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Periodic Sturm-Liouville problems related to two Riccati equations of constant coefficients

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Abstract

We consider two closely related Riccati equations of constant parameters whose particular solutions are used to construct the corresponding class of supersymmetrically-coupled second-order differential equations. We solve analytically these parametric periodic problems along the positive real axis. Next, the analytically solved model is used as a case study for a powerful numerical approach that is employed here for the first time in the investigation of the energy band structure of periodic not necessarily regular potentials. The approach is based on the well-known self-matching procedure of James (1949) and implements the spectral parameter power series solutions introduced by Kravchenko (2008). We obtain additionally an efficient series representation of the Hill discriminant based on Kravchenko's series.

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Keywords: Riccati equation; Bloch solutions; Hill discriminant

1 Introduction

Natural periodic and quasiperiodic structures have drawn the attention of mankind since old times [1]. Nowadays, in the technological world, the scientists, especially those involved in the area of material science, bring forth at a tremendous pace new artificial specimens in which finite periodic structures are the main components. A rich mathematical background related to periodicity has been developed along the years [2, 3]. The construction of new periodic potentials and the analysis of their specific properties could be valuable in guiding the modern technological design. Within this context the relationship between Riccati equations and Sturm-Liouville problems has been firmly known at least since more than half a century [4] and more recently led to supersymmetric (SUSY) quantum mechanics [5, 6, 7].

In the present work we will discuss in some detail the periodic Sturm-Liouville (PSL) problems generated by particular solutions of the very simple

Riccati equations of constant coefficients [8]

$$\frac{dR}{dx} + R^2 + k_0^2 = 0 \tag{1}$$

and

$$\frac{d\Phi}{dx} - 2S\Phi + \Phi^2 + k_0^2 + S^2 = 0 , \tag{2}$$

which is closely related to the first one. We obtain the exact PSL solutions in the Bloch form. In general, when available, the analytic solutions of a PSL equation expressed as Bloch functions allow one to analyze the band structure of the problem. Of course, this is not always possible. In many cases, even if the exact solutions are known their Bloch form is hard to disentangle. As a consequence, other well-established approaches are frequently used in order to analyze the band structure of the spectrum: either by means of the Hill discriminant (or Lyapunov function) [3] or using the band structure parameter introduced by James [9]. In general, for this goal, two linearly independent solutions are required for all values of the spectral parameter. Hence, it is essential to have an as simple form as possible for the sought solutions in terms of the spectral parameter. Therefore we show that a convenient study of the band structure of the spectrum can be achieved using a representation for solutions in the form of power series with respect to the spectral parameter.

The outline of the paper is the following. The next section is devoted to the three main points: (i) the SUSY construction of the periodic Sturm-Liouville problems of Schrödinger type starting from the aforementioned Riccati equation, (ii) solving the resulting Schrödinger equation and (iii) studying some of its properties. Next, in Section 3, we provide a numerical approach of the same problems using the self-matching method of H.M. James [9] for the Kravchenko representation of the solutions in terms of spectral parameter power series (SPPS) [10, 11]. A small Conclusion section ends up the paper.

2 Riccati-associated PSL equations

2.1 Case I: Riccati equation (1)

In the Riccati equation (1) we introduce $R(x) = \frac{f'}{f}$ leading to the second order linear differential equation

$$-f''(x) + \nu_1 f(x) = 0 , \tag{3}$$

where $\nu_1 = -k_0^2$.

The linearly independent solutions of (3) are obviously

$$f_1(x) = \cos k_0 x , \quad f_2(x) = \sin k_0 x .$$

Using f_1 one gets for the Riccati equation the solution $R_{f_1}(x) = -k_0 \tan k_0 x$. In what follows we employ f_1 to define $R_{f_1}(x)$, equally well one can use f_2

leading to $R_{f_2}(x) = k_0 \cot k_0 x$, however this brings in only minimal changes in the whole of the mathematical apparatus that follows and hereby we will deal only with the first choice.

Since ν_1 can be calculated by employing the equation

$$\nu_1 = \frac{dR_{f_1}}{dx} + R_{f_1}^2 = -k_0^2 ,$$

the supersymmetric partner potential will be given by

$$\nu_2(x) = -\frac{dR_{f_1}}{dx} + R_{f_1}^2 = k_0^2(1 + 2\tan^2 k_0 x)$$

and the supersymmetric partner equation of equation (3) is given by

$$-g''(x) + \nu_2(x)g(x) = 0 . \quad (4)$$

The supersymmetric partner linear independent solutions are

$$g_1(x) = \frac{1}{\cos k_0 x} , \quad g_2(x) = \frac{1}{k_0 \cos k_0 x} \left[\frac{k_0 x}{2} + \frac{1}{4} \sin 2k_0 x \right] .$$

Considering now the spectral issue for these two periodic potentials, the constant one ν_1 and the singular one $\nu_2(x)$:

$$\begin{aligned} -f''(x) - k_0^2 f(x) &= K^2 f(x), \\ -g''(x) + k_0^2(1 + 2\tan^2 k_0 x)g(x) &= K^2 g(x), \end{aligned}$$

we can get the K^2 spectrum of the f problem from the Bloch solutions $e^{\pm i\sqrt{k_0^2 + K^2}x}$ that provide the quasimomentum $P(K^2) = \sqrt{k_0^2 + K^2}$. On the other hand, for the g problem, being the Darboux partner of the f problem, i.e., $g(x) = (\frac{d}{dx} - R_{f_1}(x))f(x)$, we have the following Bloch solutions with the same quasimomentum $P(K^2)$

$$e^{\pm i\sqrt{k_0^2 + K^2}x} \left(\tan k_0 x \pm i\sqrt{k_0^2 + K^2} \right) .$$

As known [12], the allowed energy bands exist only for $P \in \mathbf{R}$ leading to $K^2 \geq -k_0^2$, therefore there is only one forbidden zone covering the interval $(-\infty, -k_0^2)$.

