# Calculation of Characteristic Values for Periodic Potentials

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Section II reviews the general properties of the solutions of differential equations with periodic coefficients, the so-called Hill and Mathieu equations. In Section III asymptotic formulae for the eigenvalues of the Mathieu equation in the oscillatory region (Eq. (9)) are obtained by applying the Schrödinger perturbation theory to the problem of the physical pendulum. Section IV applies the W. K. B. method to the Hill equations. Implicit equations for the eigenvalues are obtained (§9, Eq. (28), (30) §10). They are valid for $E < V_{\max}$. In the introduction (Section I) a group of physical problems are mentioned, to which the results may be applied.

## I. Introduction

In a number of physical problems differential equations with periodic coefficients occur. These include, for instance, the problems of the vibrations of the elliptic membrane (Mathieu's original problem), the diffraction of light around an elliptic cylinder,[1] the variations of the orbit of the moon due to the sun's attraction (Hill's original problem), quantum mechanics of electrons in a crystal,[2] quantum mechanics of the physical pendulum,[3] the rotation of molecules in a crystal,[4] the torsional vibrations of the $CH_2$ or $CH_3$ group in the ethylene or ethane molecule.[5]

Unfortunately our knowledge of the Mathieu functions and of the corresponding eigenvalue problem is still rather incomplete, especially on the numerical side, although valuable work in this direction has been done recently by Ince and Goldstein.[6] Some advances can be made, in my opinion, by starting from the physical problems and by the use of the approximation methods suggested by them. So we shall apply in Section III the Schrödinger perturbation theory to the problem of the physical pendulum from the "oscillator" side and obtain certain asymptotic series for the eigenvalues and the Mathieu functions themselves. In Section IV we shall apply the well-known W. K. B. method to a slightly more general problem and obtain asymptotic expressions also for certain Mathieu functions of fractional order.

In Section II we will first give a more qualitative discussion of the properties of the Hill equation, of which the Mathieu equation is a special case. For all details and further developments, especially on the mathematical side, I refer to Whittaker and Watson,[7] Ince[8] and to the recent monograph of M. J. O. Strutt.[9]

## II. General Theorems on the Hill Equation

### §1. The Floquet theorem

We will write the Hill equation in the form:

$$d^2y/dx^2+(\lambda-gF(x))y=0, \tag{1}$$

in which $\lambda$ and $g$ are constants; $F(x)=F(x+\pi)$ and $F(x)$ is so normalized that:

$$\int_0^\pi F(x)dx=0 \quad |F(x)|\leqq 1. \tag{2}$$

The Mathieu equation is the special case corresponding to $F(x)=\cos 2x$. The Floquet theorem[10] states that the general solution of (1) is of the form:

$$y=C_1e^{\sigma_1 x}u_1(x)+C_2e^{\sigma_2 x}u_2(x) \tag{3a}$$

[1] See P. Epstein, Enc. der Math. Wiss. Vol. **5**, p. 507.

[2] F. Bloch, Zeits. f. Physik **52**, 555 (1929). Ph. Morse, Phys. Rev. **35**, 1310 (1930).

[3] E. U. Condon, Phys. Rev. **31**, 891 (1928).

[4] L. Pauling, Phys. Rev. **31**, 430 (1930).

[5] H. Nielsen, Phys. Rev. **40**, 445 (1932).

[6] Ince, Proc. Roy. Soc. Edinburgh **46**, 20, 316 (1926); **47**, 294 (1927). J. London Math. Soc. **2**, 46 (1927). Goldstein, Trans. Camb. Phil. Soc. **23**, 303 (1927).

[7] Whittaker and Watson, *Modern Analysis*, Chapter 19.

[8] Ince, *Differential Equations.*

[9] M. J. O. Strutt, *Lamé sche, Mathieusche und verwandte Funktionen in Physik und Technik*, Springer, Berlin, 1932.

[10] It is analogous to the Bloch theorem in the theory of metals.

or of the form:

$$y = e^{\sigma x}[C_1 u_1(x) + C_2\{x u_1(x) + u_2(x)\}]. \quad (3b)$$

In here $u_1$ and $u_2$ are periodic in $x$ with the period $\pi$; $\pi\sigma_1$ and $\pi\sigma_2$ in (3*a*) are the logarithms of the roots of a quadratic equation:[11]

$$s^2 - 2bs + 1 = 0. \quad (4)$$

From this it follows that $\sigma_1 = -\sigma_2$ and $\sigma_1$, $\sigma_2$ are either both real or conjugate complex. Therefore $\sigma_1$ and $\sigma_2$ can only be either both real or both pure imaginary. Eq. (3*b*) corresponds to the case that the quadratic Eq. (4) has two equal roots, of which $\pi\sigma$ is then the log. Because the double root of (4) can be only $\pm 1$, $\sigma$ must be either zero or $\pm i$.

### §2. Stable and unstable solutions

The $\sigma_1$ and $\sigma_2$ in (3*a*) are certain complicated functions of $\lambda$ and $g$, the determination of which is the main problem in the theory.

