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A new method to compute Mathieu functions

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Abstract. We propose to evaluate the Mathieu functions by their modulus and phase. The modulus is independent of the characteristic exponent. In our approach, this exponent can be evaluated by integration of a first-order differential equation. For the Hamiltonian of the time-dependent harmonic oscillator, we do not need this exponent, only the modulus.

1. Introduction: the former method

The time-dependent harmonic oscillator can be described by Mathieu's differential equation [1–4]

$$\ddot{x} + f(t)x = 0 \qquad \text{with} \qquad f(t) = f(t-T) = (\tfrac{1}{2}\Omega)^2(a - 2q\cos\Omega t). \tag{1}$$

The physical parameters Ω, a and q are given†: all three are real, $\Omega > 0$ and $q > 0$ (otherwise we move the time origin by $\frac{1}{2}T = \pi/\Omega$). The parameter a may be negative; however, then the solutions with $q = 0$ are not stable‡. The possible instability for $q > 0$ will be discussed.

For $q > 0$, we can write down the linear independent *Floquet* solutions in the form§

$$x_\pm(t) = \sum_{n=-\infty}^{\infty} C_n \exp\left(\pm \mathrm{i}\frac{2n+\nu}{2}\Omega t\right) \tag{2}$$

with real coefficients C_n. Here ν is the *characteristic exponent*: it is real but is not an integer if the solutions are stable‖. From Mathieu's differential equation (1), we obtain the recurrence relation

$$C_{n-1} + C_{n+1} = \frac{a - (2n+\nu)^2}{q} C_n. \tag{3}$$

† We are looking here for the solutions of the *initial-value problem* and defer the discussion of the related *boundary-value problem* with purely periodic solutions to section 3: that problem is solved by an infinite system of characteristic values $a_n(q)$.

‡ i.e. linear combinations of $x_\pm(t) = \exp(\pm\mathrm{i}\frac{1}{2}\sqrt{a}\Omega t)$.

§ Blanch [4] writes c_{2n} instead of C_n.

‖ For unstable solutions, ν becomes complex with an integer real part.

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Setting $G_{\pm n} \equiv C_{\pm n}/C_{\pm(n-1)}$ for $n \geqslant 0$ and using $\lim_{n\to\infty} G_{\pm n} \to 0$ gives

$$G_{\pm n} = \frac{q}{a - (2n \pm \nu)^2 - qG_{\pm(n+1)}}. \tag{4}$$

The characteristic value ν must be chosen such that (3) has a non-trivial solution† or, equivalently, $G_0 G_{-1} = 1$. (We may take $\nu > 0$ for stable solutions and $\mathrm{Im}\,\nu > 0$ for unstable solutions, otherwise we have to interchange x_+ and x_-.)

From the set $\{G_n\}$, we obtain all C_n except C_0 which is determined by $x_\pm(0) = 1$, i.e. $\sum_n C_n = 1$ or

$$C_0{}^{-1} = 1 + G_1(1 + G_2(1 + \ldots)) + G_{-1}(1 + G_{-2}(1 + \ldots)). \tag{5}$$

In this normal procedure, we first have to compute ν to obtain the Floquet solutions. As

$$x_\pm(t+T) = \exp(\pm\mathrm{i}\nu\pi)x_\pm(t) \tag{6}$$

this quantity has a physical meaning apart from the factor π: for stable solutions it is the phase shift‡ picked up during the period T. This quasiperiodicity is characteristic of Floquet's solutions $x_\pm$. Another *fundamental system* x_1 and x_2 can be determined by the initial values $x_1(0) = 1 = \dot{x}_2(0)$ and $\dot{x}_1(0) = 0 = x_2(0)$.

2. A new method

By introducing the modulus and phase of the Floquet solutions (see [5] or [6])

$$x_\pm(t) = \alpha(t)\exp\{\pm\mathrm{i}\varphi(t)\} \tag{7}$$

we obtain two differential equations with a constant w§.

$$\dot{\varphi} = \frac{w}{\alpha^2} \qquad \text{and} \qquad \ddot{\alpha} + f\alpha = \frac{w^2}{\alpha^3}. \tag{8}$$

Apart from the factor $\exp(\pm\frac{1}{2}\mathrm{i}\nu\Omega t)$, the solutions $x_\pm$ must be periodic. This leads to $\alpha(t+T) = \alpha(t)$ and $\varphi(t+T) = \varphi(t) + \nu\pi$.