Using the following two Pauli matrices

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \text{and} \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} ,$$

a single matrix equation for the two-component spinor $W = \begin{pmatrix} g_1 \\ f_1 \end{pmatrix}$ can be written down:

$$\sigma_y W'(x) + i\sigma_x R_{f_1} W(x) = 0 . \quad (5)$$

The two components of the spinor W have a sort of hidden coupling through the same particular Riccati solution but otherwise they look independent one of the other.

2.2 Case II: Riccati equation (2)

A simple way to perform a direct coupling of the two components f and g is to add two constant parameters as follows: K as a spectral parameter of the Dirac-like equations and a potential coupling parameter S

$$[\sigma_y \frac{d}{dx} + i\sigma_x(R_{f_1} + S)]W_c(x) = iKW_c(x), \quad W_c = \begin{pmatrix} g_c \\ f_c \end{pmatrix}. \quad (6)$$

For related mathematical procedures the reader is directed to a textbook of Lanczos [13] and to a paper of Nogami and Toyama [14] and references therein for similar supersymmetric structure of the Dirac equation in particle physics. Equation (6) is equivalent to the following system of coupled equations

$$g'_c(x) + (k_0 R_{f_1} + S)g_c(x) = Kf_c(x) \quad (7)$$

$$f'_c(x) - (k_0 R_{f_1} + S)f_c(x) = -Kg_c(x). \quad (8)$$

This leads to:

$$-\left(\frac{d}{dx} + \Phi_1\right)\left(\frac{d}{dx} - \Phi_1\right)f_c = K^2 f_c(x), \quad (9)$$

$$-\left(\frac{d}{dx} - \Phi_1\right)\left(\frac{d}{dx} + \Phi_1\right)g_c = K^2 g_c(x), \quad (10)$$

where $\Phi_1 = R_{f_1} + S = -k_0 \tan k_0 x + S$ is a particular solution of the Riccati equation (2). In unfactorized form, (9) and (10) turn into the following equations

$$-f''_c(x) + (-k_0^2 + S^2 - 2Sk_0 \tan k_0 x)f_c(x) = K^2 f_c(x) \quad (11)$$

$$-g''_c(x) + (k_0^2 + S^2 - 2Sk_0 \tan k_0 x + 2k_0^2 \tan^2 k_0 x)g_c(x) = K^2 g_c(x). \quad (12)$$

The latter two equations define two new classes of parametric singular potentials. To see the changes with respect to the initial equations (3) and (4) for f and g , respectively, we write the previous system in terms of modified ν functions $\nu_{1,c}(x)$ and $\nu_{2,c}(x)$:

$$-f''_c(x) + \nu_{1,c}(x)f_c(x) = K^2 f_c(x), \quad -g''_c(x) + \nu_{2,c}(x)g_c(x) = K^2 g_c(x), \quad (13)$$

where

$$\nu_{1,c}(x) = \nu_1 + \Delta\nu(x), \quad \nu_{2,c}(x) = \nu_2(x) + \Delta\nu(x), \quad \Delta\nu(x) = S^2 - 2Sk_0 \tan k_0 x.$$

Note that all the solutions f_c of (11) for any value of K^2 are square integrable on any finite interval. This is due to Weyl's alternative theorem, see for example the book of Hellwig [15], all singular points $\frac{n\pi}{2k_0}$, (n odd) of $\nu_{1,c}(x)$ are limit circle points. Indeed, it is sufficient to prove square integrability of two linearly independent solutions for any fixed value of K^2 . Taking $K^2 = 0$ we see that both linearly independent solutions

$$h_1(x) = e^{Sx} \cos k_0 x \quad \text{and} \quad h_2(x) = e^{Sx} \cos k_0 x \int \frac{e^{-2Sx}}{\cos^2 k_0 x} dx$$

are square integrable on any finite interval.

The limit circle points of equation (11) become limit point singularities of (12). This can be demonstrated considering the solution $\frac{1}{h_1(x)}$ of (12) for $K^2 = 0$. Thus, Weyl's alternative guarantees that exactly one square integrable solution of (12) exists for K^2 with a nonvanishing imaginary part whereas for real K^2 such a solution cannot even exist.

In order to solve the equations (11),(12) we begin with the first equation in (13). With the aid of its solution f_c the solution of the second equation in (13) can be simply obtained by applying the Darboux transformation

$$g_c(x) = f'_c(x) - \Phi_1(x)f_c(x). \quad (14)$$

Thus, we focus next on the f_c equation which will be reduced to a hypergeometric equation. The reduction is done with the help of a procedure similar to the one described in [16].