The solutions where the $\sigma$ are real are called "unstable" solutions because they become infinite with $\pm x$. So if, e.g., $y$ represents the displacement of a body from its orbit and $x$ the time (as in Hill's problem), in such a solution the body would go farther and farther away from its orbit. The solutions where the $\sigma$ are pure imaginary are called "stable" solutions. They remain oscillatory in infinity.

Because $\sigma = f(\lambda, g)$ we can draw curves in a $\lambda$, $g$ diagram on which $\sigma$ is a constant. One can prove that an infinite set of curves arises for each value of $\sigma$. The $\sigma$ imaginary curves fill regions which we will call the stable regions. The $\sigma$ real curves fill the rest of the diagram; they give the unstable regions (see Fig. 1). The solutions of type (3*b*), contain one stable and one unstable solution. They correspond to the curves which separate the stable and unstable regions. Each stable region is bounded by a curve corresponding to $\sigma = 0$ and one corresponding to $\sigma = \pm i$. In the case of the Mathieu equation the stable solutions corresponding to these double root values of $\sigma$ are the Mathieu functions of even ($\sigma = 0$) and odd ($\sigma = \pm i$) order. The corresponding solutions of the Hill equation might be called the Hill functions.

[11] The principal values of the log have to be taken. The coefficient $b$ is real. For a proof of these statements see Note 1.

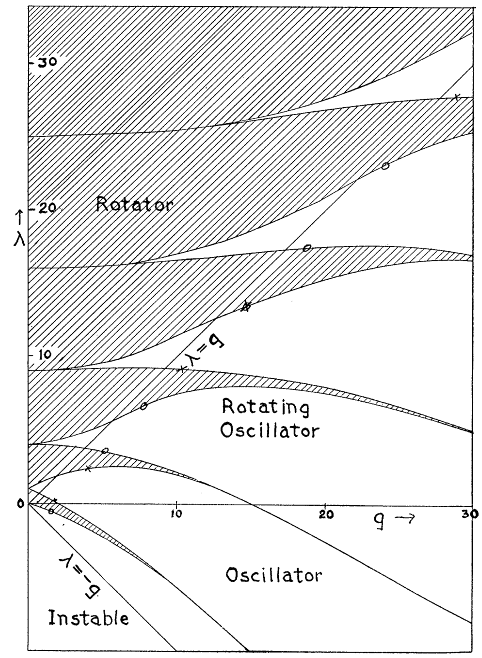


FIG. 1. Plot of regions of stable and unstable solution for $y'' + (\lambda + g \cos 2x)y = 0$. Regions of stable solution are shaded. Points used to plot curves taken from Strutt's monograph, page 24.

### §3. The extreme cases

In Fig. 1 we have four distinct regions: $\lambda < -g$, no stable solutions; $-g < \lambda < 0$, almost all points correspond to unstable solutions; $0 < \lambda < g$, regions of unstable solutions and regions of stable solutions both present with regions of unstable solution covering greater area; $\lambda > g$, greater part of area covered by regions of stable solutions.

The region $\lambda > g$ is called the rotator side since in a quantum mechanical problem it is the case when the total energy which corresponds to $\lambda$ is always greater than the potential energy, the maximum value of which is $g$.[12] The region

[12] In the quantum theory of metals this region corresponds to the case of nearly free electrons. It seems paradoxical that there are still unstable or "forbidden" regions, although they are narrow. It becomes clear, when one observes that there the de Broglie wave-length fulfills the Bragg total reflection condition.[13]

[13] See further L. Brillouin, *Die Quantenstatistik*, etc., Berlin, Springer, 1931.

$-g<\lambda<0$ is called the oscillator side since, in a quantum mechanical problem, it corresponds to the case when the system oscillates about a potential minimum.[14]

The transition region $0<\lambda<g$ may be called the rotating oscillator region. In here the very broad stable bands of the rotator side go over into the extremely narrow stable regions of the oscillator side.

## §4. The proper solutions

The proper solutions are those stable solutions having a preassigned period in $x$. Since $u_1$ and $u_2$ have the period $\pi$, the solutions having a period $\nu\pi$ where $\nu$ is an integer, are those for which $\sigma=2ri/\nu$ where $|r|$ is any integer $\leqq \nu/2$ or zero.

The problem of finding these proper solutions and the corresponding values of $\lambda$ (the eigenvalues) as function of $g$ usually arises in quantum mechanics where the potential $V(\theta)$ has a period $2\pi/\nu$ in an angle $\theta$. Then $\theta$ and $\theta+2\pi$ correspond to the same position so $\psi(\theta)=\psi(\theta+2\pi)$ if $\psi$ is to be single valued. Then after we transform to $x$ so that $V(x)=V(x+\pi)$ we must have:

$$\psi(x)=\psi(x+\nu\pi).$$

In the following chapters we will only be concerned with these eigenvalue problems. We will distinguish between one, two, three, etc., minima problems according to the value of $\nu(=1, 2, 3,$ etc.). The general character of the eigenvalues in these different cases can be easily seen from the Floquet theorem. Take first $\nu=1$; then $r$ can be only zero and we get, because $\sigma=0$ and we only want the stable solution, the Mathieu or Hill functions of even order. Because the other solution in (3*b*) must be discarded as being unstable, it is clear that the corresponding eigenvalues are not degenerated.[15] They are given by the curves marked with a circle in Fig. 1. For $\nu=2$, $r=0$ or $\pm 1$; we get, according to the definition in §2, both the Mathieu or Hill functions of even and odd order; the eigenvalues are again not degenerated. They are represented by the lines marked with either a circle or a cross. The case $\nu=3$ gives something new (see

