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A variational modification of the Harmonic Balance method to obtain approximate Floquet exponents

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We propose a modification of a method based on Fourier analysis to obtain the Floquet characteristic exponents for periodic homogeneous linear systems, which shows a high precision. This modification uses a variational principle to find the correct Floquet exponents among the solutions of an algebraic equation. Once we have these Floquet exponents, we determine explicit approximated solutions. We test our results on systems for which exact solutions are known to verify the accuracy of our method including one-dimensional periodic potentials of interest in quantum physics. Using the equivalent linear system, we also study approximate solutions for homogeneous linear equations with periodic coefficients.

KEYWORDS

Floquet exponents, harmonic balance, variational methods

MSC CLASSIFICATION

34A34, 34A99

1 | INTRODUCTION

Linear periodic differential equations and systems of equations have an enormous presence in theoretical physics and engineering: harmonic oscillator, little oscillations, vibrations, etc. However, there is a limited number of them that can be exactly solvable. In most cases, numerical methods are the only available. In order to obtain solutions of linear systems with periodic coefficients, one obtains the so called Floquet or characteristic exponents that determine a fundamental matrix for the system. This determination is usually given by a numerical approximation. In the case of linear equations with periodic non-constant coefficients, we always have the possibility of constructing the associated linear system, where the coefficients are again periodic, and then solving the system by means of the Floquet exponents.

One of the most popular procedures to give approximate solutions for linear differential equations with periodic coefficients uses truncated Fourier series, whose coefficients are determined by the widely used Harmonic Balance method.¹⁻⁴ A modification of this method, which is particularly suitable for the Mathieu equation and other Hill type equations, has been proposed in Gadella et al.⁵ This modification consists in a non-perturbative semi-analytic method to find approximate solutions of Hill type equations. The characteristic value is determined through algebraic functions so as to obtain the periodic solution. This method does not restrict the value of the Mathieu coefficient.

Precisely, the Harmonic Balance method has been used as an intermediate tool in order to obtain an approximation of the Floquet exponents for linear systems with periodic coefficients.⁶ Lazarus and Thomas⁶ mix the Harmonic Balance, one numerical asymptotic method, and the Hill method in order to compute the stability of the continued periodic solutions.

In the present paper, we introduce a modification of the procedure in Lazarus and Thomas⁶ including a variational principle, which gives the Floquet exponents as the critical values of this variational principle. This is easy to use and provides a great accuracy for the Floquet exponents and solutions as an added value. We have tested our procedure in specific examples such as the Mathieu equation and others. This method is primarily targeted to obtain the Floquet exponents of linear periodic systems, although the application to obtain analytic algebraic approximate solutions of linear differential equations with periodic coefficients is then straightforward.

This consideration of the Floquet coefficients as critical points of a variational problem is what makes our point of view different from previous methods including those in Lazarus and Thomas.⁶

Before a description of our method and for the benefit of the reader, let us begin with an account of some important and well known results, which are relevant in our presentation.⁷

Let $A(t)$ be an $n \times n$ real matrix with continuous entries on the variable t and $\mathbf{x}(t) \in \mathbb{R}^n$ for each value of t . In addition, all these entries are periodic with the same period T , so that $A(t + T) = A(t)$ for all t . Let us consider a linear system of the form

$$\dot{\mathbf{x}}(t) = A(t)\mathbf{x}(t), \quad (1)$$

where the dot means derivative with respect to t . The Floquet theory that refers to this type of systems is well known.⁷⁻¹⁰ In the sequel, we recall some interesting well known facts that are useful in our discussion⁷:

- i. If $\Phi(t)$ is a fundamental matrix of (1), $\Phi(t + T)$ is again a fundamental matrix. As is the case for any pair of two fundamental matrices, there must be a constant invertible matrix C such that

$$\Phi(t + T) = \Phi(t)C. \quad (2)$$

Since C is invertible, it must exist a $n \times n$ matrix B such that

$$C = e^{BT}, \quad (3)$$

where T is again the period for $A(t)$.

- ii. Consider the matrix $P(t) := \Phi(t)e^{-Bt}$. Then, $P(t)$ is periodic with period T and $P(t)$ is invertible.
- iii. Let us consider the following new indeterminate $\mathbf{y}(t)$ as

$$\mathbf{y}(t) = P^{-1}(t)\mathbf{x}(t). \quad (4)$$

Since $\Phi(t)$ is a fundamental matrix of (1) and, considering the definition of $P(t)$, we have that

$$\dot{P}(t) = A(t)P(t) - P(t)B, \quad (5)$$

where $A(t)$ and B are as in (1) and (3), respectively. Since $P(t)$ is invertible, using (4) gives

$$\dot{\mathbf{y}} = B\mathbf{y}. \quad (6)$$

Thus, system (1) is equivalent to a system with constant coefficients. We shall recall in a moment on the importance of the matrix B .

- iv. Then, if we define an initial condition $\mathbf{x}(t_0) := P(t_0)\mathbf{y}(t_0)$ and taking into account that the solution of (6) satisfying the initial condition $\mathbf{y}(t_0)$ is given by

$$\mathbf{y}(t) = e^{(t-t_0)B}\mathbf{y}(t_0), \quad (7)$$

we have that

$$\mathbf{x}(t) = P(t)e^{(t-t_0)B}P^{-1}(t_0)\mathbf{x}(t_0). \quad (8)$$

Let us choose as $\mathbf{y}(t_0)$ the eigenvector \mathbf{y}_0 of B with eigenvalue λ_0 , i.e., $B\mathbf{y}_0 = \lambda_0\mathbf{y}_0$, where λ_0 is any of the eigenvalues of B . Then, if $\mathbf{x}_0 := P(t_0)\mathbf{y}(t_0) = P(t_0)\mathbf{y}_0$, one has

$$\mathbf{y}(t) = e^{(t-t_0)\lambda_0}\mathbf{y}_0 \implies \mathbf{x}(t) = P(t)e^{(t-t_0)\lambda_0}P^{-1}(t_0)\mathbf{x}_0, \quad (9)$$

expression, which may be written as

$$\mathbf{x}(t) = \boldsymbol{\eta}(t)e^{(t-t_0)\lambda_0}, \quad \text{with} \quad \boldsymbol{\eta}(t) = P(t)P^{-1}(t_0)\mathbf{x}_0. \quad (10)$$

Since $P(t)$ is periodic with period T , Equations (9) and (10) show that $\boldsymbol{\eta}(t)$ is also periodic with period T .

In summary, we can obtain particular solutions of (1) if we can determine the eigenvalues of the matrix B . This eigenvalues are usually called *Floquet characteristic exponents* or *Floquet exponents* or simply *characteristic exponents*. We shall keep this terminology along our manuscript. There are no general analytic methods to obtain these characteristic exponents, and, hence, numerical methods for their determination are in order.

In the present article, we propose an analytic approximate method in order to obtain the characteristic coefficients, with the following organization: In Section 2, we give a standard method to obtain the Floquet characteristic coefficients, important for a comparison with our proposed method. We introduce our analytic algebraic approximation method in Section 3, more precisely on Section 3.1, where we propose the variational principle to obtain the Floquet critical exponents. Section 4 is devoted to a test using the Mathieu equation. In Section 5, we consider two or more dimensional systems in which each component may have different variation rates. In Section 6, we test our results on models of interest in physics. We close the paper with some concluding remarks.

2 | DETERMINATION OF THE CHARACTERISTIC EXPONENTS: STANDARD METHOD

Let us go back to Equation (1), in which $A(t)$ is periodic with period T . As initial values, we may choose any of the vectors of the canonical basis in \mathbb{R}^n , i.e., those vectors with all components equal to zero except the i th component, which is equal to one. Once we have chosen an initial value, a numerical integration such as a fourth order Runge-Kutta¹³ permits us to obtain n discrete linearly independent solutions on the finite interval $(0, T)$, where T is the period. Then, by using interpolation, for instance with splines, we obtain an approximate continuous solution. Using the initial conditions, we obtain n approximate linearly independent solutions $X_1(t), X_2(t), \dots, X_n(t)$, whose columns determine an approximate fundamental matrix $\Phi(t)$. This procedure is rather simple for $n = 2$, which will be our case.