2.3 Hypergeometric solutions

Consider the simultaneous change of the independent variable $\chi = \frac{1}{2}(1 - i \tan k_0 x) = \frac{e^{-ik_0 x}}{2 \cos k_0 x}$ and of the dependent variable $y(\chi) = (\chi^2 - \chi)^{1/2} f_c$. Then the first equation in (13) takes the following Schrödinger-like form

$$\frac{d^2 y}{d\chi^2} + I_{f_c} y = 0 \quad (15)$$

where

$$I_{f_c} = \frac{S^2 - K^2 + 2iSk_0 - 4iSk_0\chi}{4k_0^2\chi^2(\chi - 1)^2}.$$

Finally, in order to bring (15) to the hypergeometric form, the following substitution can be used [17]

$$y(\chi) = \chi^p(\chi - 1)^q U(\chi),$$

where

$$p_{1,2} = \frac{1}{2} \left(1 \pm \sqrt{\frac{(k_0 - iS)^2 + K^2}{k_0^2}} \right), \quad q_{1,2} = \frac{1}{2} \left(1 \pm \sqrt{\frac{(k_0 + iS)^2 + K^2}{k_0^2}} \right).$$

Thus, one gets

$$\chi(\chi - 1) \frac{d^2 U}{d\chi^2} + 2[(p_{1,2} + q_{1,2})\chi - p_{1,2}] \frac{dU}{d\chi} + \left[2p_{1,2}q_{1,2} - \frac{S^2 - K^2}{2k_0} \right] U = 0 \quad (16)$$

Choosing the pair p_1 and q_1 , we obtain the following solutions

$$U_1 = {}_2F_1(p_1 + q_1 - 1, p_1 + q_1; 2p_1; \chi), \quad U_2 = x^{1-2p_1} {}_2F_1(-p_1 + q_1 + 1, -p_1 + q_1; 2 - 2p_1; \chi). \quad (17)$$

Using properties of hypergeometric functions (the change of variable $\chi \rightarrow \frac{\chi}{\chi-1}$), the f_c linearly independent solutions can be written in the form

$$f_{c,1}(x) = (-1)^{q_1 - \frac{1}{2}} e^{-i(2p_1-1)k_0x} {}_2F_1(p_1 + q_1 - 1, p_1 - q_1; 2p_1; -e^{-2ik_0x}), \quad (18)$$

$$f_{c,2}(x) = (-1)^{q_1 - \frac{1}{2}} e^{i(2p_1-1)k_0x} {}_2F_1(-p_1 + q_1, -p_1 - q_1 + 1; 2 - 2p_1; -e^{-2ik_0x}). \quad (19)$$

Application of the Darboux transformation (14) to the solutions $f_{c,1}(x)$ and $f_{c,2}(x)$ leads to the following solutions $g_{c,1}(x)$ and $g_{c,2}(x)$ of the second equation in (13)

$$g_{c,1}(x) = (-1)^{q_1 - \frac{1}{2}} e^{-i(2p_1-1)k_0x} \times \left[(k_0 \tan k_0x - S - ik_0(2p_1-1)) {}_2F_1(p_1 + q_1 - 1, p_1 - q_1; 2p_1; -e^{-2ik_0x}) + \frac{(p_1 + q_1 - 1)(p_1 - q_1)}{p_1} ik_0 e^{-2ik_0x} {}_2F_1(p_1 + q_1, p_1 - q_1 + 1; 2p_1 + 1; -e^{-2ik_0x}) \right], \quad (20)$$

$$g_{c,2}(x) = (-1)^{q_1 - \frac{1}{2}} e^{i(2p_1-1)k_0x} \times \left[(k_0 \tan k_0x - S + ik_0(2p_1-1)) {}_2F_1(-p_1 + q_1, -p_1 - q_1 + 1; 2 - 2p_1; -e^{-2ik_0x}) + \frac{(p_1 + q_1 - 1)(p_1 - q_1)}{1 - p_1} ik_0 e^{-2ik_0x} {}_2F_1(-p_1 + q_1 + 1, -p_1 - q_1 + 2; 3 - 2p_1; -e^{-2ik_0x}) \right], \quad (21)$$

Though the Darboux transformation is applied to regular solutions $f_{c,1}$ and $f_{c,2}$ the singularity of the superpotential Φ implies the singularity of $g_{c,1}$ and $g_{c,2}$.