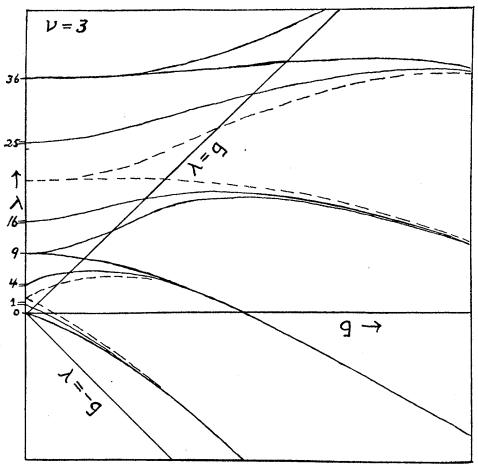


FIG. 2. Eigenvalue curves for a $\nu=3$ problem: $y''+(\lambda+g\cos 2x)y=0$; $y(x)=y(x+3\pi)$. Curves marked = represent eigenvalues degenerate for all values of $g$. Dotted curves represent the $\sigma=\pm i$ curves and are not eigenvalue curves for this problem.

Fig. 2). The value $r=0$ gives again the even order Mathieu functions with non-degenerate eigenvalues; $r=+1$ and $r=-1$ correspond to the two distinct solutions of Eq. (3*a*) with $\sigma_1=2i/3$, $\sigma_2=-2i/3$. The eigenvalues are therefore clearly doubly degenerate. For $\nu=4$ (see Fig. 3), we get the even and odd order Mathieu functions ($r=0$, $r=\pm 2$) and a doubly degenerate eigenvalue corresponding to $r=\pm 1$.

And so we can go on. In general it is easy to draw qualitatively the eigenvalues as function of $g$ or to connect the eigenvalues at the oscillator

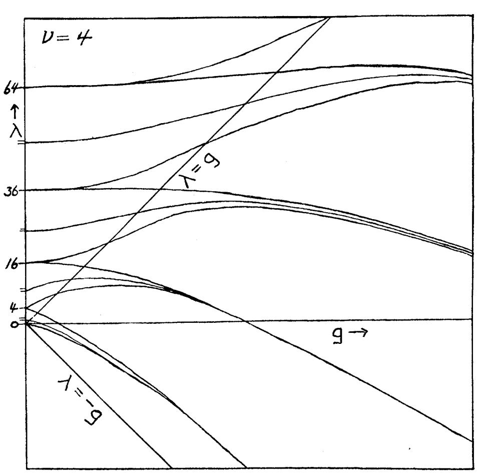


FIG. 3. Eigenvalue curves for a $\nu=4$ problem. Same as in Fig. 2 in all other respects.

[14] In the theory of metals this region corresponds to the case of nearly bound electrons.

[15] Except for certain discrete values of $g$, where the eigenvalue curves may cross. See Note I.

side with those at the rotator side. In the $\nu$-minima problem for $g=0$, the eigenvalues are given by:

$$\lambda(0)=[n+\tfrac{1}{2}-(-1)^n\tfrac{1}{2}+(-1)^n|i\sigma|]^2 \quad (5a)$$

when $\sigma$ is again $2ir/\nu$; they are then all doubly degenerate except the lowest. On the extreme oscillator side ($g\rightarrow+\infty$), one finds easily (see Section III):

$$\lambda(\infty)+g=4(n+\tfrac{1}{2})g^{\frac{1}{2}}. \quad (5b)$$

The eigenvalues here are $\nu$-fold degenerate. To connect the eigenvalues for one extreme of $g$ to those at the other extreme we need the *oscillation theorem*.[16] This theorem states that the eigenvalues are ordered in such a manner that if $\lambda_m$ corresponds to a proper solution having $m$ nodes in the interval $0\leq x<\nu\pi$ then $\lambda_m>\lambda_n$ if $m>n$. It is easy to see that the number of nodes $m$ corresponds to the integer $n$ of (5$a$) and (5$b$) by:

$$m=\nu[n+\tfrac{1}{2}-(-1)^n\tfrac{1}{2}+(-1)^n|i\sigma|].$$

So the $\nu$ lowest levels on the rotator side must join to the lowest $\nu$-fold degenerate level of the oscillator side; the second group of $\nu$ rotator levels joins the next oscillator level, etc. This enables us to draw the connecting lines, if one still remembers that all the levels are in the whole range of $g$ doubly degenerated except those corresponding to the even and odd order Hill functions. The curves corresponding to these cannot be drawn without further analysis because, as is remarked in Note I, those with the same $n$ may cross a finite number of times.[17]

