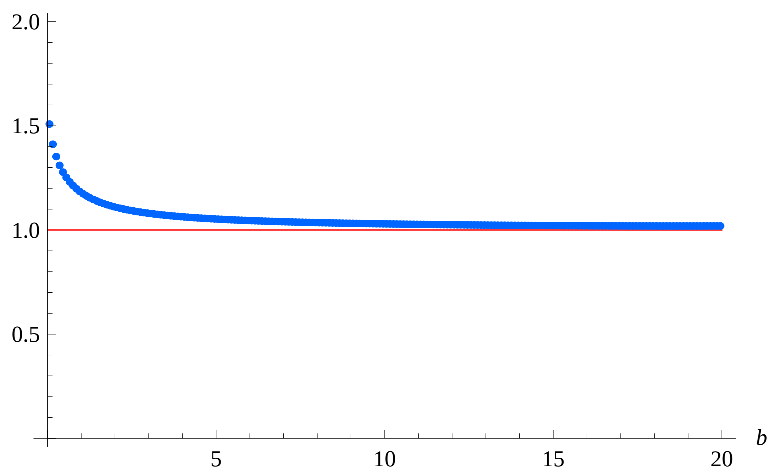

Figure 2: Thick dotted line: the rescaled Stokes multiplier $e^{-\frac{\sqrt{\frac{\pi}{3}}\Gamma(1/3)}{2^{2/3}\Gamma(11/6)} b^{\frac{5}{6}}} \sigma_0(b)$ evaluated with our algorithm; thin continuous line: 1, the WKB prediction for the rescaled Stokes multiplier.

5 Concluding Remarks

Starting from Nevanlinna's theory, we have developed an algorithm for computing Stokes multipliers of the Schrödinger equations (1, 2) that are relevant in the study of the Painleve first equation (3).

Our algorithm gives a numerical solution of the direct monodromy problem for the Painleve first equation. Indeed, given the Cauchy data y, y', z of a particular solution of P-I we are able to compute the Stokes multipliers corresponding to it via (1). We stress that our method is valid also when singular Cauchy data (i.e. poles) are given and in that case equation (2) must be used.

We have tested our algorithm in a particular case and we have shown that WKB predictions for the cubic oscillator (2) are impressively good.

We plan to pursue our study in relation with the numerical solution of the Painlevé first equation (3). In particular we plan to analyze the inverse monodromy problem for the Painlevé first equation, i.e. to compute y and y' once z and the Stokes multipliers are given. We will develop a numerical solution of the inverse problem through the numerical inversion of the solution of the direct problem presented here.

Recently [Olv10] S. Olver has constructed an algorithm for computing inverse monodromy problems through a Riemann-Hilbert approach. Once our method will have been developed, it will be interesting to compare the two methods, which are based on completely different approaches.

6 Appendix

The reader expert in anharmonic oscillators theory will skip this Appendix; for her, it will be enough to know that we denote $\sigma_k(a,b)$ the $k-th$ Stokes multipliers of equation (2). Here we review briefly the standard way, i.e. by means of Stokes multipliers, of introducing the monodromy problem for equation (2). All the statements of this section are proved in Appendix A of author's paper [Mas10a] and in Sibuya's book [Sib75] .

Lemma 4. *Fix $k \in \mathbb{Z}_5 = \{-2, \dots, 2\}$ and define a cut in the $\mathbb{C}$ plane connecting $\lambda = y$ with infinity such that its points eventually do not belong to $S_{k-1} \cup \overline{S_k} \cup S_{k+1}$. Choose the branch of $\lambda^{\frac{1}{2}}$ by requiring*

$$\lim_{\substack{\lambda \to \infty \\ \arg \lambda = \frac{2\pi k}{5}}} \mathrm{Re} \lambda^{\frac{5}{2}} = +\infty \,,$$

while choose arbitrarily one of the branch of $\lambda^{\frac{1}{4}}$. Then there exists a unique solution $\psi_k(\lambda; a, b)$ of equation (2) such that

$$\lim_{\substack{\lambda \to \infty \\ \left|\arg \lambda - \frac{2\pi k}{5}\right| < \frac{3\pi}{5} - \varepsilon}} \frac{\psi_k(\lambda; a, b)}{\lambda^{-\frac{3}{4}} e^{-\frac{4}{5}\lambda^{\frac{5}{2}} + \frac{a}{2}\lambda^{\frac{1}{2}}}} \to 1, \ \forall \varepsilon > 0 \,. \tag{13}$$

Definition. *We denote ψ_k the k-th subdominant solution or the solution subdominant in the k-th sector.*

From the asymptotics (13), it follows that ψ_k and ψ_{k+1} are linearly independent. If one fixes the same branch of $\lambda^{\frac{1}{4}}$ in the asymptotics (13) of $\psi_{k-1}, \psi_k, \psi_{k+1}$ then the following equations hold true

$$\begin{aligned} \psi_{k-1}(\lambda; a, b) &= \psi_{k+1}(\lambda; a, b) + \sigma_k(a, b)\psi_k(\lambda; a, b)\,, \\ -i\sigma_{k+3} &= 1 + \sigma_k(a, b)\sigma_{k+1}(a, b)\,,\ \forall k \in \mathbb{Z}_5\,. \end{aligned} \tag{14}$$

Definition. *The entire functions $\sigma_k(a, b)$ are called Stokes multipliers. The quintuplet of Stokes multipliers $\sigma_k(a, b), k \in \mathbb{Z}_5$ is called the monodromy data of equation (2).*

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