After (2) and (3), we readily obtain

$$C := \exp\{BT\} = \Phi^{-1}(0)\Phi(T). \quad (11)$$

The relation between the eigenvalues δ_i of C and the characteristic coefficients λ_i is well known:

$$\lambda_i = \frac{1}{T} \log \delta_i, \quad i = 1, 2, \dots, n. \quad (12)$$

Thus, we have determined the characteristic coefficients and the numerical solution $X(t)$. We have to take into account that the imaginary part of the characteristic coefficients is not uniquely determined since

$$\delta_i = \exp\{\lambda_i + 2\pi i/T\}T = e^{\lambda_i T}. \quad (13)$$

Our choice will always fix this imaginary part in such a way that the exponent coincides with $\lambda_i T$, being λ_i an eigenvalue of B .

The objective of the present article is to show that a good approximation on the characteristic coefficients may be obtained through an algebraic analytic approximation based on Fourier analysis.

3 | APPROXIMATED ANALYTIC SOLUTION

The relation between first-order linear systems of the form (1) and linear equations of order n is well known.⁷ With this idea in mind, let us illustrate our method with second-order linear differential equations of the form:

$$\ddot{y}(t) + a(t)\dot{y}(t) + b(t)y(t) = 0, \quad (14)$$

where $a(t)$ and $b(t)$ are periodic functions with respective periods T_a and T_b , which are not arbitrary, since we have to impose the condition that the ratio T_a/T_b be rational. In addition, $a(t)$ is continuously differentiable and $b(t)$ continuous. The linear system equivalent to (14) is $(z_1(t) := y(t), z_2(t) = \dot{y}(t))$

$$\begin{pmatrix} \dot{z}_1(t) \\ \dot{z}_2(t) \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -b(t) & -a(t) \end{pmatrix} \begin{pmatrix} z_1(t) \\ z_2(t) \end{pmatrix} \iff \dot{\mathbf{z}}(t) = A(t)\mathbf{z}(t). \quad (15)$$

With the change

$$y(t) = x(t) \exp \left\{ -\frac{1}{2} \int a(t) dt \right\}, \quad (16)$$

Equation (14) yields to

$$\ddot{x}(t) + f(t)x(t) = 0, \quad (17)$$

with

$$f(t) = b(t) - \frac{1}{2}a'(t) - \frac{1}{4}a^2(t). \quad (18)$$

The function $f(t)$ is continuous and periodic with a period $T = \max(T_a, T_b)$. By the Floquet characteristic exponents, or just characteristic exponents, of (14), we mean the characteristic exponents of the associated system (15). Analogously, the characteristic exponents of (17) are the characteristic exponents of its related system.

Let us list in the sequel some of the properties of Equation (14):

- Assume that

$$f(t) > 0 \quad \text{and} \quad T \int_0^T f(t) dt \leq 4. \quad (19)$$

Then, it has been proven in Chicone⁸ that all solutions are bounded. Consequently, the characteristic exponents of (14) do not have positive real part.

- If $f(t) < 0$, let us multiply (14) by $y(t)$ and integrate by parts. Then, we have

$$\frac{d}{dt} y^2(t) = \int [y'(t)]^2 dt - \int f(t) y^2(t) dt > 0. \quad (20)$$

Since $y^2(t) \leq 0$, we note that for large values on the variable t , $t \mapsto \infty$, the solution $y(t)$ is not bounded.

Consequently, the characteristic coefficients must have a positive real part.

- Let us go to Equation (17). It can be proven^{8,9} that the sum of its characteristic exponents is equal to zero.

3.1 | The method

Consider Equation (17) and assume that λ is one of its characteristic exponents. Choosing for simplicity $t_0 = 0$, we go back to (17) where it was stated that for each Floquet exponent, there is a solution of the type $x(t) = \eta(t)e^{\lambda t}$, where $\eta(t)$ is periodic with period T .^{*} The point is that $\eta(t)$ and λ are unknown, and our objective is to find an approximate expression for them. Using this result in (17), we obtain the following differential equation:

$$\ddot{\eta}(t) + 2\lambda\dot{\eta}(t) + (\lambda^2 + f(t))\eta(t) = 0. \quad (21)$$

^{*}We may assume that a basis of solutions is of this form, provided that B be diagonalizable.

We have obtained a second-order equation with a periodic coefficient $f(t)$ with period T . Let us expand $\eta(t)$ into Fourier series and then truncate this series. The truncated solution $\eta_n(\lambda, t)$ is

$$\eta_n(\lambda, t) = \frac{a_0}{2} + \sum_{k=1}^n \{a_k \cos(k\omega t) + b_k \sin(k\omega t)\}, \quad (22)$$

with $\omega := 2\pi/T$. Now, $x_n(t) = z_n(t, \lambda) \exp(\lambda t)$.

In order to determine the characteristic exponent λ , we propose the following strategy:

- i. First of all, we determine the coefficients a_k and b_k by means of the Harmonic Balance (HB) method.¹⁻³ In summary, we replace (22) into (21) so as to obtain a new Fourier polynomial. Since Equation (20) must be satisfied, coefficients for the harmonics in this Fourier polynomial must vanish. This yields to an homogeneous linear algebraic system of dimension $2n + 1$, with indeterminates a_0, a_k and b_k and $k = 1, 2, \dots, n$. In order to obtain non-trivial solutions, the determinant Δ of the matrix of the system of the coefficients must vanish. Since (21) is linear, this determinant is a polynomial on λ , so that

$$\Delta(\lambda) = 0 \quad (23)$$

gives λ in terms of ω and any other parameter appearing in (20). Although (23) has at most n roots, only two of them could be the characteristic exponents we are looking for. Moreover, it is not difficult to check that the coefficients a_k and $b_k, k = 1, 2, \dots, n$ are rational polynomial functions on λ .

- ii. After we have completed the previous step, we shall determine the approximate value of λ by a variational principle. Since the exact solution $x(t)$ satisfies

$$\int_0^T (\ddot{x}(t) + f(t)x(t))^* (\ddot{x}(t) + f(t)x(t)) dt = 0, \quad (24)$$

where the star denotes complex conjugation, we propose that the *approximate characteristic exponent*, λ_k , we are searching for is a *critical point* (usually a minimum) of $E(\lambda)$ defined as

$$E(\lambda) := \int_0^T (\ddot{x}_n(t) + f(t)x_n(t))^* (\ddot{x}_n(t) + f(t)x_n(t)) dt. \quad (25)$$

Note that λ may have an imaginary part and thus $x(t)$. This is the reason why we have to include a complex conjugation in (24)–(25).

Once we have the Floquet characteristic exponents for the given equation, we determine the coefficients a_0, a_k , and $b_k, k = 1, 2, \dots, n$ for the truncated Fourier series that approximates the solution.

Our variational principle is just an Ansatz, which should be confirmed by numerical experiments. This is the main objective of the next section.

4 | APPLICATION: THE MATHIEU EQUATION

The Mathieu equation is a simple non-trivial equation with periodic coefficients which is well suitable as a laboratory in order to test the above ideas as shown by previous work of our group.⁵ The Mathieu equation has been largely studied, as for instance in previous works.¹⁴⁻¹⁹ Let us write the Mathieu equation as

$$\ddot{x}(t) + \omega^2(1 - \alpha \cos t)x(t) = 0. \quad (26)$$

As is well known, two linearly independent solutions are

$$x_1(t) = C \left(4\omega^2, 2\alpha\omega^2, \frac{t}{2} \right), \quad x_2(t) = S \left(4\omega^2, 2\alpha\omega^2, \frac{t}{2} \right), \quad (27)$$

where C and S stand for the Mathieu sine and cosine.¹⁹ These are exact solutions, so that we can determine *exact* characteristic exponents just by constructing a fundamental matrix with them and, then, making use of Equations (12) and (13), which in this case give the exact results.