The solutions (18), (19) and (20), (21) are quasiperiodic or Bloch functions with the quasimomentum

$$P_S(K^2) = (2p_1 - 1)k_0 = \sqrt{(k_0 - iS)^2 + K^2},$$

which defines the Brillouin zone as follows: $\text{Re}(P_S) \in [-k_0, k_0]$. The allowed energies exist only for $P_S \in \mathbf{R}$ [12]. This condition holds when $(k_0 - iS)^2 + K^2 \in \mathbf{R}^+$. To specify the spectrum we should make some additional considerations. Limiting ourselves to the real values of the spectral parameter K^2 we have that for $k_0 \in \mathbf{R}$, S should be of the form $S = is$, where $s \in \mathbf{R}$. Moreover, K^2 must satisfy the inequality $K^2 \geq -(k_0 + s)^2$ or equivalently $K^2 \in (-(k_0 + s)^2, \infty]$. It is worth mentioning that for $s = 0$ we get the spectrum of the uncoupled potentials ν_1 and ν_2 . Another apparently possible case: $S \in \mathbf{R}$, $k_0 = i\gamma$, where $\gamma \in \mathbf{R}$ that also leads to a real P_S is not meaningful for the analysis of issues related to the quasimomentum since the potentials $\nu_{1,c}$ and $\nu_{2,c}$ are not periodic any more. Thus the spectrum of (11) and (12) is real only for purely imaginary values of the parameter S .

Notice that periodic potentials with purely imaginary coupling constants have been considered for the case of Mathieu equation [18] and have applications to the alternating flow of electromagnetic fields along conducting elliptic cylinders.

At the band edges we have $P_S = \begin{cases} 2nk_0 \\ (2n+1)k_0 \end{cases}$, $n = 0, \pm 1, \pm 2, \dots$. The solutions $f_{c,1}$ and $f_{c,2}$ are periodic when

$$P_S = 2nk_0 \implies K^2 = (2nk_0)^2 - (k_0 - iS)^2 \quad (22)$$

and antiperiodic for

$$P_S = (2n+1)k_0 \implies K^2 = ((2n+1)k_0)^2 - (k_0 - iS)^2. \quad (23)$$

For these special values of K^2 corresponding to the band edges two pairs of Bloch solutions $f_{c,1}(x, K^2)$, $f_{c,2}(x, K^2)$ and $g_{c,1}(x, K^2)$, $g_{c,2}(x, K^2)$ degenerate to single solutions $f_{c,1}(x, K^2) \equiv f_{c,2}(x, K^2)$ and $g_{c,1}(x, K^2) \equiv g_{c,2}(x, K^2)$. Indeed, the solutions (18) and (19) in the periodic case $P_S = 2nk_0$ have the form

$$f_{c,1}^{per}(x) = (-1)^{q_1(n) - \frac{1}{2}} e^{-2ink_0 x} {}_2F_1 \left(n - \frac{1}{2} + q_1(n), n + \frac{1}{2} - q_1(n); 1 + 2n; -e^{-2ik_0 x} \right),$$

$$f_{c,2}^{per}(x) = (-1)^{q_1(m) - \frac{1}{2}} e^{2imk_0 x} {}_2F_1 \left(-m - \frac{1}{2} + q_1(m), -m + \frac{1}{2} - q_1(m); 1 - 2m; -e^{-2ik_0 x} \right),$$

where $q_1(n) = \frac{1}{2} + \sqrt{n^2 + i\frac{S}{k_0}}$.

It is clear that in order to have the same value of P_S in both functions we should take $m = -n$, thus the solutions are periodic and $f_{c,1}^{per}(x) \equiv f_{c,2}^{per}(x)$.

In the antiperiodic case $P_S = (2n+1)k_0$ we have $q_1(n) = \frac{1}{2} + \sqrt{(n + \frac{1}{2})^2 + i\frac{S}{k_0}}$ and

$$f_{c,1}^{aper}(x) = (-1)^{q_1(n) - \frac{1}{2}} e^{-i(2n+1)k_0 x} {}_2F_1 \left(n + q_1(n), n + 1 - q_1(n); 2n + 2; -e^{-2ik_0 x} \right),$$

$$f_{c,2}^{aper}(x) = (-1)^{q_1(m) - \frac{1}{2}} e^{i(2m+1)k_0 x} {}_2F_1 \left(-m - 1 + q_1(m), -m - q_1(m); -2m; -e^{-2ik_0 x} \right).$$

Taking $m = -(n+1)$ we obtain that $f_{c,1}^{aper} \equiv f_{c,2}^{aper}$ are antiperiodic. Note that in both cases $q_1(n) = q_1(m)$. Analogously we obtain

$$g_c^{per}(x) = (-1)^{q_1(n) - \frac{1}{2}} e^{-2ink_0 x} \left[(k_0 \tan k_0 x - S - 2ink_0) \times \right. \\ \left. \times {}_2F_1 \left(n - \frac{1}{2} + q_1(n), n + \frac{1}{2} - q_1(n); 1 + 2n; -e^{-2ik_0 x} \right) + \right. \\ \left. + \frac{S}{n + \frac{1}{2}} e^{-2ik_0 x} {}_2F_1 \left(n + \frac{1}{2} + q_1(n), n + \frac{3}{2} - q_1(n); 2 + 2n; -e^{-2ik_0 x} \right) \right],$$

and

$$g_c^{aper}(x) = (-1)^{q_1(n)-\frac{1}{2}} e^{-i(2n+1)k_0x} \left[(k_0 \tan k_0x - S - (2n+1)ik_0) \times \right. \\ \left. \times {}_2F_1(n+q_1(n), n+1-q_1(n); 2n+2; -e^{-2ik_0x}) + \right. \\ \left. + \frac{S}{n+1} e^{-2ik_0x} {}_2F_1(n+1+q_1(n), n+2-q_1(n); 2n+3; -e^{-2ik_0x}) \right].$$

The value $P_S = 0$ and consequently $K_0^2 = -(k_0 + s)^2$ give us the following periodic nodeless solution of (11) which we denote by $f_0(x)$

$$f_0(x) = (-1)^{i\sqrt{\frac{s}{k_0}}} {}_2F_1\left(i\sqrt{\frac{s}{k_0}}, -i\sqrt{\frac{s}{k_0}}; 1; -e^{-2ik_0x}\right). \quad (24)$$

This eigenfunction will be used later on.

