A modification of a classical method to obtain Floquet exponents and solutions for linear periodic differential equations.

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September 22, 2022

Abstract

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.

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 obtain 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 [5].

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].

In the present paper, we introduce a modification of the procedure in [6] 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. This efficiency as well as the accuracy of our modification has been tested in specific examples (like for instance in the Mathieu equation), as is well known the difficulty to establish error bounds for Fourier series based approximation methods. 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 of previous methods including those in [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

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

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

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

$$\Phi(t+T) = \Phi(t)\,C\,. \tag{2}$$

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

$$C = e^{BT}\,, \tag{3}$$

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:

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

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

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

where $A(t)$ and B are as in (1) and (3), respectively. Then and taking into account that $P(t)$ is invertible and using (4), we have that

$$\dot{\mathbf{y}} = B\,\mathbf{y}\,. \tag{6}$$

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 that the solution of (6) satisfying the initial condition $\mathbf{y}(t_0)$ is given by

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

we have that

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

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 eigevalues of B. Then if $\mathbf{x}_0 := P(t_0)\,\mathbf{y}(t_0) = P(t_0)\,\mathbf{y}_0$, one has

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

expression which may be written as

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

Since $P(t)$ is periodic with period T, equation (9) shows 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 not 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 order: 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 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 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-Kutta [12] 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 $X_1(t), X_2(t), \ldots, X_n(t)$, 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

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

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

$$\lambda_i = \frac{1}{T}\log\delta_i\,, \qquad i = 1, 2, \ldots, n\,. \tag{12}$$

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:

$$\delta_i = \exp\{\lambda_i + 2\pi i/T\}T = e^{\lambda_i T}\,. \tag{13}$$

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:

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

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 (16) is $(z_1(t) := y(t),\ z_2(t) = \dot{y}(t))$

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

With the change

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

equation (16) yields to

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

with

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

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

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

  Then, it has been proven in [8] 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

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

  Since $y^2(t) \leq 0$, we note that for large values on the variable t, $t \longmapsto \infty$, 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 exponent. Choosing for simplicity $t_0 = 0$, we go back to (17) were it was stated that for each Floquet exponent there is a solution of the type $x(t) = \eta(t)\, e^{t\lambda}$, where $\eta(t)$ is periodic with period T[1]. 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:

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

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

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

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 $k = 1, 2, \ldots, n$. 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

$$\Delta(\lambda) = 0 \tag{23}$$

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, $k = 1, 2, \ldots, n$ 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

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

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:

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

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).

[1] We may assume that a basis of solutions is of this form, provided that B be diagonalizable.

Once we have the Floquet characteristic exponents for the given equation, we determine the coefficients a_0, a_k and b_k, $k = 1, 2, \ldots, n$ 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 [13–18]. Let us write the Mathieu equation as

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

As is well known, two linearly independent solutions are

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

where C and S stand for the Mathieu sine and cosine [18]. 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), that 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 ten:

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

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

$$c_0 = 16\,\omega^2 + \,8\,(-5 + \alpha^2)\,\omega^4 + (33 - 14\,\alpha^2)\,\omega^6\alpha^2 - \frac{1}{2}(20 - 14 + \,\alpha^4)\,\omega^8 -$$
$$-8\,(1 - \,\alpha^2 + \frac{3}{16}\alpha^4)\,\omega^{10}\,,$$

$$c_2 = \frac{1}{16}(256 + (560 - 96\alpha^2)\omega^4 + 160(\alpha^2 - 2)\omega^6 + (80 - 48\alpha^2 + 3\alpha^4)\omega^8)\,,$$

$$c_4 = 40 + 35\omega^2 + 3\alpha^2\omega^4 + (10 - 3\alpha^2)\,\omega^6\,,$$

$$c_6 = 33 + 20\omega^2 - (-10 + \alpha^2)\omega^4\,,$$

$$c_8 = 5(2 + \omega^2)\,,$$

$$c_{10} = 304 + 80\,\omega^2\,. \tag{29}$$

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:

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

$$\begin{aligned} a_0 = \frac{1}{\alpha\omega^2}\{3(-2 + \lambda^2 + \omega^2) - \frac{1}{8\lambda}[(16 + 4\lambda^4 - 20\omega^2 - (-4 + \alpha^2)\omega^4 + \\ +\lambda^2(-52 + 8\omega^2))(-\lambda\alpha^2\omega^4 + 2\lambda(-16\lambda^2 - (-4 + \lambda^2 + \omega^2)^2)]/d_1\}\,, \\ a_1 = 1\,, \\ a_2 = -\frac{1}{2}[\alpha\omega^2(-16 - 4\lambda^4 + 20\omega^2 + (-4 + \alpha^2)\omega^4 + \lambda^2(52 - 8\omega^2))]/d_2\,, \end{aligned} \tag{31}$$

where,

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

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:

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

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, span $\eta(t)$ into Fourier series. We obtain an explicit expression of the form:

$$x_e(t) = \exp\left(-\frac{1}{43}t\right)\left(\frac{66}{265} + \frac{486}{487}\cos t - \frac{4}{45}\cos 2t + \right.$$

$$\left. + \frac{1}{340}\cos 3t - \frac{131}{60}\sin t + \frac{7}{39}\sin 2t - \frac{1}{176}\sin 3t + ...\right). \tag{34}$$

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:

$$x_A(t) = \exp\left(-\frac{1}{43}t\right)\left(\frac{267}{1069} + \cos t - \frac{5}{56}\cos 2t + \right.$$

$$\left. + \frac{1}{346}\cos 3t - \frac{376}{171}\sin t + \frac{19}{105}\sin 2t - \frac{1}{178}\sin 3t\right) \tag{35}$$

and

$$x_e(t) = \exp\left(-\frac{1}{43}t\right)\left(\frac{285}{1141} + \cos t - \frac{5}{56}\cos 2t + \frac{1}{346}\cos 3t - \right.$$

$$\left. - \frac{596}{271}\sin t + \frac{19}{105}\sin 2t - \frac{1}{178}\sin 3t\right) + ... \tag{36}$$

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

$$x_A(t) = \exp\left(-\frac{1}{10}t\right)\left(\frac{1}{2} + \cos t - \frac{1}{5}\cos 2t + \frac{1}{69}\cos 3t - \right.$$

$$\left. -\frac{19}{9}\sin t + \frac{1}{3}\sin 2t - \frac{1}{50}\sin 3t\right) \tag{37}$$

and

$$x_e(t) = \exp\left(-\frac{1}{10}t\right)\left(\frac{1}{2} + \cos t - \frac{1}{5}\cos 2t + \frac{1}{69}\cos 3t - \right.$$

$$\left. -\frac{19}{9}\sin t + \frac{1}{3}\sin 2t - \frac{1}{51}\sin 3t\right) + \ldots \tag{38}$$

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.

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.

In **Table 1**, we compare the values of the approximate characteristic exponent given by our method, λ_A, the exact, λ_e, and the one detemined 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

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

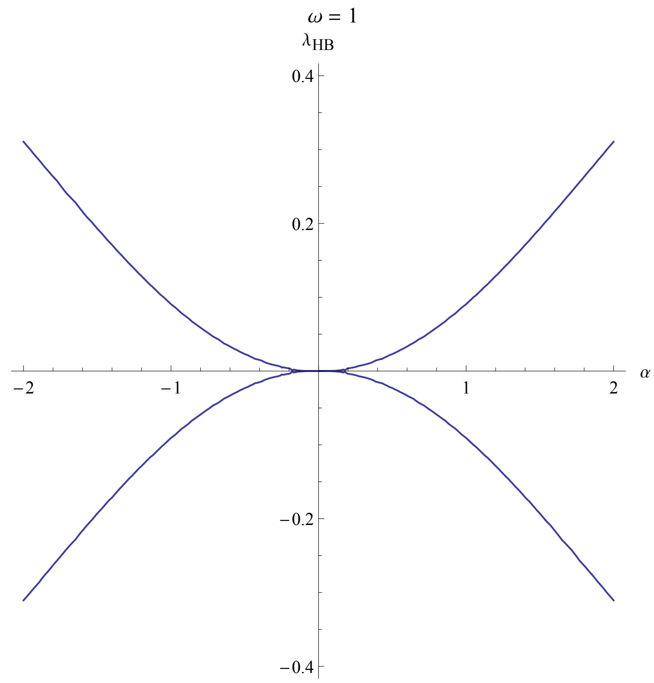

Figure 1: Variation of λ_A in terms of α for $n = 2$ and $\omega = 1$.