Now, the objective is clear and is the comparison of the results obtained with our proposed variational method with the exact results that can be obtained as described above. In addition, we shall also compare both with those obtained following the lines introduced in Section 2.

Before proceeding, a couple of comments are in order. First of all, using (19), we see that for $\omega < 1/4$ and for all values of α , the solutions are bounded. Also note that whenever $\lambda = ik$, k being an integer number, the solution is periodic with period equal to 2π . Finally, let us recall that the sum of the critical exponents is equal to zero, an interesting property to take into account when testing our results.

Let us go back to the determinant (23), which we write now as $\Delta(\lambda) \equiv \Delta_{\alpha,\omega}(\lambda)$, due to its dependence on all these three variables. In our case, it is an even polynomial of degree $2(2n + 1)$. Furthermore, in all cases studied, it is also an even polynomial on the variables α and ω . As an example, let us take $n = 2$, so that the polynomial on λ has degree 10:

$$\Delta_{\alpha,\omega}(\lambda) = \sum_{k=0,\text{even}}^{10} c_k \lambda^k. \quad (28)$$

In (28), all odd coefficients vanish, while the even coefficients are given by

$$\begin{aligned} c_0 &= 16\omega^2 + 8(-5 + \alpha^2)\omega^4 + (33 - 14\alpha^2)\omega^6\alpha^2 - \frac{1}{2}(20 - 14 + \alpha^4)\omega^8 - 8\left(1 - \alpha^2 + \frac{3}{16}\alpha^4\right)\omega^{10}, \\ c_2 &= 16 + (35 - 6\alpha^2)\omega^4 + 10(\alpha^2 - 2)\omega^6 + \left(5 - 3\alpha^2 + \frac{3}{16}\alpha^4\right)\omega^8, \\ c_4 &= 40 + 35\omega^2 + 3\alpha^2\omega^4 + (10 - 3\alpha^2)\omega^6, \\ c_6 &= 33 + 20\omega^2 - (-10 + \alpha^2)\omega^4, \\ c_8 &= 5(2 + \omega^2), \\ c_{10} &= 304 + 80\omega^2. \end{aligned} \quad (29)$$

Then, using the Harmonic Balance method that, in this case, is a simple algebraic problem in which the equations that determine the coefficients a_k and b_k are homogeneous and starting with the initial condition $a_1 = 1$, we obtain for the first coefficients the following values:

$$\begin{aligned} b_1 &= \left(-\lambda\alpha^2\omega^4 + 2\lambda\left(-16\lambda^2 - (-4 + \lambda^2 + \omega^2)^2\right)\right) / d_1, \\ b_2 &= -12\lambda\alpha\omega^2(-4 + \lambda^2 + \omega^2) / d_2, \end{aligned} \quad (30)$$

$$\begin{aligned} a_0 &= \frac{1}{\alpha\omega^2} \left\{ 3(-2 + \lambda^2 + \omega^2) - \frac{1}{8\lambda} \left[(16 + 4\lambda^4 - 20\omega^2 - (-4 + \alpha^2)\omega^4 \right. \right. \\ &\quad \left. \left. + \lambda^2(-52 + 8\omega^2) \right) \left(-\lambda\alpha^2\omega^4 + 2\lambda\left(-16\lambda^2 - (-4 + \lambda^2 + \omega^2)^2\right) / d_1 \right] \right\}, \end{aligned} \quad (31)$$

$$a_1 = 1,$$

$$a_2 = -\frac{1}{2} \left[\alpha\omega^2(-16 - 4\lambda^4 + 20\omega^2 + (-4 + \alpha^2)\omega^4 + \lambda^2(52 - 8\omega^2)) \right] / d_2,$$

where

$$\begin{aligned} d_1 &= \frac{1}{4}\alpha^2\omega^4(-4 + \lambda^2 + \omega^2) + (-1 + \lambda^2 + \omega^2)\left(-16\lambda^2 - (-4 + \lambda^2 + \omega^2)^2\right), \\ d_2 &= 4\lambda^6 + 4\lambda^4(7 + 3\omega^2) + \lambda^2(32 - 8\omega^2 - (-12 + \alpha^2)\omega^4) - (-4 + \omega^2)(-16 + 20\omega^2 + (-4 + \lambda^2)\omega^4). \end{aligned} \quad (32)$$

We may obtain similar expressions for higher values of n , although they are increasingly complicated and do not provide of any new information. Once we have obtained the roots λ_k of (23), only two of them can be chosen to be the critical exponents. They are precisely those which minimize (25). Once we have obtained the critical exponents, we readily determine an explicit approximated solution of (17).

As an example, let us choose $\alpha = 0.5$, $\omega = 1$ and $n = 2$. We obtain the following approximate solution:

$$x_A(t) = \exp\left(-\frac{1}{43}t\right) \left(\frac{267}{1069} + \cos t - \frac{4}{45} \cos 2t - \frac{185}{84} \sin t + \frac{15}{83} \sin 2t \right). \quad (33)$$

Note that the general exact solution has the form $x_e(t) = c_1 x_1(t) + c_2 x_2(t)$, where $x_i(t)$, $i = 1, 2$ are given in (26). The constants c_i , $i = 1, 2$ should be determined through the initial conditions $x_e(0) := x_A(0)$ and $\dot{x}_e(0) := \dot{x}_A(0)$, where the dot represents derivative with respect to t . These values are obtained with the expression for $x_A(t)$ in (33).

We know the exact value of the characteristic exponents, which validates our comparison, take one and denote it as λ_e . These characteristic exponents are $\lambda = \pm 1/43$. In order to compare the exact solution with the approximation given in (33), it is natural to choose the exponent with minus sign, so that $\lambda_e = -1/43$. Thus, the exact solution has the form $x_e(t) = e^{\lambda_e t} \eta(t)$; see comments before (21). Since we have determined already $x_e(t)$ through the above initial conditions, we have $\eta(t)$. Then, expand $\eta(t)$ into Fourier series. We obtain an explicit expression of the form:

$$x_e(t) = \exp\left(-\frac{1}{43}t\right) \left(\frac{66}{265} + \frac{486}{487} \cos t - \frac{4}{45} \cos 2t + \frac{1}{340} \cos 3t - \frac{131}{60} \sin t + \frac{7}{39} \sin 2t - \frac{1}{176} \sin 3t + \dots \right). \quad (34)$$

The coefficients in both solutions have been adjusted to a rational number with an error upper bound of 0.07%. The relative difference between approximate (33) and exact (34) solutions is at most less than 0.9%. This is certainly satisfactory. As expected, a higher value of n gives a higher precision. For instance, take $n = 3$, $\alpha = 0.5$ and $\omega = 1$. We have for the approximate and exact solution, respectively, the following results:

$$x_A(t) = \exp\left(-\frac{1}{43}t\right) \left(\frac{267}{1069} + \cos t - \frac{5}{56} \cos 2t + \frac{1}{346} \cos 3t - \frac{376}{171} \sin t + \frac{19}{105} \sin 2t - \frac{1}{178} \sin 3t \right) \quad (35)$$

and

$$x_e(t) = \exp\left(-\frac{1}{43}t\right) \left(\frac{285}{1141} + \cos t - \frac{5}{56} \cos 2t + \frac{1}{346} \cos 3t - \frac{596}{271} \sin t + \frac{19}{105} \sin 2t - \frac{1}{178} \sin 3t \right) + \dots \quad (36)$$