## III. Perturbation Theory Attack

### §5. The quantum theory of the physical pendulum

The Schrödinger equation for a pendulum of length $r$ and having a bob of mass $m$ oscillating in the gravitational field of the earth is:[18]

$$d^2\psi/d\theta^2+(8\pi^2mr^2/h^2)(E-2mgr\sin^2\tfrac{1}{2}\theta)\psi=0, \quad (6)$$

where $\theta$ is the angle between the vertical and the string of the pendulum. We introduce the new variables given below and expand the $\sin^2\frac{1}{2}\theta$ term in a power series.

$$x=\tfrac{1}{2}r\theta; \qquad k=4\pi mg^{\frac{1}{2}}/r; \qquad \alpha=32\pi^2mr^2E/h^2; \qquad \mu^2=1/r. \quad (7)$$

The equation now takes a form allowing the Schrödinger perturbation theory to be applied quite readily.

$$d^2\psi/dx^2+[\alpha-2k^2\sum_{i=0}^{\infty}(-\mu)^i(2x)^{2i+2}/(2i+2)!]\psi=0. \quad (8)$$

The perturbation parameter is $\mu$. The zero order equation is then the well-known equation for the harmonic oscillator, with the eigenvalues $\alpha_n{}^0=4k(n+\frac{1}{2})$ and the eigenfunctions:

$$\psi_n{}^0=(2k/\pi)^{1/4}2^{-n/2}(n!)^{-\frac{1}{2}}e^{-kx^2}H_n(x(2k)^{\frac{1}{2}}),$$

where $H_n$ is the $n$th order Hermite polynomial. Without any trouble one can carry out the perturbation calculation to the second order in the eigenfunction and to the third order in $\alpha$.[19] The

[16] Ince, *Ordinary Differential* equation, p. 246. This question of connection was considered by Nielsen (reference 5) where one finds a figure in the case $\nu=6$.

[17] For an example where they cross once, see Strutt, reference 9, Fig. 3. In the case of the Mathieu functions (Fig. 2) they don't cross at all.

[18] A more likely problem is a dipole oscillating in a plane in a homogeneous electric field.

[19] The matrix elements involved in the perturbation formulae can all be obtained with the help of the integrals:

$$\int_{-\infty}^{+\infty}x^{2p}e^{-x^2}H_n(x)H_m(x)dx=\sum_{j=0}^{p-(m+n)/2}\binom{2p}{2j}\binom{2p-2j}{p-j+(m+n)/2}\frac{2^{(m+n)/2+j-p}}{((m+n)/2+j-p)!}\Gamma(j+\tfrac{1}{2}),$$

where $m+n$ must be even. If $m+n$ is odd the integral vanishes.

results are given below:

$$\alpha_n=\sum_0^\infty \alpha_n{}^j\mu^j$$

$$\alpha_n{}^0=4(n+\tfrac{1}{2})k,$$

$$\alpha_n{}'=-\tfrac{1}{4}(2n^2+n+1),$$

$$\alpha_n{}^2=-\frac{1}{4k}\frac{1}{4!}(6n^3+9n^2+9n+3),$$

$$\alpha_n{}^3=-\frac{3}{4k^2}\left(\frac{1}{4!}\right)^3\frac{1}{5!}(3600n^5+68611n^4+276241n^3+304691n^2+281690n+61480).$$

The coefficients in the development of the perturbed eigenfunctions in terms of $\psi_n{}^0$, i.e., the coefficients $d_{nm}{}^j$ in:

$$\psi_n=\sum_{j=0}^\infty \mu^j\psi_n{}^j;\qquad \psi_n{}^j=\sum_{m=0}^\infty d_{nm}{}^j\psi_m{}^0$$

have also been calculated, at least for $j=1$ and 2. Because they take up much space and because they will not be used later, we will not reproduce them here. The writer will be glad, though, to communicate the results by letter to anybody who is interested in them.

## §6. Discussion

For small values of $\mu$ or large values of $k$ the above formulae are very convenient for the numerical calculation of the eigenvalues. For the first three eigenvalues we have:

$$\alpha_0/k=2-0.25\rho-0.0312^5\rho^2-0.0278^+\rho^3-\cdots,$$
$$\alpha_1/k=6-1.25\rho-0.2813^-\rho^2-0.4602^-\rho^3-\cdots, \quad (9)$$
$$\alpha_2/k=10-2.75\rho-1.0938^-\rho^2-2.3761^+\rho^3-\cdots,$$

where $\rho=\mu/k$. To compare these results with the exact calculations of Goldstein we must first transform (8) to the standard form

$$d^2\psi/dx^2+(4a+16q\cos 2x)\psi=0, \quad (10)$$

so that

$$4a\rho^2=4+\alpha\rho/k, \quad (11a)$$

$$8q=1/\rho^2. \quad (11b)$$

For the comparison see Table I. The first column gives $q$, which determines $\rho$. From (9) one then calculates $\alpha_n/k$, which, substituted in (11$a$), gives our value of $a$ tabulated in column 2. The third column gives the exact values of $a$ according to Goldstein and his symbols for the eigenfunctions, the even order Mathieu functions. We see that if $q$ is large enough the error is very small.