The constant w must be chosen properly—otherwise we would not have the correct periodicity of the modulus—and depends on the initial values. Choosing $x_\pm = x_1 \pm \mathrm{i}wx_2$, we have $\alpha(0) = 1$, $\dot{\alpha}(0) = 0$ and $\varphi(0) = 0$ besides $\dot{\varphi}(0) = w$. Since $\nu > 0$, we have $w > 0$ and w is then the *Wronskian* $w = (\dot{x}_+ x_- - x_+\dot{x}_-)/(2\mathrm{i})$. Since $\dot{\alpha}(0) = 0$, we obtain $\alpha(t)$ as an even function in t, simplifying our procedure.

† After Hill (see e.g.[3] p 124), this gives the condition $\sin^2 \frac{1}{2}\pi\nu = \Delta \sin^2 \frac{1}{2}\pi\sqrt{a}$ where Δ is the determinant of an infinite tridiagonal matrix with 1 as its diagonal elements and $q/(4n^2 - a)$ as the neighbours of these elements. For high precision we have to use a high-dimensional matrix because of the slow convergence of Δ.

‡ For unstable solutions, ν characterizes the instability.

§ This follows from the integration of $\alpha\ddot{\varphi} + 2\dot{\alpha}\dot{\varphi} = 0$. For unstable solutions, we set $x_\pm(t) = \alpha(t)\exp\{\pm\varphi(t)\}$ and get $\ddot{\alpha} + f\alpha = -w^2/\alpha^3$ while the differential equation for φ remains unchanged. Thus, we can use all equations for unstable solutions α as well by substituting w^2 by $-w^2$.

Evidently, we first need a solution of the inhomogeneous and nonlinear differential equation for $\alpha(t)$. Afterwards, we can determine the phase $\varphi(t)$—and the characteristic exponent $\nu = \varphi(T)/\pi$—from a differential equation of *first order*.

Actually, we work with

$$y = \alpha^2 \qquad \text{as function of } \tau = \Omega t \tag{9}$$

instead of α. Indicating differentiation with respect to τ by a prime, we obtain the nonlinear inhomogeneous differential equation

$$yy'' - \tfrac{1}{2}y'^2 + 2\Omega^{-2} f y^2 = 2\Omega^{-2} w^2 \tag{10}$$

with $2\Omega^{-2} f = \frac{1}{2}(a - 2q\cos\tau)$. Since y is even and periodic like α, we have the even Fourier expansion†

$$y = \sum_{n=0}^{\infty} b_n \cos n\tau \tag{11}$$

and we insert this into the differential equation (10). Comparing the time-independent terms, we find

$$\left(\frac{2w}{\Omega}\right)^2 = \sum_{n=0}^{\infty}(1 + \delta_{n0})\left(\frac{a - 3n^2}{2} {b_n}^2 - q b_n b_{n+1}\right). \tag{12}$$

The terms connected with $\cos n\tau$ for $n \in \{1, 2, \ldots\}$) yield a bilinear system of equations

$$\begin{aligned}
&\sum_{k=0}^{n} \frac{[a - (n-k)^2](n-k) + [a - k^2]k}{2n} b_k b_{n-k} \\
&\qquad + \sum_{k=0}^{\infty} \frac{[a - (n+k)^2](n+k) - [a - k^2]k}{n} b_k b_{n+k} \\
&\qquad = q\frac{b_1 b_n + b_0 b_{n+1} + {b_0}^2 \delta_{n1}}{2} + q\sum_{k=0}^{n-1} b_k \frac{b_{n-k-1} + b_{n-k+1}}{2} \\
&\qquad + q\sum_{k=0}^{\infty} b_k (b_{n+k-1} + b_{n+k+1})
\end{aligned}$$

that can be solved by the recurrence relation

$$\frac{2n-1}{2n-\delta_{n1}} b_{n-1} + \frac{2n+1}{2n} b_{n+1} = \frac{a - n^2}{q} b_n. \tag{13}$$

This relation may be compared with (3) giving the usual coefficients C_n: we do not need the characteristic exponent ν and have only positive indices n.

In order to keep rounding errors small, it is advisable to calculate, as a first step, the ratio $g_n \equiv b_n/b_{n-1}$ from the recurrence relation

$$g_n = \frac{2n-1}{2n-\delta_{n1}} \frac{q}{a - n^2 - (1 + \frac{1}{2}/n) q g_{n+1}}. \tag{14}$$

† For an unstable solution, we have to substitute $\cos n\tau$ by $\cosh n\tau$.

