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On the solution of Hill's equation using Milne's method

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Abstract. Milne's method is applied to the Hill equation, i.e. the Schrödinger equation for a periodic one-dimensional potential. The method allows a compact discussion of the organization and parameter dependence of the stability bands as well as an efficient numerical computation of the band edges. As an example a class of potentials which show a transition from two to one minimum per period is studied numerically. Furthermore, periodic solutions of the Milne equation are discussed and constructed.

1. Introduction

In this paper we study the one-dimensional Hill equation [1], which appears in numerous problems in physics. Typical examples are the classical harmonic oscillator with periodic parametric excitation [2]

$$\frac{d^2x}{dt^2}+\omega^2(t)x=0 \tag{1}$$

where $\omega(t+T)=\omega(t)$, or the propagation in periodic structures, i.e. the one-dimensional Schrödinger equation

$$\frac{d^2\psi}{dx^2}+\frac{2m}{\hbar^2}(E-V(x))\psi=0 \tag{2}$$

with a periodic potential $V(x+L)=V(x)$. A well-known example from mathematical physics is the Mathieu equation. Despite their appearance in many textbooks on mechanics or quantum mechanics the Hill equation is still not fully understood, as the recent appearance of various articles on this subject [3-10] demonstrates.

The purpose of the present paper is to develop certain aspects of the so-called 'amplitude-phase' method in more detail, namely, to study the connection between the Hill equation and the Milne equation [11] under periodic conditions. The Milne equation has been studied before in many articles, references to which can be found in previous papers by one of the authors (HJK) [12-14] covering the non-periodic case (bound and resonance states for the Schrödinger equation). Although being nonlinear, the Milne equation offers various advantages in comparison to the original linear equations and provides a powerful tool for many applications, including numerical ones. Here we demonstrate its usefulness for the investigation of the Hill equation.

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A second aim of the present study is a discussion of the existence, properties and numerical construction of periodic solutions of the Milne equation. Such solutions are essential for a forthcoming article about the quasienergy (Floquet) spectrum of the (periodically) parametrically excited quantum mechanical harmonic oscillator [15].

2. The Hill and the Milne equations

The Hill equation (e.g. see [1, 16]) in its standard form is given by

$$y''(x)+Q(x)y(x)=0 \tag{3}$$

where $Q(x)$ is periodic with period T:

$$Q(x+T)=Q(x). \tag{4}$$

In our discussion we will furthermore assume that $Q(x)$ satisfies the symmetry condition

$$Q(x)=Q(-x). \tag{5}$$

In particular we will discuss the periodic Schrödinger equation, i.e.

$$Q(x)=\frac{2m}{\hbar^2}(E-V(x)) \tag{6}$$

where the periodic, symmetric potential has a global minimum at $x_0=0$ in the interval $[-T/2, T/2]$. There is an intimate connection between the linear equation (3) and the nonlinear Milne equation [11]

$$\rho''(x)+Q(x)\rho(x)=\frac{1}{\rho^3(x)}. \tag{7}$$

The general solution of (3) can be constructed from a single (arbitrary) solution of (7) as

$$y(x)=b\rho(x)\sin(\varphi(x)+\beta) \tag{8}$$

where b and β are arbitrary constants, and $\varphi(x)$ is related to $\rho(x)$ by the integral

$$\varphi(x)=\int_{x_0}^{x}\frac{dx'}{\rho^2(x')}. \tag{9}$$

On the other hand the general solution of Milne's equation (7) can be written in terms of two independent solutions y_1, y_2 of the linear equation (3) [14, 17, 18] as

$$\rho(x)=(Ay_1^2(x)+By_2^2(x)+2Cy_1(x)y_2(x))^{1/2}. \tag{10}$$

The constants A, B and C are related to the Wronskian W of $y_1(x)$ and $y_2(x)$ by $AB-C^2=W^{-2}$ and determined by the initial condition for $\rho(x_0)$ and $\rho'(x_0)$ at some point x_0. It should be stressed that they—as well as $y_1(x)$, $y_2(x)$ and W—are generally dependent on the parameters of $Q(x)$, i.e. energy dependent for the case of the Schrödinger equation (6).