TABLE I.

| $q$ | $1/\rho$ | Our $-a$ | Goldstein $-a$ | Function |
|---|---|---|---|---|
| 2 | 4 | 6.065 | 6.065 | $n=0$ |
| 3 | 4.898 | 9.615 | 9.615 | $Ce_0$ |
| 2 | 4 | 2.3373 | 2.3326 | $n=1$ |
| 3 | 4.898 | 4.9593 | 4.9791 | |
| 4 | 5.656 | 7.8450 | 7.8385 | $Se_2$ |
| 5 | 6.325 | 10.839 | 10.838 | |
| 5 | 6.325 | 5.183 | 5.110 | $n=2$ |
| 10 | 8.942 | 18.371 | 18.481 | |
| 20 | 12.65 | 49.087 | 49.382 | $Ce_2$ |
| 40 | 17.94 | 115.854 | 116.202 | |
| 100 | 28.28 | 329.972 | 330.137 | |

One must not expect that taking the higher order perturbations into account will always improve the result. It is fairly certain that (9) are not convergent but asymptotic developments of the eigenvalues in the extreme oscillator side. Even should the series for $\alpha_n$ and $\psi_n$ converge, one cannot be sure that they would converge to the required solution because one does not take the periodicity condition into account. For this reason one must expect that the series for $\psi_n(x)$ represents the even order Mathieu function fairly well only for $-\pi<x\mu^{\frac{1}{4}}<+\pi$. For values of $x$ outside this region we may continue the solution periodically. Furthermore one sees from Fig. 1 that on the extreme oscillator side the stable regions are extremely narrow so that one may expect that the series (9) will also represent the eigenvalues of all other stable solutions to within their inherent error. In Section IV we will calculate these extremely small splittings.

## IV. The W.K.B. Solution

### §7. Introduction

We will treat in this chapter the $\nu$-minima problem with the well-known W.K.B. method. The physical problem which it may represent is, e.g., the quantum theory of a wheel (symbolizing a molecule or a radical like $CH_2$) of $2\nu$ spokes of equal length. The wheel is rotating about a fixed axis and the ends of neighboring spokes carry opposite but equal charges. The wheel is placed in an inhomogeneous electric field (symbolizing the crystal or interatomic forces). The Schrödinger equation would be:

$$d^2\psi/d\theta^2+(8\pi^2I/h^2)(E-V(\theta))\psi=0 \quad (12)$$

where $V(\theta)=V(\theta+2\pi/\nu)$ and we will suppose that $V(\theta)$ has in each period $2\pi/\nu$ one maximum and one minimum and is even around each of them. We measure $\theta$ from one of these minima and take $\theta$ increasing counterclockwise. We choose the zero energy so that

$$\int_0^{2\pi} V(\theta)d\theta=0.$$

To apply the W.K.B. method we must distinguish between the classical and non-classical regions. The $2\nu$ roots of $E-V(\theta)=0$ are:

$$\theta_i=-a+2(i-1)\pi/\nu, \qquad \theta_i'=+a+2(i-1)\pi/\nu, \quad (13)$$

where $a$ is the first positive root. The region between $\theta_i$ and $\theta_i'$ will be called the $i$th classical region $(E-V>0)$ and the region $\theta_i'<\theta<\theta_{i+1}$, the $i$th non-classical region $(E-V<0)$.

In each classical region the solution of (12) will be oscillatory and be given by:

$$\psi_i=C_ip^{-\frac{1}{2}}\cos\left((2\pi/h)\int_{b_i}^{\theta}pd\theta+\delta_i\right), \quad (14)$$

where $b_i$ abbreviates $2(i-1)\pi/\nu$ and $p$ is the angular momentum $[2I(E-V)]^{\frac{1}{2}}$. In each non-classical region the solution of (12) will consist of a decreasing and an increasing exponential:

$$\psi_i'=A_i\bar{p}^{-\frac{1}{2}}\exp\left((2\pi/h)\int_{b_i'}^{\theta}\bar{p}d\theta\right)+B_i\bar{p}^{-\frac{1}{2}}\exp\left(-(2\pi/h)\int_{b_i'}^{\theta}\bar{p}d\theta\right), \quad (15)$$

where

$$b_i'=2(i-\tfrac{1}{2})\pi/\nu, \qquad \bar{p}=[2I(V-E)]^{\frac{1}{2}}.$$

### §8. Application of the connection formulae and of the periodicity condition

The relations between the constants $A_i$, $B_i$, $C_i$ and $\delta_i$ are determined by the connection formulae of Kramers.[20] Applying these to extend the solution in the $i$th non-classical region to the $i$th classical