Table 1. Fourier coefficients b_n for two examples with $a = 0$ (one in the stable region ($q = \frac{1}{2}$) and one at the boundary ($q \approx 0,9$)) and the example $a = 3$, $q = \frac{1}{2}$ (in the stable region).

n	$a = 0$ $q = 0,5000$	$a = 0$ $q = 0,9080$	$a = 3$ $q = 0,5000$
0	$2,0 \times 10^{+00}$	$1,3 \times 10^{+04}$	$8,8 \times 10^{-01}$
1	$-1,1 \times 10^{+00}$	$-1,6 \times 10^{+04}$	$1,9 \times 10^{-01}$
2	$1,0 \times 10^{-01}$	$2,8 \times 10^{+03}$	$-7,5 \times 10^{-02}$
3	$-4,6 \times 10^{-03}$	$-2,4 \times 10^{+02}$	$5,2 \times 10^{-03}$
4	$1,3 \times 10^{-04}$	$1,2 \times 10^{+01}$	$-1,8 \times 10^{-04}$
5	$-2,3 \times 10^{-06}$	$-3,9 \times 10^{-01}$	$3,6 \times 10^{-06}$
6	$2,9 \times 10^{-08}$	$8,9 \times 10^{-03}$	$-5,0 \times 10^{-08}$
7	$-2,7 \times 10^{-10}$	$-1,5 \times 10^{-04}$	$5,1 \times 10^{-10}$
8	$2,0 \times 10^{-12}$	$2,0 \times 10^{-06}$	$-3,9 \times 10^{-12}$
9	$-1,2 \times 10^{-14}$	$-2,2 \times 10^{-08}$	$2,4 \times 10^{-14}$
10	$5,6 \times 10^{-17}$	$1,9 \times 10^{-10}$	$-1,2 \times 10^{-16}$

This is as in the usual numerical calculation. For high n we can ignore g_{n+1} compared to $n^2 - a$ as well and thus, can find all g_n up to $n = 1$. Subsequently, we can determine b_0 from $\alpha(0) = 1$ or $y(0) = \sum_{n=0}^{\infty} b_n = 1$ to get

$$b_0{}^{-1} = 1 + g_1(1 + g_2(1 + \ldots)) \tag{15}$$

and then all b_n from $b_n = g_n b_{n-1}$.

Equation (12) can be converted by the recurrence relation into the fast converging series

$$\left(\frac{2w}{\Omega}\right)^2 = a\left(b_0{}^2 - \sum_{n=1}^{\infty} b_n{}^2\right) + q\left(2\sum_{n=1}^{\infty} b_n b_{n+1} - \frac{1}{2} b_0 b_1 + \frac{3}{4}\sum_{n=1}^{\infty} \frac{b_n b_{n+1}}{n(n+1)}\right). \tag{16}$$

(For unstable solutions we get a factor -1 as mentioned in footnote § on page 5566.)

From (8), we get the phase

$$\varphi(t) = \frac{w}{\Omega} \int_0^{\Omega t} \frac{\mathrm{d}\tau}{\sum_{n=0}^{\infty} b_n \cos n\tau}. \tag{17}$$

As a consequence of the even Fourier series, we have $y(\tau) = y(2\pi - \tau)$ and thus, can restrict ourselves to $0 \leqslant \Omega t \leqslant \pi$, obtaining the characteristic exponent from

$$\nu = \frac{2}{\pi} \varphi\left(\frac{1}{2} T\right). \tag{18}$$

The integrals can be calculated numerically by Simpson's method. (Using intervals of equal length has advantages when computing Fourier series: we should compute the often used cosines at $2\pi/(2N)$ once and store them. This is more profitable than the Gauss–Legendre method.)

3. Discussion

The Fourier series $\sum_n b_n \cos n\tau$ converges very fast because the coefficients b_n get smaller, nearly as $q^n/(n!)^2$, with increasing n as a result of the recurrence relation. The convergence is also shown in table 1. Besides avoiding the parameter ν, we also have only positive n.