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 which 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

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

  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:

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

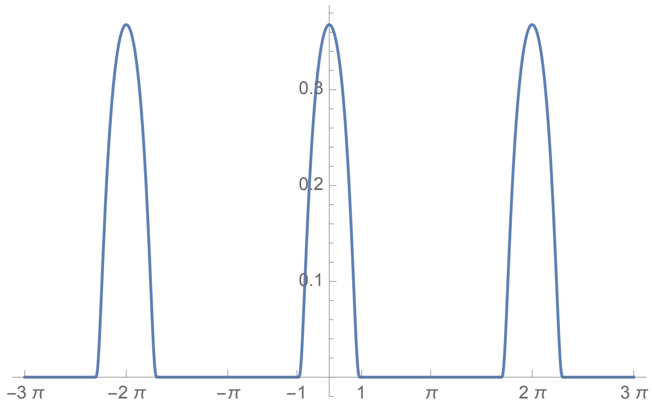

Figure 2: The potential of compact support (44) extended by periodicity

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 which is reducible to the Mathieu equation is the one dimensional Schrödinger equation with potential given by

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

where $V_0 > 0$ and λ is the wave length of two interfering lasers [19].

5 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 $(\hbar/(2m) = 1)$

$$-\frac{d^2}{dx^2}\,\psi(x) + V(x,a)\psi(x) = E\psi(x)\,, \tag{43}$$

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

$$V(x,a) := \left\{ \begin{array}{ccc} 0 & \text{if} & |x| \ge a\,, \\ N\,\exp\left(\frac{1}{x^2-a^2}\right) & \text{if} & -a \le x \le a\,. \end{array} \right. \tag{44}$$

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

$$N = \frac{e^{1/a^2}}{\sqrt{\pi}\, a\, U\left(\dfrac{1}{2}, 0, \dfrac{1}{a^2}\right)}\,, \tag{45}$$

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

Prior to the study of (43), let us make some considerations. To begin with, let us write the Hill equation

$$\psi''(x) + \alpha(x)\psi(x) = 0\,, \tag{46}$$

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 $\alpha(x)$:

$$\alpha(x) = E - V(x)\,, \tag{47}$$

with a normalization condition of the type

$$\int_{-T/2}^{T/2} V(x)\, dx = 1\,. \tag{48}$$

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

$$0 < T \int_{-T/2}^{T/2} \alpha(x)\, dx \leq 4\,. \tag{49}$$

Then, all solutions of (46) are bounded. In particular and taking into account (47) and (48), we have bounded solutions of (46) and, therefore, of (43) if and only if E satisfies the inequalities

$$T < E \leq T + \frac{4}{T}\,. \tag{50}$$

This result is an obvious consequence of (19).

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

$$\psi\left(-\frac{T}{2}\right) = \psi\left(\frac{T}{2}\right)\,, \qquad \psi'\left(-\frac{T}{2}\right) = \pm\psi'\left(\frac{T}{2}\right)\,, \tag{51}$$

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

$$\psi(x) = \exp\{\lambda x\}\, P(x)\,, \tag{52}$$

where λ is the Floquet exponent and $P(x)$ is T-periodic. Note that we write $\psi(x)$ in the form (52) 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 menas 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 (52) into (43), so as to obtain the following differential equation:

$$P''(x) + 2\lambda\, P'(x) + (\lambda^2 + E - V(x,a))P(x) = 0\,. \tag{53}$$

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

$$P_n(x) = \frac{a_0}{2} + \sum_{k=1}^{n} \{a_n\, \cos(k\omega x) + b_k\, \sin(k\omega x)\}\,, \tag{54}$$