[20] H. A. Kramers, Zeits. f. Physik **39**, 828 (1926); H. A. Kramers and G. P. Ittmann, Zeits. f. Physik **58**, 217 (1929); A. Zwaan, Diss. Utrecht (1929). These formulae are collected in a paper by L. A. Young and G. E. Uhlenbeck, Phys. Rev. **36**, 1154 (1930). For the application of the method to the two identical minima problem see D. M. Dennison and G. E. Uhlenbeck, Phys. Rev. **41**, 313 (1932) and to the problem of two unequal minima, Ta-You Wu, Phys. Rev. in press. From the standpoint of these papers I treat the case of an infinite number of identical minima, where one requires periodic solutions. This problem has also been considered by M. J. O. Strutt (Math. Ann. **101**, 559 (1929) using an analogous method with incorrect connection formulae.

region and requiring the result to be identical with (14) we obtain:

$$A_i = C_i\beta \cos(\gamma/2+\delta_i+\pi/4), \qquad B_i = (C_i/2\beta)\sin(\gamma/2+\delta_i+\pi/4), \tag{16}$$

where:

$$\beta = \exp\left((2\pi/h)\int_{b_i'}^{\theta_{i+1}} \bar{p}d\theta\right) = \exp\left((\pi/h)\int_{\theta_1'}^{\theta_2} \bar{p}d\theta\right), \tag{17}$$

$$\gamma = (2\pi/h)\int_{\theta_i}^{'_i} p d\theta = (2\pi/h)\int_{\theta_1}^{\theta_1'} p d\theta. \tag{18}$$

We extend the solution in the $i$th non-classical region to the succeeding $(i+1)$th classical region in the same manner and obtain:

$$A_i = (C_{i+1}/2\beta)\sin(\gamma/2-\delta_{i+1}+\pi/4), \qquad B_i = \beta C_{i+1}\cos(\gamma/2-\delta_{i+1}+\pi/4). \tag{19}$$

Eqs. (16) and (19) immediately lead to a recurrence relation between the phases $\delta_i$:

$$2\beta^2\cot(\gamma/2+\delta_i+\pi/4) = (1/2\beta^2)\,\mathrm{tg}(\gamma/2-\delta_{i+1}+\pi/4) \tag{20}$$

and to a set of linear homogeneous equations for the amplitudes $C_i$ [21]

$$C_i\beta\cos(\gamma/2+\delta_i+\pi/4) = (C_{i+1}/2\beta)\sin(\gamma/2-\delta_{i+1}+\pi/4). \tag{21}$$

Since $\psi$ must have the period $2\pi$, we must require:

$$\delta_i = \delta_{i+\nu}, \qquad C_i = C_{i+\nu}. \tag{22}$$

Therefore (21) are $\nu$ homogeneous linear equations in the $\nu$ unknowns $C_i$. In order that the solution be not identical zero, the determinant of the coefficients must vanish giving:

$$\beta^\nu \prod_{k=1}^{\nu}\cos(\gamma/2+\delta_k+\pi/4) = (2\beta)^{-\nu}\prod_{k=1}^{\nu}\sin(\gamma/2-\delta_k+\pi/4). \tag{23}$$

At least one of the $C_i$ will now be arbitrary, which is just what one needs to normalize the solution. From (20) and (23) the simpler form follows:

$$\prod_{k=1}^{\nu}\cos(\gamma+2\delta_k) = \prod_{k=i}^{\nu}\cos(\gamma-2\delta_k). \tag{24}$$

Because of (22) Eqs. (20) and (24) become $\nu+1$ equations for the $\nu$ $\delta_i$ and $\gamma$, which may be solved for $\gamma$ in terms of $\beta$ and integers (the quantum numbers) only. Since, if $V(\theta)$ is given, $\gamma$ and $\beta$ depend on $E$ only, this will give an implicit equation for the eigenvalues of $E$.

## §9. Solution in special cases

This solution of (20) and (24) for small values of $\nu$ is given below. Introducing the abbreviations:

$$\varphi_1 = 2\tan^{-1}(1/2\beta^2), \qquad \varphi_2 = 2\tan^{-1}[2\beta^2/1+4\beta^4+(1+4\beta^4+16\beta^8)^{\frac{1}{2}}]$$

we obtain:

$$\nu=1: \quad \gamma=(n+\tfrac{1}{2})\pi-(-1)^n\varphi_1; \qquad 4\delta_1=\pi-(-1)^n\pi, \tag{a}$$

$$\nu=2: \quad \gamma=(n+\tfrac{1}{2})\pi\pm\varphi_1; \qquad 4\delta_1=-4\delta_2=\pi-(-1)^n\pi, \tag{b}$$

$$\nu=3: \quad \gamma=(n+\tfrac{1}{2})\pi-(-1)^n\varphi_1; \qquad 4\delta_1=4\delta_2=4\delta_3=\pi-(-1)^n\pi, \tag{a}$$

$$\gamma=(n+\tfrac{1}{2})\pi+(-1)^n\varphi_2; \qquad 4\delta_1=\pi\mp(-1)^n\pi, \quad \delta_2=-\delta_3=\pm\tfrac{1}{2}(-1)^n\varphi_2, \tag{c}$$

[21] They arise from equating the first relations (16) and (19). Equating the second relations will give the same set of linear equations because of (20).