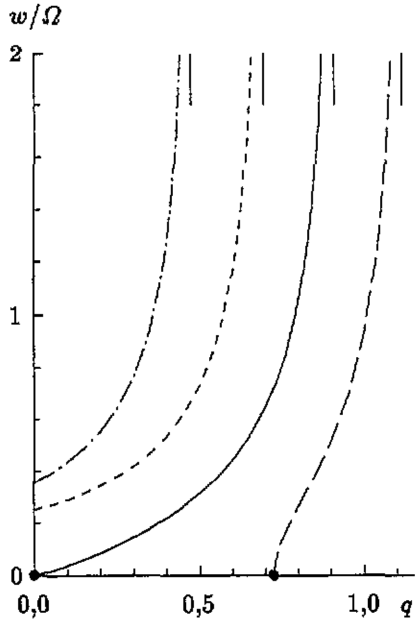

Figure 1. Wronskian w divided by driving frequency Ω as a function of q; shown for $a = -\frac{1}{4}$ (long broken curve), $a = 0$ (full curve), $a = \frac{1}{4}$ (broken curve) and $a = \frac{1}{2}$ (chain curve). Vertical lines and bullets mark the boundary of stability.

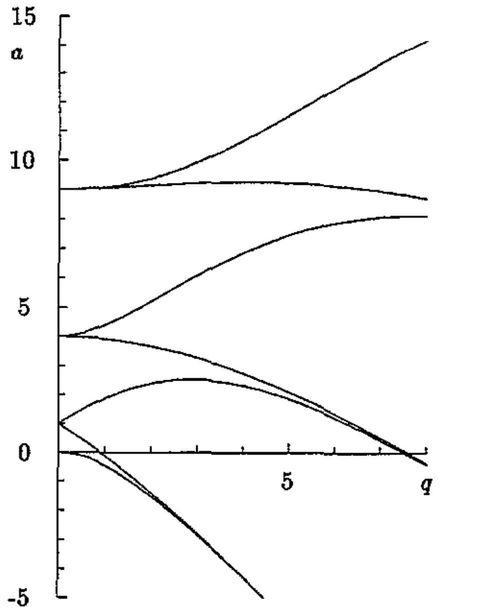

Figure 2. Stability chart for the Mathieu functions with $0 \leqslant q \leqslant 8$ and $-5 \leqslant a \leqslant 15$ as derived from (12). The curves display the boundaries, which apparently increasingly restrict the stable regions with growing q.

The Wronskian w is determined by the fundamental solutions $x_\pm$ and can be calculated from (16) as a function of parameters a and q (without using the characteristic exponent). Figure 1 displays $w(q)/\Omega$ for some parameters a.

At the boundary of stability, the Wronskian diverges (or vanishes). Even this boundary can be determined without the use of ν: we only need to find the change of sign in (16) as a function of a and q. The result is plotted in figure 2 for $0 \leqslant q \leqslant 8$ and $-5 \leqslant a \leqslant 15$.

Applications [1, 2] often need periodic Mathieu functions with integer values of ν. This *boundary problem* can be solved only for special characteristic values a_ν with integer ν. At these values of a, the solutions change from stable to unstable and can thus be found from the stability chart (figure 2).

In figure 3, we show α and φ as functions of t/T in the interval of periodicity [0, 1] for $a = 0$ and several values of q. In figure 4, we display the respective functions $\alpha \cos \varphi$ for the larger interval $0 \leqslant t/T \leqslant 8$ since the periodicity cannot be seen as well.

The decomposition in modulus and phase is useful for physical applications too: according to Brown [5], the Hamiltonian of the time-dependent oscillator

$$H = \frac{p^2}{2m} + \frac{m}{2} f(t) x^2 \tag{19}$$

can be transformed with the generating function $G(t, p, x') = -\alpha(px' - \frac{1}{2}m\dot{\alpha}x'^2)$, i.e. by $x = -\partial G/\partial p = \alpha x'$ and $p' = -\partial G/\partial x' = \alpha(p - m\dot{\alpha}x')$ into the form

$$H' = \frac{1}{\alpha^2}\left(\frac{p'^2}{2m} + \frac{m}{2} w^2 x'^2\right). \tag{20}$$