In terms of (10) the phase integral $\varphi(x)$ can be evaluated in closed form [14]:

$$\varphi(x)=-\tan^{-1}\left[W\left(C+A\frac{y_1(x)}{y_2(x)}\right)\right]_{x_0}^{x}. \tag{11}$$

Unless otherwise stated, we will in the following always use symmetric solutions of Milne's equation, i.e. we choose the initial condition $\rho'(0)=0$.

The use of the Milne equation has various advantages despite its nonlinearity. Numerical integration is straightforward and the solutions are well behaved and smooth, in particular for so-called '*classical initial conditions*'

$$\rho(0)=Q^{-1/4}(0) \qquad \text{and} \qquad \rho'(0)=0 \tag{12}$$

where 0 is the position of the maximum of the $Q(x)$ function (a minimum of $V(x)$). In this case $\rho^{-2}(x)$ closely resembles the classical wavenumber $Q^{1/2}(x)$ [12, 13].

For symmetric solutions the constant β is equal to $\pi/2$, for antisymmetric solutions we have $\beta=0$ (note that $\rho(-x)=\rho(x)$ and $\varphi(x)=-\varphi(-x)$). Furthermore one can construct solutions $y_n^{(+)}(x)$, which vanish at the end of the unit potential box,

$$y_n^{(+)}\left(\pm\frac{T}{2}\right)=0 \tag{13}$$

by imposing the condition

$$\Phi(E)=2\varphi\left(\frac{T}{2}\right)=2\int_0^{T/2}\frac{\mathrm{d}x}{\rho^2(x)}=(n+1)\pi \qquad n=0,1,2,\ldots. \tag{14}$$

Equation (13) is only satisfied for special values $E=\varepsilon_n^+$ and (14) is recognized as the quantization condition [12] for the box potential

$$\tilde{V}(x)=\begin{cases} V(x) & \text{for } |x|<\dfrac{T}{2} \\ \infty & \text{for } |x|\geqslant\dfrac{T}{2} \end{cases} \tag{15}$$

It will be helpful to construct solutions $y_n^{(-)}(x)$ with vanishing derivatives at the box boundaries:

$$y_n^{(-)\prime}\left(\pm\frac{T}{2}\right)=0. \tag{16}$$

The energies satisfying (16) are denoted as $E=\varepsilon_n^-$.

From (8) we obtain

$$y'(x)=b\left(\rho'\sin(\varphi+\beta)+\frac{1}{\rho}\cos(\varphi+\beta)\right) \tag{17}$$

and (16) leads to the condition

$$\tan\left(\frac{\Phi}{2}\right)=\Delta \tag{18}$$

for symmetric and

$$\tan\left(\frac{\Phi}{2}\right)=-\frac{1}{\Delta} \tag{19}$$

for antisymmetric solutions. Δ is determined by the ρ-function at the boundary

$$\Delta=\rho'\left(\frac{T}{2}\right)\rho\left(\frac{T}{2}\right) \tag{20}$$

and the index n is defined by $n\pi<\Phi<(n+1)\pi$ for $\Delta>0$ and by $(n-1)\pi<\Phi<n\pi$ for $\Delta<0$. The functions $y_n^{(\pm)}(x)$ are symmetric for even n and antisymmetric for odd n and n counts the number of zeros inside the unit potential box $|x|\leqslant T/2$. Each of

the two sets ε_n^+ and ε_n^- is non-degenerate. However, a member of ε_n^- can be degenerate with one of ε_n^+. A direct consequence of (18), (19) and (14) are the inequalities

$$\begin{aligned} &\varepsilon_{n-1}^+ \leqslant \varepsilon_n^- < \varepsilon_n^+ \qquad \text{for } \Delta > 0 \\ &\varepsilon_{n-2}^+ < \varepsilon_n^- \leqslant \varepsilon_{n-1}^+ \qquad \text{for } \Delta < 0. \end{aligned} \tag{21}$$

Hence, a degeneracy occurs for $\Delta = 0$ and is restricted to the case $\varepsilon_n^- = \varepsilon_{n-1}^+$.