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 $b_k(E)$, $n = 1, 2, \ldots, n$. Let us use (54) in (53). These coefficients must vanish, which gives a homogeneous linear system in the indeterminates a_0, a_k and b_k, $k = 1, 2, \ldots, n$, so that the determinant of the coefficients must vanish. This determinant is a polynomial $\Delta(E)$, which yields to the algebraic equation:

$$\Delta(E) = 0\,. \tag{55}$$

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-Lioville problem should satisfy:

$$\int_0^T (\psi''(x) + (E - V(x,a))\psi(x))^*\, (\psi''(x) + (E - V(x,a))\psi(x))\, dx = 0\,. \tag{56}$$

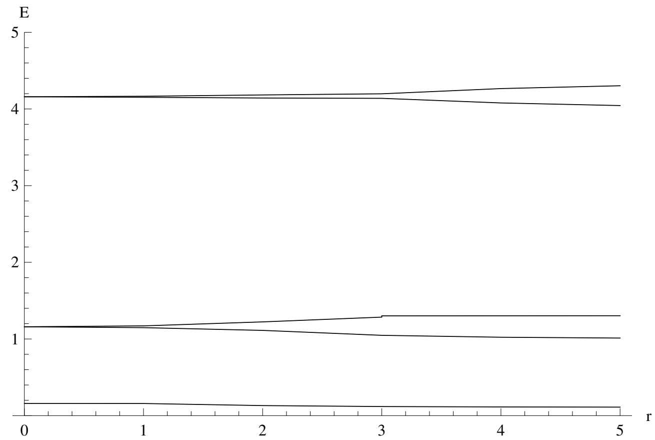

Figure 3: Three first energy levels in terms of r. The growing and decreasing curves correspond to even and odd solutions, respectively.

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

$$D(E_r) = \int_0^T (\psi''_{n,r}(x)+(E_r-V(x,a))\,\psi_{n,r}(x))^*\,(\psi''_{n,r}(x)+(E_r-V(x,a))\,\psi_{n,r}(x))\,dx\,, \quad (57)$$

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 which depends on the number of harmonics chosen in (54). 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 (44), $a = T/(2r)$, we have the following:

i.) The limit $\lim_{r\to\infty} V(x,a) = N_\infty\,\delta(x)$, where N_∞ is a constant.

ii.) The limit $\lim_{r\to 0} V(x,a) = 1/T$, for $-T/2 < x < T/2$.

iii.) If we consider just the odd solutions and take the limit $r \longmapsto 0$, we may obtain the exact value of all energy levels. These values are:

$$E_n = \frac{1}{T} + n^2\,, \qquad n = 0, 1, 2, \dots . \quad (58)$$

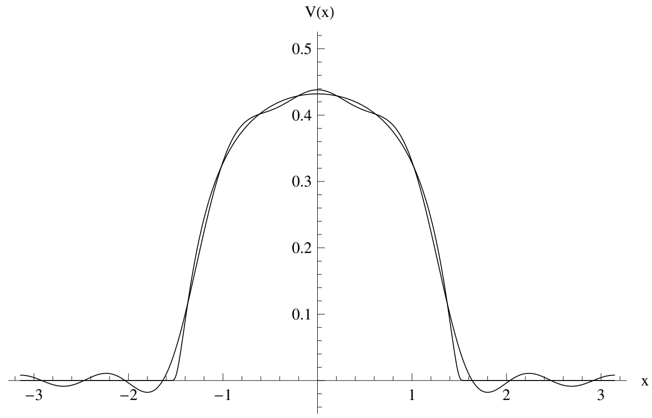

Figure 4: Potential for $r = 2$ and $\lambda = i$.

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

$$E_n = \frac{1}{T} + \frac{(2n+1)^2}{4}\,, \qquad n = 0, 1, 2, \dots . \tag{59}$$

Finally, in Figure 4, we depict the potential (43) 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:

- **The Harbola comb.**

  This is a periodic potential, for which the basic cell is given by the function [20]:

$$f(x, a, b) := \frac{N}{\sqrt{x^2 + b^2}}\,, \qquad x \in [-a, a]\,, \qquad N = \frac{1}{2\,\mathrm{arcsinh}\,(a/b)}\,. \tag{60}$$

  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 [21].

- **One dimensional periodic Coulomb potential.**

  Here, the function for the basic cell is

$$f(x, a, \varepsilon) = \begin{cases} -\dfrac{k}{\varepsilon} & \text{if} \quad |x| \le \varepsilon\,, \\ -\dfrac{k}{x} & \text{if} \quad \varepsilon < |x| < \pi\,, \end{cases} \tag{61}$$

  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.