For $n = 3$, $\alpha = 1$ and $\omega = 1$, we obtain analogously:

$$x_A(t) = \exp\left(-\frac{1}{10}t\right) \left(\frac{1}{2} + \cos t - \frac{1}{5} \cos 2t + \frac{1}{69} \cos 3t - \frac{19}{9} \sin t + \frac{1}{3} \sin 2t - \frac{1}{50} \sin 3t \right) \quad (37)$$

and

$$x_e(t) = \exp\left(-\frac{1}{10}t\right) \left(\frac{1}{2} + \cos t - \frac{1}{5} \cos 2t + \frac{1}{69} \cos 3t - \frac{19}{9} \sin t + \frac{1}{3} \sin 2t - \frac{1}{51} \sin 3t \right) + \dots \quad (38)$$

It is important to stress that for $n = 2$ and $n = 3$, we have used different initial conditions so that the exact solutions (36) and (37) do not coincide. These initial conditions are given by the values of $x_A(t)$ and its first derivative at the origin. In particular, for $n = 2$, we have $x(0) = 1.16088$ and $\dot{x}(0) = -1.86793$. For $n = 3$, we have $x(0) = 1.16337$ and $\dot{x}(0) = -1.88083$. Since we have changed the initial conditions, we have changed the solution and therefore the critical exponents could be different, which is the case here.

Observe that we have achieved a better precision. The conclusion is that the higher the harmonic number n is the better accuracy is obtained. This result is quite satisfactory.

In Table 1, we compare the values of the approximate characteristic exponents given by our method, λ_A , the exact, λ_e , and the one determined by the method sketched in Section 2, λ_{num} , for $n = 3$, $\omega = 1$ and different values of α . The precision of $x_A(t)$ is evaluated through the second moment

α	1/10	3/10	5/10	7/10	1
λ_e	9.31603 10^{-4}	8.37695 10^{-3}	2.32152 10^{-2}	4.52826 10^{-2}	9.10175 10^{-2}
λ_A	9.31603 10^{-4}	8.37695 10^{-3}	2.32152 10^{-2}	4.52825 10^{-2}	9.10172 10^{-2}
λ_{num}	9.31620 10^{-4}	8.37697 10^{-3}	2.32151 10^{-2}	4.52826 10^{-2}	9.10175 10^{-2}
S^2	0.	4. 10^{-9}	9. 10^{-8}	6. 10^{-7}	4. 10^{-6}
$E(\lambda)$	2. 10^{-10}	4. 10^{-7}	6. 10^{-6}	7. 10^{-5}	5. 10^{-4}

TABLE 1 Values of λ_e , λ_A , λ_{num} , S^2 and $E(\lambda)$ for some selected values of the parameter α

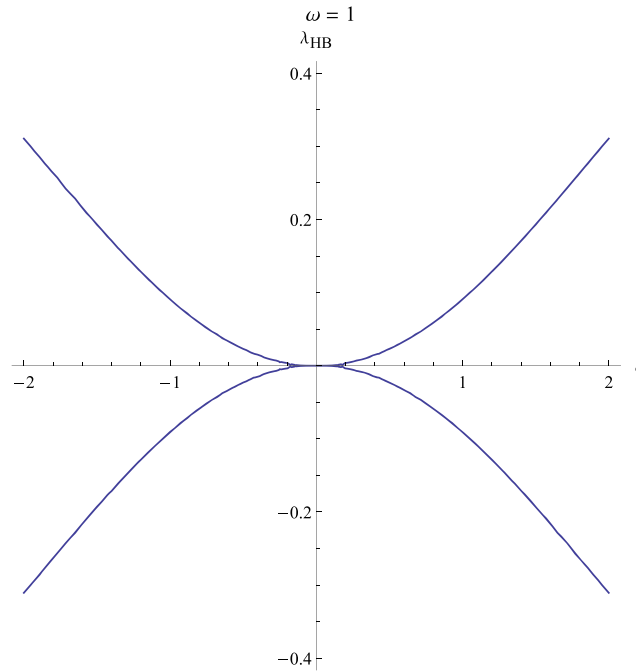


FIGURE 1 Variation of λ_A in terms of α for $n = 2$ and $\omega = 1$ [Colour figure can be viewed at wileyonlinelibrary.com]

$$S^2 := \frac{1}{T} \int_0^T (x_e(t) - x_A(t))^* (x_e(t) - x_A(t)) dt. \quad (39)$$

Finally, we include $E(\lambda)$ given in (24), which measures the deviation of the solution $x_A(t)$ from the exact solution of the differential equation (16). Since the sum of the exponents vanish, we refer only to one of them. Nevertheless, we must say that errors in the method that are always present in this kind of estimations make the sum of both critical exponents not exactly equal to zero. An estimation with six digits of λ_A exactly matches the exact result, while λ_{num} has a minor discrepancy of three units in the last digit. Computational results have been preformed with the use of Mathematica, the CPU time being negligible.

In Figure 1, we plot the dependence of λ_A with α for $n + 2$ and $\omega = 1$. Note that both solutions appear symmetric with respect to the abscise axis. Recall that there are always two solutions whose sum is equal to zero.

We finish this discussion with the presentation of some simple physical models, which can be described via the Mathieu equation. Among all possibilities, let us choose the following one dimensional models:

- The Schrödinger equation of the quantum pendulum is given by

$$-\frac{\hbar^2}{2ml^2} \frac{d^2\psi(\eta)}{d\eta^2} + mgl(1 + \cos \eta)\psi(\eta) = E\psi(\eta), \quad (40)$$

where η is the angle variable.

- The Kapitza pendulum: This is an inverted pendulum for which one point have fast oscillations upwards and downwards. Its equation is given by

$$\ddot{\theta}(t) - \frac{g}{\ell} \sin \theta(t) = \frac{A}{l} \ell \omega^2 \sin \omega t \sin \theta(t). \quad (41)$$

For small oscillations, we have $\sin \theta \approx \theta$ and, consequently, (41) becomes the Mathieu equation, which is now periodic for the variable time t .

- One equation that is reducible to the Mathieu equation is the one-dimensional Schrödinger equation with potential given by

$$V(x) = V_0 \cos^2 \left(\frac{2\pi}{\lambda} x \right), \quad (42)$$

where $V_0 > 0$ and λ is the wave length of two interfering lasers.²⁰

5 | SOLUTIONS GROWING AT DIFFERENT RATES

Along this section, we shall investigate a situation in which the behavior of solutions grow at different rates. Tian and Wang¹⁰ discuss the case in which $A(t)$ and the matrix obtained by integrating its entries with respect to the variable t commute. We are going to explore how to apply our method when this is the case. It is noteworthy that we now have an explicit expression for the fundamental matrix $\Phi(t)$. Let us go back to (1) and pose a result that has been proven in Tian and Wang.¹⁰ Here, we use the following hypothesis:

- i. All entries of $A(t)$ in (1) are integrable on the interval $[0, t]$.
- ii. The matrix $A(t)$ fulfills the following commutation relation:

$$\left[\int_0^t A(v) dv \right] A(t) = A(t) \left[\int_0^t A(v) dv \right], \quad (43)$$

where the integral of a matrix is the matrix resulting of integrating all its entries. A sufficient condition for this commutation is given by Tian and Wang.^{10, corollary 2.3} However, it is not necessary, and we are not using it in this presentation. Our hypothesis is just (43).