$\nu=4:\quad \gamma=(n+\frac{1}{2})\pi\pm\varphi_1;\qquad 4\delta_1=-4\delta_2=4\delta_3=-4\delta_4=\pi-(-1)^n\pi,\qquad (b)$

$\gamma=(n+\frac{1}{2})\pi;\qquad \delta_1=\delta_3=0,\quad \pi/2;\qquad \delta_2=\delta_4=\delta_1+\pi/2,\qquad (c)$

$\nu=6:\quad \gamma=(n+\frac{1}{2})\pi\pm\varphi_1;\qquad 4\delta_1=-4\delta_2=+4\delta_3=-4\delta_4=4\delta_5=-4\delta_6=\pi-(-1)^n\pi,\qquad (b)$

$\gamma=(n+\frac{1}{2})\pi+(-1)^n\varphi_2;\qquad 4\delta_1=4\delta_4=\pi\mp(-1)^n\pi;\qquad \delta_2=-\delta_3=\delta_5=-\delta_6=\pm(-1)^n\frac{1}{2}\varphi_2,\quad (c)$

$\gamma=(n+\frac{1}{2})\pi-(-1)^n\varphi_2;\qquad 4\delta_1=4\delta_4=\pi\pm(-1)^n\pi;\qquad \delta_2=-\delta_3=\delta_5=-\delta_6=\mp(-1)^n\frac{1}{2}\varphi_2.\quad (c)$

The equations marked (*a*) correspond to the even order Hill functions, those marked (*b*) to the Hill functions of both orders, those marked (*c*) to the doubly degenerate solutions (see Figs. 2 and 3, Section II).

TABLE II. *Splitting of first three eigenvalues for* $\nu=4$, $V(\theta)=-g\cos 4\theta$.

| $n$ | $q$ | $a'_1$ | $a'_2$ | $a'_3$ | $n$ | $q$ | $a'_1$ | $a'_2$ | $a'_3$ |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 1 | 10.49 | 10.75 | 11.01 | 2 | 3 | 78.64 | 80.93 | 83.05 |
| | 2 | 15.26 | 15.27 | 15.28 | | 5 | 112.03 | 112.65 | 113.27 |
| | 3 | 17.79 | 17.80 | 17.81 | | 8 | 146.48 | 146.52 | 146.56 |
| 1 | 2 | 42.19 | 43.63 | 44.97 | 3 | 5 | 143.47 | 147.48 | 152.25 |
| | 3 | 51.26 | 52.15 | 53.04 | | 8 | 194.43 | 194.96 | 195.49 |
| | 5 | 72.17 | 72.17 | 72.17 | | 12.5 | 251.72 | 251.76 | 251.80 |

Table II shows the splitting of the first three eigenvalues in the case $\nu=4$, $V(\theta)=-g\cos 4\theta$. We set:

$$16q=8\pi^2Ig/h^2 \quad\text{and}\quad a'=8\pi^2I(E+g)/h^2$$

to approach the standard form (10). The $a'$ is connected with the $a$ of (10) by:

$$a=a'-4q.$$

The middle column gives the doubly degenerate eigenvalues (see Fig. 3).

## §10. The general solution

We wish to correlate our W.K.B. solution with the Floquet theorem. To obtain the same notation as in Section II we introduce the variable $x=\nu\theta/2$, so that $V(x)=V(x+\pi)$ and $\psi(x)=\psi(x+\nu\pi)$. As in the proof of the Floquet theorem (see Note I) we will start with a fundamental set of W.K.B. solutions $y_1(x)$ and $y_2(x)$. For $y_1$ we choose the solution for which the phase $\delta_1$ in the first classical region is zero and which is then extended over the whole region without regard for the periodicity condition. For $y_2$ we choose the analogous solution with $\delta_1=\pi/2$. With the help of the connection formulae (20) and (21) we can write the characteristic equation analogous to (4) immediately:

$$s^2-2bs+c=0, \tag{25}$$

where now

$$2b=-(1/2\beta^2)(1+4\beta^4)\sin(\gamma+\pi/2), \tag{26}$$

$$c=[1+32\beta^8/[(1+16\beta^8)^2+64\beta^4\csc^2(\gamma+\pi/2)]]^{\frac{1}{2}}. \tag{27}$$