3 An efficient numerical approach for the energy band structure

The potentials $\nu_{1,c}$ and $\nu_{2,c}$ are periodic functions of period $\Lambda = \frac{\pi}{k_0}$, and have singularities at the points $\frac{n\pi}{2k_0}$. Following James [9] we choose the first period as $[0, \Lambda]$ and call it the zeroth cell, the second period $[\Lambda, 2\Lambda]$ as the first cell, and so forth. Following the fundamental procedure of James [9], we construct the so-called self-matching solutions of the SUSY-related equations (11) and (12) for the zeroth cell which allows us to build the Bloch solutions on the entire range of x . We proceed further by writing the SPPS representation of the associated Hill discriminants which allows us to describe the spectrum of the SUSY-related equations (11) and (12) in a simple way. For doing this we choose to use a numerically calculated solution instead of the exact one given in the preceding section. First, because the SPPS approach is clearly more universal and can be applied in situations when the exact solution is unavailable. Second, and more important for this work is that all the following constructions imply the computation of solutions for a large set of different values of the spectral parameter K^2 , while the exact solutions involving the hypergeometric functions have been proved considerably less practical than the approximate solutions obtained below. The SPPS method allows one to construct a solution in the form of a power series with respect to the parameter K^2 which is ideally suited for our purposes. Compared to the use of exact solutions it gives us the possibility to calculate a solution for different values of K^2 in a more efficient way. From Figs. (1) and (2) one can assess the excellent agreement displayed by the zeroth-cell solutions obtained using both methods for a given set of the spectral parameter K^2 .

3.1 Self-matching cell solutions

Now we begin with the equation for f_c on the zeroth cell $x \in [0, \Lambda]$ in order to construct the so-called self-matching pair of independent cell solutions F_{\pm} [9].

To obtain these special solutions it is necessary first to have two linearly independent solutions f_1 and f_2 satisfying the following initial conditions

$$\begin{aligned} f_1(0, K^2) &= 1, & f_2(0, K^2) &= 0, \\ f_1'(0, K^2) &= 0, & f_2'(0, K^2) &= 1. \end{aligned} \quad (25)$$

The method of spectral parameter power series (SPPS) [10, 11] gives these solutions in explicit form as follows. Let f_0 be a particular solution of $-f_0'' + \nu_1 f_0 = K_0^2 f_0$ such that $f_0 \in C^2(0, \Lambda)$ together with $\frac{1}{f_0}$ are bounded on $[0, \Lambda]$. The general solution f_c has the form $f_c = C_1 f_1 + C_2 f_2$, with

$$\begin{aligned} f_1(x) &= \frac{f_0(x)}{f_0(0)} \tilde{\Sigma}_0(x) + f_0'(0) f_0(x) \Sigma_1(x), \\ f_2(x) &= -f_0(0) f_0(x) \Sigma_1(x), \end{aligned} \quad (26)$$

where $\tilde{\Sigma}_0$ and Σ_1 are the spectral parameter power series $\tilde{\Sigma}_0(x) = \sum_{n=0}^{\infty} \tilde{X}^{(2n)}(x) (K^2 - K_0^2)^n$, $\Sigma_1(x) = \sum_{n=1}^{\infty} X^{(2n-1)}(x) (K^2 - K_0^2)^{n-1}$ with the coefficients \tilde{X} , X given by the following recursive relations

$$\tilde{X}^{(0)} \equiv 1, \quad X^{(0)} \equiv 1, \quad (27)$$

$$\tilde{X}^{(n)}(x) = \begin{cases} \int_0^x \tilde{X}^{(n-1)}(\xi) f_0^2(\xi) d\xi & \text{for an odd } n \\ \int_0^x \tilde{X}^{(n-1)}(\xi) \frac{d\xi}{-f_0^2(\xi)} & \text{for an even } n \end{cases} \quad (28)$$

$$X^{(n)}(x) = \begin{cases} \int_0^x X^{(n-1)}(\xi) \frac{d\xi}{-f_0^2(\xi)} & \text{for an odd } n \\ \int_0^x X^{(n-1)}(\xi) f_0^2(\xi) d\xi & \text{for an even } n. \end{cases} \quad (29)$$

The solution f_0 is given by (24) and corresponds to the particular value of $K_0^2 = -(k_0 + s)^2$ which represents a band edge.

One can check by a straightforward calculation that the solutions f_1 and f_2 fulfill the initial conditions (25). In Fig. 1 we plot the series solutions f_1 and f_2 evaluated by (26) by a solid line and the markers represent the exact solutions calculated taking the appropriate linear combinations of $f_{c,1}$ and $f_{c,2}$ given respectively by (18) and (19) in order to fulfill the same initial conditions.