Then Tian and Wang,¹⁰ its general solution can be written as $\mathbf{x}(t) = \Phi(t)\mathbf{x}(0)$, where the initial condition $\mathbf{x}(0)$ is arbitrary and the fundamental matrix $\Phi(t)$ is given by

$$\Phi(t) = \exp \left\{ \int_0^t A(v) dv \right\}. \quad (44)$$

Since we are mainly interested in equations of the type (21), we shall restrict ourselves to the case $n = 2$. First of all, let us use the following notation:

$$D(t) := \int_0^t A(v) dv, \quad (45)$$

so that (43) takes the form:

$$D(t)D'(t) = D'(t)D(t). \quad (46)$$

We construct the matrix $D'(t)$ by taken the derivative with respect to t of all entries in $D(t)$. A straightforward integration of (46) shows that there exists two non-zero constants α and β such that, if we denote by $a_{ij}(t)$ the entries of $A(t)$,

$$a_{21}(t) = \alpha a_{12}(t), \quad a_{22}(t) = a_{11}(t) + \beta a_{12}(t), \quad (47)$$

so that

$$D(t) = \begin{pmatrix} f(t) & g(t) \\ \alpha g(t) & f(t) + \beta g(t) \end{pmatrix}, \quad (48)$$

with

$$f(t) = \int_0^t a_{11}(v) dv, \quad g(t) = \int_0^t a_{12}(v) dv. \quad (49)$$

The converse is also true, in the sense that (47) implies (46).

Then, we may obtain the fundamental matrix (44) in the following form:

$$\Phi(t) = Q(t) \exp \left\{ f(t) + \frac{1}{2} \beta g(t) \right\}, \quad (50)$$

with

$$Q(t) = \begin{pmatrix} \cosh\left(\frac{1}{2}\gamma g(t)\right) - \frac{\beta}{\gamma} \sinh\left(\frac{1}{2}\gamma g(t)\right) & \frac{2}{\gamma} \sinh\left(\frac{1}{2}\gamma g(t)\right) \\ \frac{2\alpha}{\gamma} \sinh\left(\frac{1}{2}\gamma g(t)\right) & \cosh\left(\frac{1}{2}\gamma g(t)\right) + \frac{\beta}{\gamma} \sinh\left(\frac{1}{2}\gamma g(t)\right) \end{pmatrix}. \quad (51)$$

Here, $\gamma := \sqrt{4\alpha + \beta^2}$. Observe that the dependence on t of $Q(t)$ comes solely with $g(t)$ and, hence, of $a_{12}(t)$ only. An explicit expression for $\Phi(t)$ is only possible if we know the primitives for $a_{11}(t)$ and $a_{12}(t)$. Otherwise, we have to resort to numerical estimations of $f(t)$ and $g(t)$.

Let us prove that the fundamental matrix is given by (50)–(51). We perform this proof into two steps. First of all, take $\beta = 0$, and then, remove this condition.

i. The case $\beta = 0$. Now, $D(t)$ may be written as

$$D(t) = f(t)I + g(t) \begin{pmatrix} 0 & 1 \\ \alpha & 0 \end{pmatrix}, \quad (52)$$

where I is the identity matrix. Since any matrix commutes with the identity, by exponentiation, we have

$$\Phi(t) = e^{D(t)} = \exp\{f(t)I\} \cdot \exp \left[g(t) \begin{pmatrix} 0 & 1 \\ \alpha & 0 \end{pmatrix} \right]. \quad (53)$$

In order to calculate the second exponential in (53), we proceed by direct exponentiation of the involved matrix. Then, (53) becomes

$$\Phi(t) = \exp\{f(t)\} \begin{pmatrix} 1 + \frac{g^2\alpha}{2} + \frac{g^4\alpha^2}{24} + \dots & g + \frac{g^3\alpha}{6} + \frac{g^5\alpha^2}{120} + \dots \\ \alpha \left(g + \frac{g^3\alpha}{6} + \frac{g^5\alpha^2}{120} + \dots \right) & 1 + \frac{g^2\alpha}{2} + \frac{g^4\alpha^2}{24} + \dots \end{pmatrix}. \quad (54)$$

It is obvious that the entries of the matrix in (54) are Taylor series corresponding to \sinh and \cosh centered at the origin. Thus, we obtain $Q(t)$ as in (48) for $\beta = 0$.

ii. The case $\beta \neq 0$. The procedure is essentially the same. In this case, we decompose $D(t)$ as

$$D(t) = \left\{ f(t) + \frac{\beta}{2}g(t) \right\} I + g(t) \begin{pmatrix} -\beta/2 & 1 \\ \alpha & \beta/2 \end{pmatrix}, \quad (55)$$

so that

$$\Phi(t) = e^{D(t)} = \exp \left\{ f(t) + \frac{\beta}{2}g(t) \right\} \cdot \exp \left\{ g(t) \begin{pmatrix} -\beta/2 & 1 \\ \alpha t & \beta/2t \end{pmatrix} \right\}. \quad (56)$$

Since $A(t)$ is periodic with period T , we have from (2), (3), and $\Phi(T) = e^{D(T)}$, the following relation:

$$C = e^{BT} = \Phi(T) = e^{D(T)}, \quad (57)$$

so that

$$B = \frac{1}{T}D(T). \quad (58)$$

We see that the matrix B of (6) is the average in the mean of $A(t)$. Since the Floquet exponents are the eigenvalues of B , we easily determine these Floquet coefficients. In addition, we provide of an interesting interpretation to the entries of the matrix $A(t)$. Here, the Floquet exponents have the following form:

$$\lambda_{\pm} = \frac{1}{T} \left(f(T) + \frac{1}{2}(\beta \pm \gamma)g(T) \right). \quad (59)$$

It is important to remark that this procedure makes sense if (45) holds. Otherwise, the eigenvalues of $A(t)$ may differ from the critical exponents, as in the case of the Marcus-Yamabe equation to be discussed next. In addition, in our case, the critical exponents also coincide with the eigenvalues of the average of $A(t)$ over a period, which is the matrix given by

$$\overline{A(t)} := \frac{1}{T} \int_0^T A(t) dt. \quad (60)$$

5.1 | An example

The results of the previous subsection allow us to test the method introduced in Section 3. Now, $A(t)$ is a 2×2 periodic matrix so that relations (48) are valid. For the independent entries and parameters in (48), we choose

$$a_{11}(t) = -1, \quad a_{12}(t) = 2 + \sin t, \quad \alpha = -1, \quad \beta = 0. \quad (61)$$

Relations (61) fully determine $A(t)$, which is periodic with period 2π . Using (10) and (11), we have

$$\Phi(t) = e^{-t} \begin{pmatrix} \cos(1 + 2t - \cos t) & \sin(1 + 2t - \cos t) \\ -\sin(1 + 2t - \cos t) & \cos(1 + 2t - \cos t) \end{pmatrix}. \quad (62)$$

Using these data, let us write Equation (1) as a second order linear equation. This gives

$$(2 + \sin t)\ddot{x}(t) + (4 - \cos t + 2 \sin t)\dot{x}(t) + (10 - \cos t + 13 \sin t + 6\sin^2 t + \sin^3 t)x(t) = 0. \quad (63)$$

Next, we determine the critical exponents by our method for $n = 3$. The result is a double $\lambda_A = -1 - 1.9998i$ (we recall that the exponents are unique modulus $k\pi i/T$, k being integer). Here, it is possible to obtain the exact value, which gives $\lambda_e = -1 - 2i$. The conclusion is that our method gives far more precision than the standard numerical method.