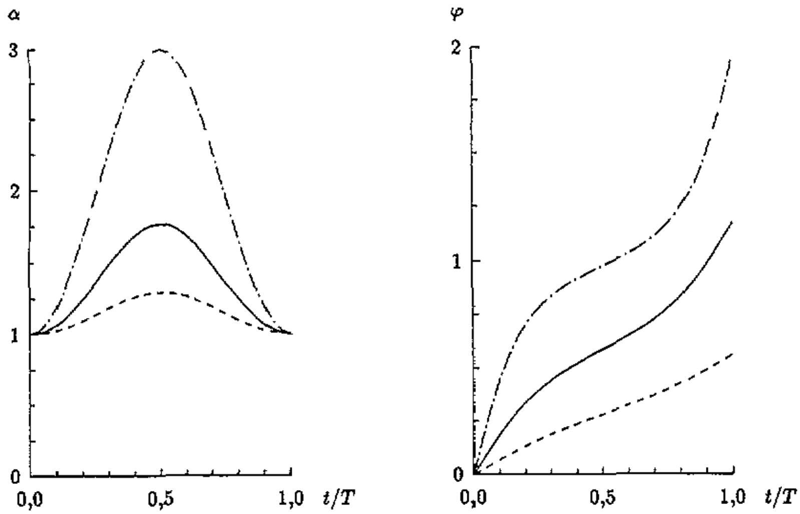

Figure 3. Modulus α and phase φ of the Mathieu functions with $a = 0$ as functions of t/T; shown for $q = \frac{1}{4}$ (broken curve), $q = \frac{2}{4}$ (full curve) and $q = \frac{3}{4}$ (chain curve).

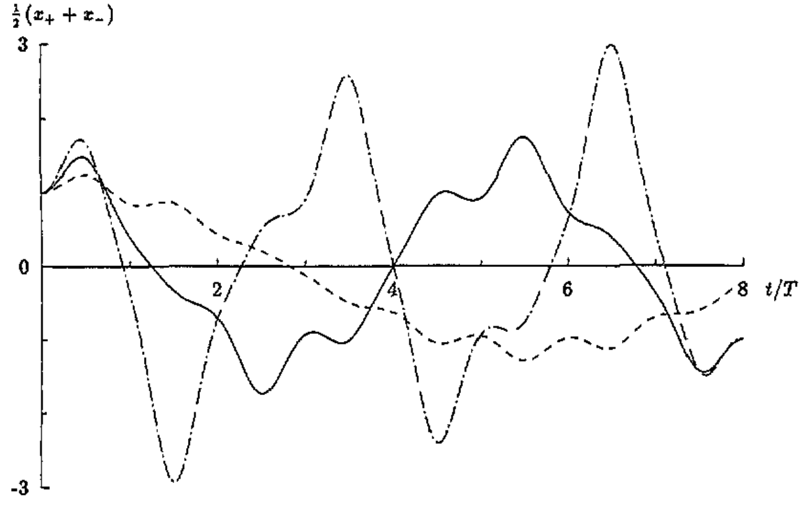

Figure 4. The real part of the Mathieu functions $x_\pm$ with the same parameters as in figure 3.

Thus, we need only the modulus of the Mathieu functions and the Wronskian w and can ignore the characteristic exponent ν. Thus, our method is most effective in this case.

In [7], we propose to write

$$H' = \frac{Iw}{\alpha^2} = I\dot{\varphi} \tag{21}$$

with the invariant†

† The connection between $H(t)$ and an invariant divided by a known time-dependent function is already known [8–10].

$$Iw = \frac{p'^2}{2m} + \frac{m}{2}w^2x'^2. \tag{22}$$

That is, I does not depend on time like the Hamiltonian of the time-independent harmonic oscillator of mass m and frequency w. In quantum mechanics, the eigenvalues of I are $(n+\frac{1}{2})\hbar$.

For all observables B, the Hamiltonian H' determines their time dependence by

$$\frac{\mathrm{d}B}{\mathrm{d}t} = [B, H'] + \frac{\partial B}{\partial t} = \left([B, I] + \frac{\partial B}{\partial \varphi}\right)\frac{\mathrm{d}\varphi}{\mathrm{d}t}. \tag{23}$$

Thus, it seems to be favourable to take $\varphi(t)$, instead of t, as the independent variable giving

$$\frac{\mathrm{d}B}{\mathrm{d}\varphi} = [B, I] + \frac{\partial B}{\partial \varphi}. \tag{24}$$

For example, we get $x' = \sqrt{2I/mw}\sin\varphi$ and $p' = \sqrt{2Imw}\cos\varphi$.

In conclusion, the modulus of the Mathieu functions and their Wronskian can be calculated directly without the characteristic exponent with a very effective numerical algorithm. For the Hamiltonian of the time-dependent oscillator and the stability, only the modulus and Wronskian are relevant. With these quantities, we can determine the phase and the characteristic exponent by a differential equation of first order. In this way, Mathieu functions can be calculated more accurately than with the usual methods.

Acknowledgments

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