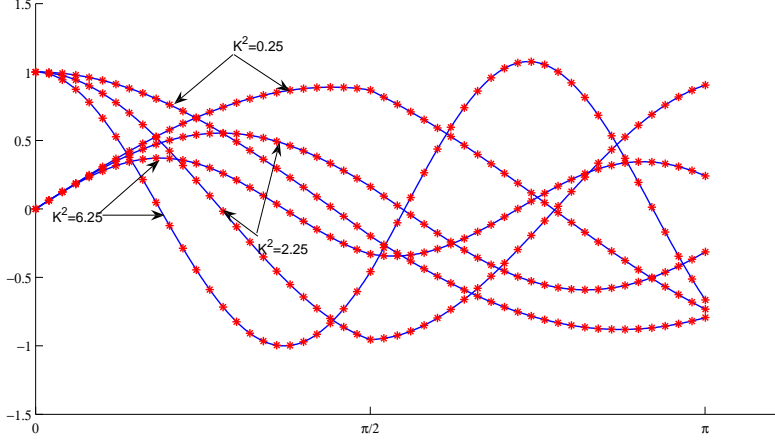


Fig. 1. The solid lines represent the series solutions f_1 and f_2 evaluated by (26) and the markers represent the exact solutions (18) and (19). The values of the parameters S and k_0 are $0.1i$ and 1 , respectively.

Denoting now

$$\begin{aligned} f_1(\Lambda, K^2) &= a_{11}(K^2), & f_2(\Lambda, K^2) &= a_{12}(K^2), \\ f'_1(\Lambda, K^2) &= a_{21}(K^2), & f'_2(\Lambda, K^2) &= a_{22}(K^2), \end{aligned}$$

one can write the self-matching solutions F_{\pm} in the form

$$F_{\pm}(x, K^2) = f_1(x, K^2) + \alpha_{\pm} f_2(x, K^2),$$

where α_{\pm} solve the equation $a_{12}\alpha_{\pm}^2 + (a_{11} - a_{22})\alpha_{\pm} - a_{21} = 0$ [9].

To obtain the self-matching solutions to the equation (12) we first construct the solutions g_1 and g_2 which satisfy the initial conditions $g_1(0, K^2) = g'_2(0, K^2) = 1$ and $g_2(0, K^2) = g'_1(0, K^2) = 0$. For this taking the following linear combinations

$$\tilde{f}_1(x) = \frac{1}{K^2} (Sf_1(x) + (S^2 + K^2) f_2(x)) \quad \text{and} \quad \tilde{f}_2(x) = \frac{1}{K^2} (f_1(x) + Sf_2(x))$$

and applying the Darboux transformation (14) to them gives

$$g_1(x) = \tilde{f}'_1(x) - \Phi_1(x)\tilde{f}_1(x) \quad \text{and} \quad g_2(x) = \tilde{f}'_2(x) - \Phi_1(x)\tilde{f}_2(x). \quad (30)$$

Illustrative plots of the latter solutions are displayed in Fig. (2) in solid lines, while the markers correspond to the exact formulas (20) and (21). Notice also that all the singularities of the above solutions are contained in the Darboux transformation function $\Phi_1(x) = S - k_0 \tan k_0 x$.

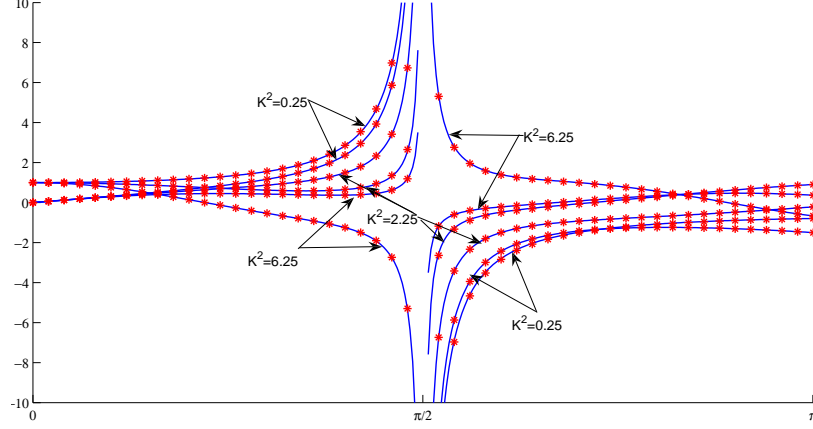


Fig. 2. Series and exact solutions g_1 and g_2 evaluated by (30) and (20) and (21), respectively, for the same parameters as in Fig. 1.

By analogy with the f -case we denote

$$\begin{aligned} g_1(\Lambda, K^2) &= b_{11}(K^2), & g_2(\Lambda, K^2) &= b_{12}(K^2), \\ g'_1(\Lambda, K^2) &= b_{21}(K^2), & g'_2(\Lambda, K^2) &= b_{22}(K^2), \end{aligned}$$

and the self-matching solutions G_{\pm} have the form

$$G_{\pm}(x, K^2) = g_1(x, K^2) + \beta_{\pm} g_2(x, K^2),$$

where β_{\pm} are roots of the equation $b_{12}\beta_{\pm}^2 + (b_{11} - b_{22})\beta_{\pm} - b_{21} = 0$.