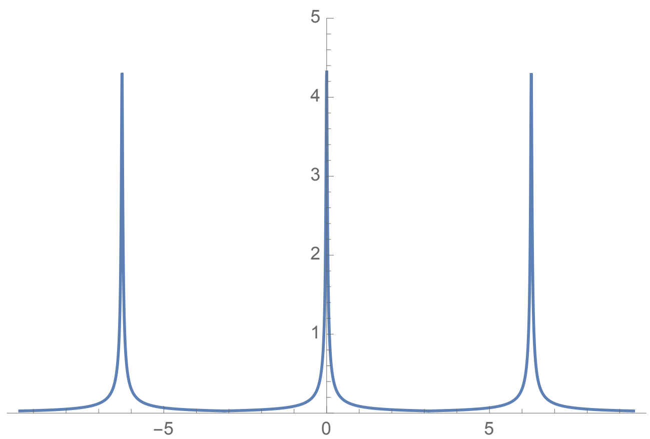

Figure 5: Harbola comb.

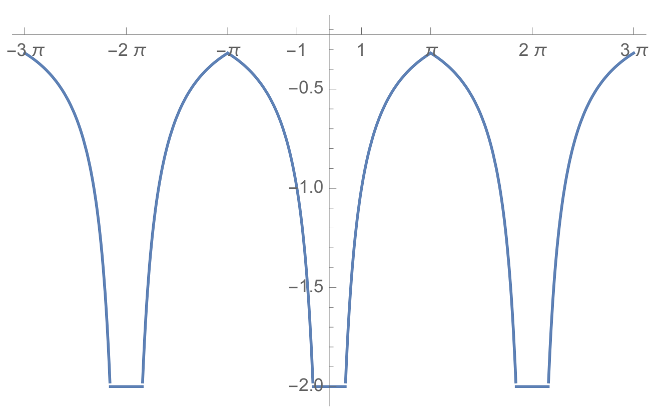

Figure 6: Periodic Coulomb potential with $k = 1$ and $\varepsilon = 1$.

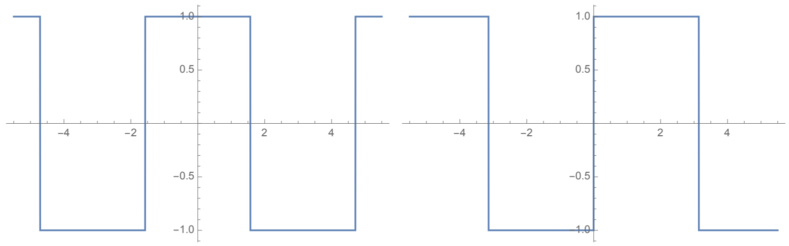

Figure 7: Meissner potential given in (62) (to the left) and (63) (to the right).

- **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 [22].

  ii.) *The Meissner equation*, which is a particular case of the Hill equation [23]. 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

$$\frac{d^2y(t)}{dt^2} + (\alpha^2 + \omega^2 \,\mathrm{sgn}(\cos t))y(t) = 0\,, \tag{62}$$

  or

$$\frac{d^2y(t)}{dt^2} + \left(1 + r\,\frac{\sin(\omega t)}{|\sin(\omega t)|}\right) y(t) = 0\,. \tag{63}$$

  Here, the Floquet exponents may be exactly determined [24]. In Figure 7, we see the form of periodic potential.

  iii.) *Lamé equation*. It has the form [25]:

$$\frac{d^2y(x)}{dx^2} + (A + B\wp(x))y(x) = 0\,, \tag{64}$$

  where A and B are constants and $\wp(x)$ the Weierstrass elliptic function [26, 27].

6 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.

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.

Acknowledgements

This work was supported by MCIN with funding from the European Union NextGenerationEU (PRTRC17.I1) and the Consejería de Educación through QCAYLE project, as well as the PID2020-113406GB-I0 project by MCIN of Spain, as well as to the National University of Rosario (Argentina) grant ING19/i402. We acknowledge suggestions from Prof. Luis Miguel Nieto.

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