Finally, let us integrate (63) using our method, approaching coefficients by their nearest rational number and use trigonometric relations. We have the following approximation for the solution:

$$x_A(t) = e^{-t} \left(\frac{1}{8}i + \frac{8}{17} \cos t - \frac{7}{8}i \cos(2t) + \frac{1}{2} \cos(3t) + \frac{1}{8}i \cos(4t) - \frac{1}{42} \cos(5t) - \frac{10}{19}i \sin t - \frac{26}{30} \sin(2t) - \frac{1}{2}i \sin(3t) + \frac{1}{8} \sin(4t) + \frac{1}{42}i \sin(5t) + \dots \right). \quad (64)$$

Using (62), let us obtain the first terms of the exact solution by using the initial conditions $x(0) = x_A(0)$ and $\dot{x}(0) = \dot{x}_A(0)$ and expanding the entries of $\Phi(t)$ in Fourier series. The result is

$$x_e(t) = e^{-t} \left(\frac{1}{8}i + \frac{7}{15} \cos t - \frac{7}{8}i \cos(2t) + \frac{1}{2} \cos(3t) + \frac{1}{8}i \cos(4t) - \frac{1}{45} \cos(5t) - \frac{6}{7}i \sin t - \frac{26}{30} \sin(2t) - \frac{1}{2}i \sin(3t) + \frac{1}{8} \sin(4t) + \frac{1}{45}i \sin(5t) + \dots \right). \quad (65)$$

The coincidence between both results is high showing the remarkable accuracy of our method.

5.2 | A second example: The Marcus-Yamabe equation

As a second example, let us consider the Marcus-Yamabe system, which is of second order. This has been given as a counter-example of a periodic system such that the eigenvalues of $A(t)$ are constant, i.e., independent of t , equal to $(-1 \pm \sqrt{7}i)/4$ and yet being the zero solution not stable.^{9,11} The Marcus Yamabe system is of the form (1), with matrix $A(t)$ given by

$$A(t) = \begin{pmatrix} -1 + \frac{3}{2} \cos^2 t & 1 - \frac{3}{2} \cos t \sin t \\ -1 - \frac{3}{2} \cos t \sin t & -1 + \frac{3}{2} \sin^2 t \end{pmatrix}. \quad (66)$$

System (64) has two linearly independent solutions of the form:

$$\mathbf{x}_1(t) = \begin{pmatrix} -\cos t \\ \sin t \end{pmatrix} e^{t/2}, \quad \mathbf{x}_2(t) = \begin{pmatrix} \sin t \\ \cos t \end{pmatrix} e^{-t}. \quad (67)$$

It is easy to write the associated differential equation of the Marcus-Yamabe system, the Marcus-Yamabe equation. This is

$$(8 - 6 \sin 2t)\ddot{x}(t) + (4 + 12 \cos 2t - 3 \sin 2t)\dot{x}(t) + (-5 + 3 \cos 2t + 9 \sin 2t)x(t) = 0. \quad (68)$$

This equation does not have singular points. Its Floquet characteristic coefficients are -1 and $1/2$; see (67). If we apply the method introduced in Section 3 with $n = 3$, we obtain the same critical exponents and the following basis of the space of solutions:

$$x_1(t) = e^{-t} \sin t, \quad x_2(t) = e^{t/2} \cos t, \quad (69)$$

with coincide with the exact solution as we see from (67). The conclusion is that our approximate method has yield to the exact solution with $n = 3$.

5.3 | A third simple example

Dieci et al¹² propose a multiple shooting method combined with continuous orthonormalization in order to solve multi-periodic problems. We want to comment one of their examples and show that we arrive to the same solution using the ideas we have introduced in the present section. In fact, we choose their example 5.2, in which

$$A(t) = \begin{pmatrix} 0 & \beta \sin(\alpha t) \\ -\beta \sin(\alpha t) & 0 \end{pmatrix}. \quad (70)$$

Let us choose $\alpha = \beta = 1$ for simplicity. Note that in (70), we have used the notation in Dieci et al,¹² so that the parameters α and β in this matrix have nothing to do with others previously introduced by us.

Then, after (60), we conclude that the average matrix $\bar{A}(t)$ is the zero matrix, so that the critical exponents are zero. In consequence, all solutions are periodic.

Following the above notation, we have

$$f(t) \equiv 0, \quad g(t) \equiv 1 - \cos t. \quad (71)$$

Consequently, matrix $D(t)$ defined in (45) satisfies the commutation relation (46). Observe that γ in (51) is here given by $\gamma = 2i$, so that the fundamental matrix $\Phi(t)$ obtained after (50)–(51), is now given by

$$\begin{pmatrix} \cos(1 - \cos t) & \sin(1 - \cos t) \\ -\sin(1 - \cos t) & \cos(1 - \cos t) \end{pmatrix}, \quad (72)$$

which is exactly the result given in Dieci et al.¹²

6 | SOME MODELS OF INTEREST IN PHYSICS

In this section, we propose some other examples of application of the general formalism as described in Sections 2 and 3. All the following examples are one-dimensional quantum models of interest in physics, are periodic and governed by a second order linear equation such as the Schrödinger equation. We intend to develop with some detail one of them and leave the others for the reader consideration.

- Schrödinger equation with potential given by a periodic function with compact support. This is ($\hbar/(2m) = 1$)

$$-\frac{d^2}{dx^2} \psi(x) + V(x, a)\psi(x) = E\psi(x), \quad (73)$$

where $a > 0$ is a fixed real number and

$$V(x, a) := \begin{cases} 0 & \text{if } |x| \geq a, \\ N \exp\left(-\frac{1}{x^2 - a^2}\right) & \text{if } -a \leq x \leq a. \end{cases} \quad (74)$$

We choose the constant N in such a way that the area under each bump be one. This gives

$$N = \frac{e^{1/a^2}}{\sqrt{\pi} a U\left(\frac{1}{2}, 0, \frac{1}{a^2}\right)}, \quad (75)$$

where $U(a, b, z)$ is the second kind Kummer function. This potential is extended by periodicity as shown in Figure 2.

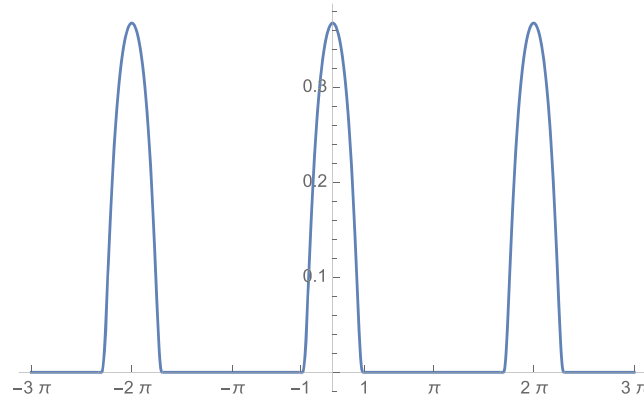


FIGURE 2 The potential of compact support (74) extended by periodicity [Colour figure can be viewed at wileyonlinelibrary.com]

Prior to the study of (73), let us make some considerations. To begin with, let us write the Hill equation

$$\psi''(x) + \alpha(x)\psi(x) = 0, \quad (76)$$

with x real and $\alpha(x)$ is periodic with period T . Since we want to compare (46) with the Schrödinger equation, let us choose the following form for $\alpha(x)$:

$$\alpha(x) = E - V(x), \quad (77)$$

with a normalization condition of the type

$$\int_{-T/2}^{T/2} V(x) dx = 1. \quad (78)$$

An interesting property of the Hill equation is the following^{8,11}: Let us assume that $\alpha(x)$ is strictly positive, $\alpha(x) > 0$ and

$$0 < T \int_{-T/2}^{T/2} \alpha(x) dx \leq 4. \quad (79)$$

Then, all solutions of (76) are bounded. In particular and taking into account (77) and (78), we have bounded solutions of (76) and, therefore, of (73) if and only if E satisfies the inequalities

$$T < E \leq T + \frac{4}{T}. \quad (80)$$

This result is an obvious consequence of (19).