3.2 Bloch solutions

We are now in a position to write down the Bloch (quasi-periodic) solutions to the equation (11) through the whole range of x divided as follows $n\Lambda \leq x < (n+1)\Lambda$ for $n = 0, \pm 1, \pm 2, \dots$

$$f_{\pm}(x, K^2) = r_{\pm}^n F_{\pm}(x - n\Lambda, K^2) = r_{\pm}^n [f_1(x - n\Lambda, K^2) + \alpha_{\pm} f_2(x - n\Lambda, K^2)]. \quad (31)$$

The Bloch factors r_{\pm} are a measure of the rate of increase (or decrease) in magnitude of the self-matching solutions $F_{\pm}(x, K^2)$ when one goes from the left end of the cell to the right one, i.e.,

$$r_{\pm}(K^2) = \frac{F_{\pm}(\Lambda, K^2)}{F_{\pm}(0, K^2)}.$$

The values of r_{\pm} can be also written as

$$r_{\pm}(K^2) = \frac{1}{2} \left(D_f(K^2) \mp \sqrt{D_f^2(K^2) - 4} \right),$$

where $D_f(K^2)$ denotes Hill's discriminant (also known as Lyapunov function) associated with (11) [3] and $D_f(K^2) = a_{11} + a_{22}$. For equation (12) the Hill discriminant is given by $D_g(K^2) = b_{11} + b_{22}$. Using the relations (30) between the solutions g_1, g_2 and f_1, f_2 the identity $D_f(K^2) \equiv D_g(K^2)$ can be easily obtained. This means that the Bloch factors for the quasi-periodic solutions to equation (12) are the same as for (11). Thus, for a numerable set of cells, $n\Lambda \leq x < (n+1)\Lambda$ for $n = 0, 1, 2, \dots$, one can write

$$g_{\pm}(x, K^2) = r_{\pm}^n G_{\pm}(x - n\Lambda, K^2) = r_{\pm}^n [g_1(x - n\Lambda, K^2) + \beta_{\pm} g_2(x - n\Lambda, K^2)]. \quad (32)$$

In Fig. 3 the Bloch solutions (31) and (32) are plotted with solid and dotted lines respectively.

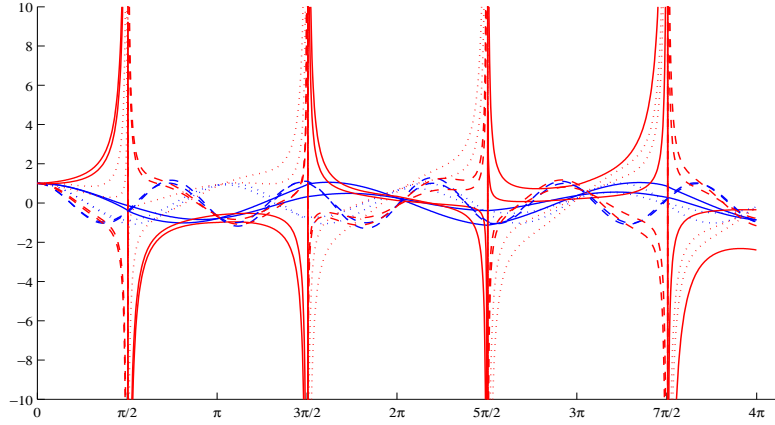


Fig. 3. The blue lines are the solutions f_{\pm} given by (31) and the red lines represent the solutions g_{\pm} given by (32) for the same values of the parameters as previously and for $K^2 = 0.25$ (solid lines), 2.25 (dotted lines), and 6.25 (dashed lines).

3.3 A power series representation for the Hill discriminant

The Hill discriminant (Lyapunov function) allows one to describe the spectrum of periodic differential equations. Namely, the spectrum of (11) and (12) is given by the following set [2] $\{K^2 : D_f(K^2) \in \mathbf{R} \text{ and } |D_f(K^2)| \leq 2\}$. The expression for $D_f(K^2) = a_{11} + a_{22}$ can be written in a simple explicit form. For this we write a_{11} and a_{22} in form of a spectral parameter power series using (26) and taking into account that $\frac{d}{dx}\Sigma_1(x) = \frac{1}{-f_0^2(x)}\Sigma_0(x)$, where $\Sigma_0(x) = \sum_{n=0}^{\infty} X^{(2n)}(x)(K^2 - K_0^2)^n$:

$$a_{11} = \frac{f_0(\Lambda)}{f_0(0)}\tilde{\Sigma}_0(\Lambda) + f_0'(0)f_0(\Lambda)\Sigma_1(\Lambda) \text{ and } a_{22} = -f_0(0)f_0'(\Lambda)\Sigma_1(\Lambda) + \frac{f_0(0)f_0(\Lambda)}{f_0^2(\Lambda)}\Sigma_0(\Lambda).$$

Since $f_0(x)$ is a Λ -periodic function: $f_0(0) = f_0(\Lambda)$. Finally, writing the explicit expressions for $\tilde{\Sigma}_0(\Lambda)$ and $\Sigma_0(\Lambda)$ we obtain a representation for the Hill

discriminant associated with (11) and (12)

$$D_f(K^2) \equiv D_g(K^2) = \sum_{n=0}^{\infty} \left(\tilde{X}^{(2n)}(\Lambda) + X^{(2n)}(\Lambda) \right) (K^2 - K_0^2)^n. \quad (33)$$

Thus, only one particular nodeless periodic solution $f_0(x)$ of (11) is needed for the construction of the Hill discriminant $D_f(K^2)$. There are other known series representations of the Hill discriminant, see [3, 19]. Nevertheless none of them allows one to represent it as a spectral parameter power series which is extremely useful for calculations involving different values of the spectral parameter.