One sees that, in contrast to the case where one starts with two exact solutions, the coefficient $c$ is now not unity. However, since $\beta$ is always $>1$, $c$ is always nearly one ($1<c<1.04$). The difference is clearly due to our approximations. In the following we will take $c=1$. Calling the log of the roots of (25) again $\pi\sigma_1$ and $\pi\sigma_2$ we have then $\sigma_1=-\sigma_2=\sigma$ and from (26) follows:

$$\sin(\gamma+\pi/2)=-4\beta^2/(4\beta^4+1)\cos i\sigma\pi=\operatorname{sech} D\cos i\sigma\pi, \tag{28}$$

where

$$D=\log 2\beta^2=\frac{\pi\nu}{h}\int_{x_1'}^{x_2}\bar{p}dx+\log 2. \tag{29}$$

For the proper solutions we must take $\sigma = 2ri/\nu$, $|r| \leqq \nu/2$ or zero and then (28) is an implicit equation for $E$.[22] Comparing these results with the exact solution in the case of the Mathieu equation one finds that (28) gives too wide stable regions if $E$ is near $V_{\max}$. We can still improve the result (28) in the following manner. From (28) follows

$$\gamma = (n+\tfrac{1}{2})\pi - (-1)^n \sin^{-1} (\text{sech } D \cos i\sigma\pi).$$

Now if $\beta$ is large, sech $D$ is very small and we may put the $\sin^{-1}$ equal to its argument. So

$$\gamma = (n+\tfrac{1}{2})\pi - (-1)^n \text{ sech } D \cos i\sigma\pi. \tag{30}$$

If we now use (30) for all values of $D$, we get considerable better results for $E$ near $V_{\max}$, i.e., $D \cong \log 2$. Furthermore, (30) exhibits for $E$ near $V_{\max}$ the so-called quarter quantization of Kramers and Ittmann (reference 16), which must be expected.[23]

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## Note I.

Because most books do not contain the complete proof of the Floquet theorem we will give it here.

Let $y_1(x)$, $y_2(x)$ be a set of fundamental solutions of (1). Then because (1) is invariant under the transformation $x' = x+\pi$, $y_1(x+\pi)$ and $y_2(x+\pi)$ will also be solutions of (1). We must have therefore:[24]

$$\begin{aligned} y_1(x+\pi) &= d_{11}y_1(x) + d_{12}y_2(x), \\ y_2(x+\pi) &= d_{21}y_1(x) + d_{22}y_2(x). \end{aligned} \tag{$\alpha$}$$

We wish now to find a solution $y = c_1y_1 + c_2y_2$ so that $y(x+\pi) = sy(x)$. Using ($\alpha$) we find that $c_1$, $c_2$ must fulfill the equations:

$$\begin{aligned} c_1(s-d_{11}) + c_2d_{12} &= 0, \\ c_1d_{21} + c_2(s-d_{22}) &= 0. \end{aligned} \tag{$\beta$}$$

The necessary and sufficient condition that ($\beta$) has at least one solution is:

$$\begin{vmatrix} s-d_{11} & d_{12} \\ d_{21} & s-d_{22} \end{vmatrix} = 0.$$

One proves easily that:

$$d_{11}d_{22} - d_{12}d_{21} = \Delta(\pi)/\Delta(0) = 1,$$

when $\Delta(x) = y_1y_2' - y_2y_1'$ is the Wronskian, which is a constant as a consequence of (1). We get therefore for $s$ the quadratic equation (Eq. (4) of Section II)

$$s^2 - (d_{11}+d_{22})s + 1 = 0. \tag{$\gamma$}$$

There are two main cases:

a. ($\gamma$) has two single roots. We can then find two of the required solutions $y(x)$ and this leads to (3*a*).

b. ($\gamma$) has one double root, which must be $\pm 1$. Supposing $d_{12}$ and $d_{21}$ not both zero, we can then find only one set of $c_i$, i.e., one required solution $\bar{y}(x)$. To find the second solution substitute $y = x\bar{y} + z$. We find for $z$:

$$z'' + (\lambda - gF(x))z = -2d\bar{y}/dx. \tag{$\delta$}$$

$\bar{y}$ has the period $\pi(s=+1)$ or $2\pi(s=-1)$. The homogeneous part of ($\delta$) has $\bar{y}$ as the only periodic solution. We will be able to find a solution of ($\delta$) with period $\pi$ or $2\pi$ if and only if $\bar{y}$ is orthogonal to the right-hand side, which is obvious. So we are led to (3*b*).

There remains the possibility that $d_{12}$ and $d_{21}$ are both zero. Then the $c_i$ are arbitrary and all solutions are periodic with period $\pi$ or $2\pi$. We get again (3*a*) but with $\sigma_1 = \sigma_2 = 0$ or $\pm i$, so that both solutions are stable. One can prove that this can only occur for discrete values of $g$. They are the points where the eigenvalue curves for the Hill functions may cross (see §4).

[22] Strutt (reference 16) obtains by his method the equation which would result if one omits the log 2 in the definition of $D$. That this cannot be correct follows immediately from the fact that then for $E = V_{\max}$ all solutions would be stable, contrary to the known results (see Fig. 1; $E = V_{\max}$ corresponds to $\lambda = g$).

[23] Quarter quantization is to be expected for the limits of the stable regions if $E$ is near $V_{\max}$. Then $\sigma = 0$, $\pm i$, and sech $D \cong 0.8 \cong \frac{1}{4}\pi$ so that (30) goes over in: $\gamma = (n+\frac{1}{2})\pi \pm \frac{1}{4}\pi$.

[24] The $y_1$, $y_2$ may be chosen real and then the $d_{ij}$ will also be real.