Next, let us consider the Sturm-Liouville associated to the boundary conditions:

$$\psi\left(-\frac{T}{2}\right) = \psi\left(\frac{T}{2}\right), \quad \psi'\left(-\frac{T}{2}\right) = \pm\psi'\left(\frac{T}{2}\right), \quad (81)$$

and E the eigenvalue to be determined. In order to connect this Sturm-Liouville problem to our original periodic potential Schrödinger equation, let us write $a = \frac{T}{2r}$ with $r > 0$, a fixed real number. On the interval of the form $[-T/2, T/2]$, the potential is equal to (70) if $|x| \leq \frac{T}{2r}$ and vanishes in the two subintervals for which $\frac{T}{2r} < |x| < \frac{T}{2}$. In Figure 2, we have chosen $a = 1$ and $T = 2\pi$.

Boundary conditions (81) imply that the solution $\psi(x)$ is periodic with period T . After the Floquet theorem, the solution can be written as

$$\psi(x) = \exp\{\lambda x\} P(x), \quad (82)$$

where λ is the Floquet exponent and $P(x)$ is T -periodic. Note that we write $\psi(x)$ in the form (82) in order to implement our method and its algorithm, as was implemented in Section 4, concerning the example after the Mathieu equation. As in Figure 2, we may choose $T = 2\pi$ without loss of generality.

Next, we want to apply our harmonic balance based method to the above situation. To this end, we write both $\alpha(x)$ and $P(x)$ by means of respective Fourier polynomials of period T , for which the coefficients depend on the Floquet exponent and the energy E , to be determined. Since we are looking for periodic solutions, then $\lambda = ik$, k being an integer number, which we choose equal to one for simplicity. Also, the sum of the two Floquet exponents for the Hill equation is zero,⁸ so that these exponents can be chosen to be $\lambda_{\pm} := \pm i$.

We obtain the energy levels with a slight modification of the application of the harmonic balance method as exposed in Section 3.1. There, the objective was the computation of the Floquet exponents. Now, it is of the energy levels. To this end, use (82) into (73), so as to obtain the following differential equation:

$$P''(x) + 2\lambda P'(x) + (\lambda^2 + E - V(x, a))P(x) = 0. \quad (83)$$

As for (21), we approximate a solution for $P(x)$ through a Fourier polynomial as

$$P_n(x) = \frac{a_0}{2} + \sum_{k=1}^n \{a_n \cos(k\omega x) + b_k \sin(k\omega x)\}, \quad (84)$$

where $\omega = 2\pi/T$.

Next, we fix λ , either i or $-i$. Then, apply the harmonic balance method so as to determine the Fourier coefficients a_k and b_k as functions of the energy, $a_k(E)$ and $b_k(E)$, $n = 1, 2, \dots, n$. Let us use (84) in (53). These coefficients must vanish, which gives a homogeneous linear system in the indeterminates a_0, a_k and b_k , $k = 1, 2, \dots, n$, so that the determinant of the coefficients must vanish. This determinant is a polynomial $\Delta(E)$, which yields to the algebraic equation:

$$\Delta(E) = 0. \quad (85)$$

In relation to the degree of this polynomial, some comments are in order. For the Mathieu equation, discussed in Section 4, if we approximate the solution with the Fourier polynomial with two frequencies, the degree is 10. With more frequencies, it must be higher. For instance, with three frequencies the polynomial degree is 14. Similar for the other worked examples. For instance, for the Harbola comb (see below) and the potential in (74), we have used a polynomial (55) of degree fourteen. This is obvious: When we use two harmonics, we have five coefficients so that the matrix for which the determinant is $\Delta(E)$ is a 5×5 matrix with argument E^2 , so that the determinant is of degree 10 on E . If we had chosen three harmonics, we need to determine seven coefficients, and this is the order of the corresponding determinant on E^2 , so that the polynomial is of order fourteen, and so on.

However, not all solutions of (55) are good solutions, since good solutions must approximate the exact solutions. This gives a manner to choose the “good” solutions. As in (23) and (24) and taking into account that the exact solution, $\{\psi(x), E\}$, for of the Sturm-Liouville problem should satisfy:

$$\int_0^T (\psi''(x) + (E - V(x, a))\psi(x))^* (\psi''(x) + (E - V(x, a))\psi(x)) dx = 0. \quad (86)$$

Then, we propose the Ansatz according to which the correct approximate value for the energy, which we denote here as E_r should minimize the following expression:

$$D(E_r) = \int_0^T (P''_{n,r}(x) + (E_r - V(x, a))P_{n,r}(x))^* (P''_{n,r}(x) + (E_r - V(x, a))P_{n,r}(x)) dx, \quad (87)$$

where $P_{n,r}(x) = \exp\{\lambda x\} \psi_{n,r}(x)$ is the solution of the form (53) with $a_k = a_k(E_r)$ and $b_k = b_k(E_r)$, $n = 1, 2, \dots, n$.

Needless to say that a Sturm-Liouville like this one under our study shows an infinite number of the energy levels. In this approximation, we obtain just a finite number of these levels, number that depends on the number of harmonics chosen in (84). The more harmonics the more solutions one may expect to find (although with increasing calculation difficulty). Also, one may look for “even” or the “odd” solutions, which are those for which we choose the b_k or the a_k coefficients equal to zero, respectively.

In Figure 3, we represent the dependence of the values of the energy with the parameter r . The growing curves in the energy represent even solutions, while the decreasing curves correspond to odd solutions. Observe that, for the ground state, no distinction is shown between the energies of even and odd solutions.

For the potential (71), $a = T/(2r)$, we have the following:

- i. The limit $\lim_{r \rightarrow \infty} V(x, a) = N_\infty \delta(x)$, where N_∞ is a constant.
- ii. The limit $\lim_{r \rightarrow 0} V(x, a) = 1/T$, for $-T/2 < x < T/2$.
- iii. If we consider just the odd solutions and take the limit $r \mapsto 0$, we may obtain the exact value of all energy levels. These values are

$$E_n = \frac{1}{T} + n^2, \quad n = 0, 1, 2, \dots \quad (88)$$

Same for even solutions. In this case, we obtain in the limit $r \mapsto 0$ the following energy levels:

$$E_n = \frac{1}{T} + \frac{(2n+1)^2}{4}, \quad n = 0, 1, 2, \dots \quad (89)$$

Finally, in Figure 4, we depict the potential (70) for $r = 2$ and $\lambda = i$.

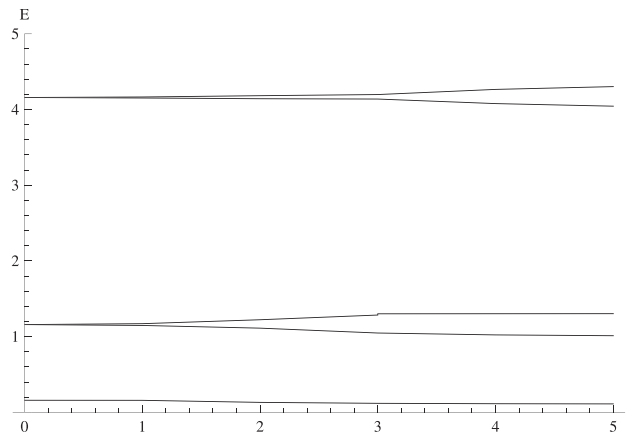


FIGURE 3 Three first energy levels in terms of r . The growing and decreasing curves correspond to even and odd solutions, respectively

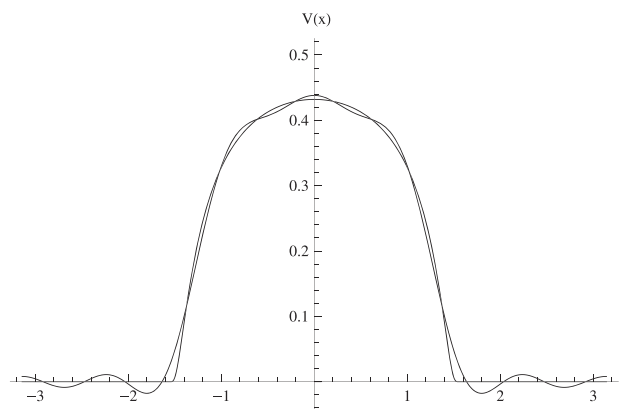


FIGURE 4 Potential for $r = 2$ and $\lambda = i$

In addition to above model, we have studied some others with detail. Methods and results are essentially identical to those discussed so far, so that there is no serious point in a detailed analysis of those. Nevertheless, an account of the models studied may be interesting. These models are as follows:

- **The Harbola comb**

This is a periodic potential, for which the basic cell is given by the function²¹:

$$f(x, a, b) := \frac{N}{\sqrt{x^2 + b^2}}, \quad x \in [-a, a], \quad N = \frac{1}{2 \operatorname{arc} \sinh(a/b)}. \quad (90)$$

Then, we extend it by periodicity outside the interval $[-a, a]$. This periodic potential (Harbola comb) is depicted in Figure 5. Observe that for high energy values, this potential resembles a Dirac comb.²²

- **One dimensional periodic Coulomb potential**

Here, the function for the basic cell is

$$f(x, a, \varepsilon) = \begin{cases} -\frac{k}{\varepsilon} & \text{if } |x| \leq \varepsilon, \\ -\frac{k}{x} & \text{if } \varepsilon < |x| < \pi, \end{cases} \quad (91)$$

so that the basic cell is the interval $[-\pi, \pi]$. Then, we extend this potential by periodicity. This potential is depicted in Figure 6. Observe that we have avoided the singularity with this choice.

- **Other potentials** We give the equations that use these potentials, being their explicit form evident.

i. *The Kroning-Penney model* is very well known in solid state.²³

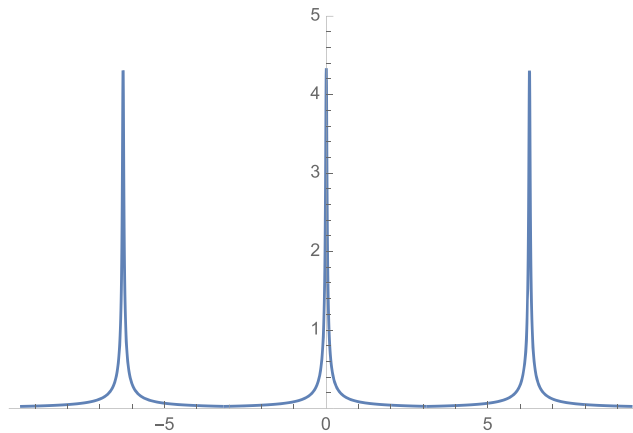


FIGURE 5 Harbola comb [Colour figure can be viewed at wileyonlinelibrary.com]

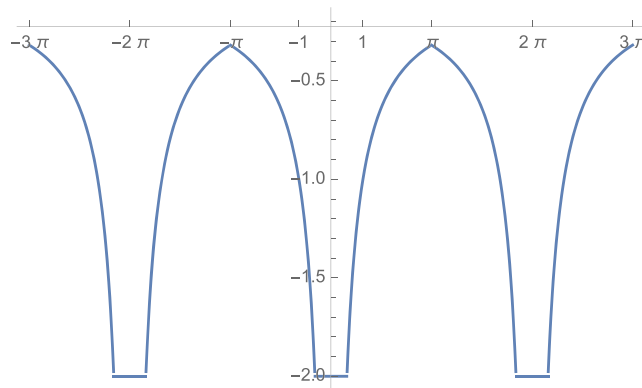


FIGURE 6 Periodic Coulomb potential with $k = 1$ and $\varepsilon = 1$ [Colour figure can be viewed at wileyonlinelibrary.com]

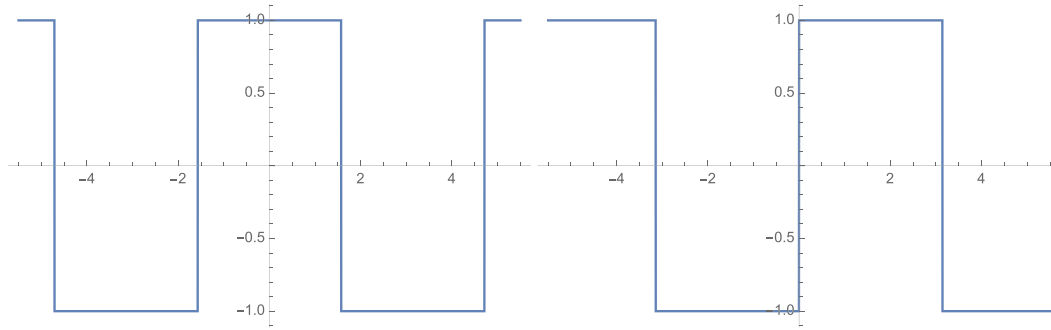


FIGURE 7 Meissner potential given in (92) (to the left) and (93) (to the right) [Colour figure can be viewed at wileyonlinelibrary.com]

- ii. *The Meissner equation*, which is a particular case of the Hill equation.²⁴ This is rather similar to the Kroning-Penney model, although in this case, the equation is periodic with respect to time instead of the spatial variable. It is usually presented into two equivalent forms, either as

$$\frac{d^2 y(t)}{dt^2} + (\alpha^2 + \omega^2 \operatorname{sgn}(\cos t))y(t) = 0, \quad (92)$$

or

$$\frac{d^2 y(t)}{dt^2} + \left(1 + r \frac{\sin(\omega t)}{|\sin(\omega t)|}\right) y(t) = 0. \quad (93)$$

Here, the Floquet exponents may be exactly determined.²⁵ In Figure 7, we see the form of periodic potential.

- iii. *Lamé equation*. It has the form²⁶:

$$\frac{d^2 y(x)}{dx^2} + (A + B\wp(x))y(x) = 0, \quad (94)$$

where A and B are constants and $\wp(x)$ the Weierstrass elliptic function.^{27,28}

7 | CONCLUDING REMARKS

The Hill-Harmonic Balance method was designed in order to obtain the Floquet characteristic exponents for linear differential equations and systems with periodic coefficients. These exponents are solutions of an algebraic equation of degree $2n + 1$, where n is the order of a Fourier polynomial that it is used in order to obtain an approximate analytic solution for the equation. Since in general, $2n + 1$ is much larger than the order of the equation, that in many practical cases is two, Hill-Harmonic Balance is not efficient. We propose a modification of this method that permits to choose the Floquet exponents among the solutions of the algebraic equation efficiently. Following our method, the Floquet coefficients are determined through a variational principle. It is precisely the use of this variational principle that determines the Floquet exponents as its critical points, which makes our procedure different from other discussed in the literature. These tools are easy to implement for practical applications. We obtain an excellent precision in function of the number of harmonics used.

We have compared our results with the exact results known for the Mathieu equation. They show a good accuracy even if we just take the first two nodes (up to $n = 2$) in the Fourier series. The precision obtained for $n = 3$ is excellent. We also have compared our results with those obtained with the standard method described in Section 2. The conclusion is that we obtain better results with little effort and negligible computational time.

One-dimensional periodic models are of great interest in Quantum Physics as they serve as toy models in the search for crystal properties, starting with the celebrated Kroning-Penney model. We have studied a variety of these models under the perspective of the formalism introduced in the present article. We have listed some of the most relevant among the studied models and give a detailed analysis on one of them. Results for the others are similar.

We have also given Floquet exponents for two-dimensional models and added some examples thereof.

In conclusion, this is a method to obtain Floquet characteristic coefficients which is simple, efficient, and with an excellent precision as shown in the testing examples. Although we have not proposed an explicit formula to evaluate the error, once we have determined critical exponents and approximate solutions, formula (24) may serve to test the accuracy of a given solution.

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CONFLICT OF INTEREST

This work does not have any conflict of interest.

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