Figure 4 shows the plot of $D_f(K^2)$ which we evaluate in two ways. With the solid line we plot the function $D_f(K^2)$ obtained by means of the SPPS solutions given by (33) and the markers correspond to $D_f(K^2)$ obtained with the exact solutions (18) and (19). From (33) the advantage of the SPPS method for calculating the Hill discriminant and hence the corresponding spectrum can be assessed. Using the SPPS the calculation of the value of the Hill discriminant for every value of its argument reduces to a simple substitution of the value of K^2 into an easily evaluated expression (33). The values of K^2 for which $D_f(K^2) = \pm 2$ correspond to the band edges of the spectrum. Notice that $D_f(K^2) = \pm 2$ is in accordance with (22) and (23), namely $D_f(K^2) = 2$ exactly for $K^2 = (k_0 - iS)^2 - (2nk_0)^2$ and $D_f(K^2) = -2$ when $K^2 = (k_0 - iS)^2 - ((2n+1)k_0)^2$.

When $D(K^2) \neq \pm 2$, the general solutions of (11) and (12) have the form (understanding that it refers to the whole x axis henceforth)

$$f_c(x) = C_+ f_+(x) + C_- f_-(x) \quad \text{and} \quad g_c(x) = \tilde{C}_+ g_+(x) + \tilde{C}_- g_-(x)$$

For the values of K^2 giving $D_f(K^2) = \pm 2$, two pairs of independent solutions $f_+(x, K^2)$, $f_-(x, K^2)$ and $g_+(x, K^2)$, $g_-(x, K^2)$ reduce to a pair of a single solutions $f_+(x, K^2) \equiv f_-(x, K^2)$ and $g_+(x, K^2) \equiv g_-(x, K^2)$, but there is a definite prescription for the construction of an independent second solution [9].

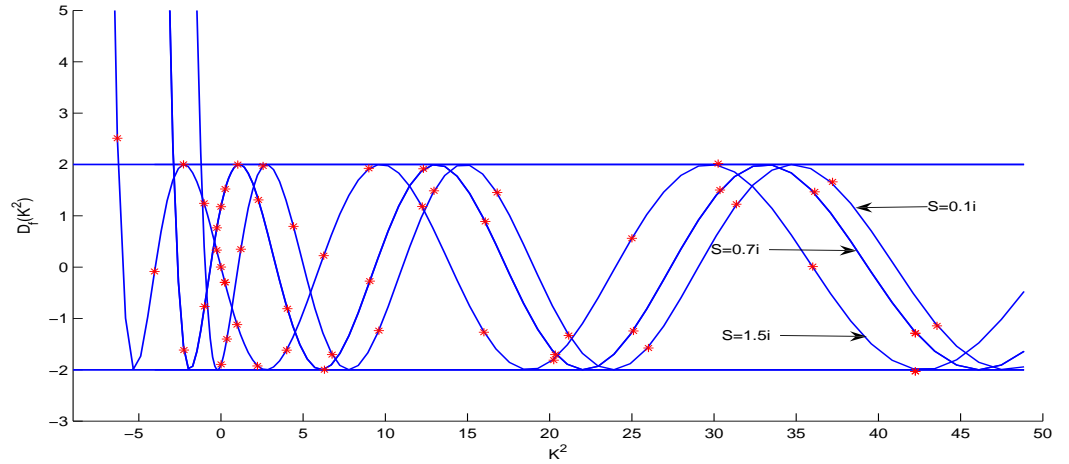


Fig. 4. The Hill discriminant $D_f(K^2)$ evaluated using SPPS solutions (26) (solid line) and by the exact solutions (18) and (19) (markers) for $S = \{0.1i, 0.7i, 1.5i\}$.

4 Conclusions

We have used one particular solution of simple Riccati equations of constant parameters to build the corresponding supersymmetric partner Sturm-Liouville equations. The latter equations are solved analytically in terms of hypergeometric functions. Furthermore we worked with Kravchenko's spectral parameter power series solutions that are better suited from the algorithmic (numerical) standpoint and allows an easy implementation of the old self-matching procedure of H.M. James [9] for solving periodic Sturm-Liouville problems of Schrödinger type in terms of Bloch solutions. We also obtain an effective power series representation of the Hill discriminant in terms of the Kravchenko series. The mathematical procedure expounded in this paper can be applied to more general periodic SL equations that abound in the area of nanostructured materials and in the form of periodic Helmholtz equations in photonics. Other applications can be foreseen in the areas of chirp technology, see for example Refs. [20] and [21].

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