Figure 1 shows results for the Mathieu equation

$$Q(x) = E - 2q\cos(2x). \tag{22}$$

The phase integral $\Phi(E)$ as well as $\Delta(E)$ are given for a value of $q = -1.5$. Figure 2 shows the typical smooth behaviour of the Milne solutions when classical initial conditions are used ($E = 8$ and $E = 28$, with $q = -4$). The Milne solutions are non-oscillatory, contrary to the $y(x)$s, and $\rho^{-2}(x)$ closely resembles the classical wavenumber $Q^{1/2}(x)$, which is also shown for comparison. It should be stressed that the observed behaviour is typical only for classical initial conditions and potentials structurally similar to (22). Different initial conditions (see [14]) and more complicated potentials can lead to a different behaviour of $\Phi(E)$ and $\Delta(E)$ (numerical examples are given below). For energies not exceeding the potential maximum, i.e. $E < 8$ for $q = -4$, part of the potential region becomes classically forbidden. A semiclassical approximation of $\rho^{-2}(x)$ for this case is discussed in [12].

Several properties concerning the function $\Phi(E)$ have been proven (e.g. see [14] and references therein):

(i) $\Phi(E) = (n+1)\pi$ has a unique solution E_n for $n = 0, 1, \ldots$ (23)

(ii) $\Phi(E_n) < \Phi(E_{n+1})$ (24)

(iii) $$\left.\frac{\mathrm{d}\Phi(E)}{\mathrm{d}E}\right|_{E_n} > 0 \tag{25}$$

(iv) $\Phi(E_n) < \Phi(E) < (E_{n+1})$ for $E_n < E < E_{n+1}$. (26)

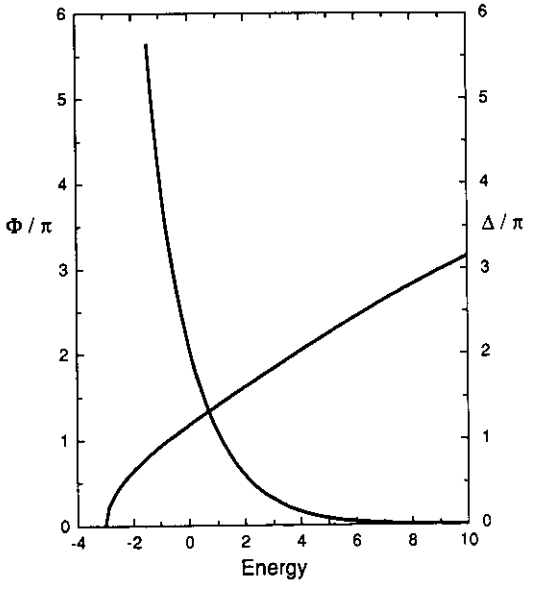

Figure 1. $\Phi(E)$ and $\Delta(E)$ as functions of the energy for the Mathieu potential with $q = -1.5$. Classical initial conditions are used.

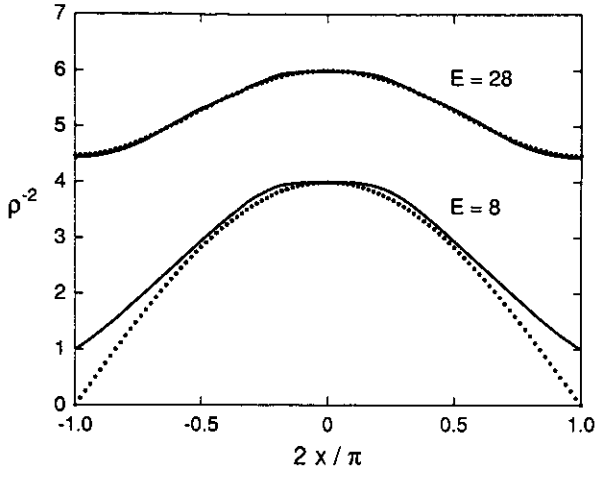

Figure 2. The function $\rho^{-2}(x)$ for the Mathieu potential ($q=-4$) for energies $E=8$ and 28. Also shown is the classical wavenumber $Q^{1/2}(x)$ (dotted curves).

It is possible for $\Phi(E)$ to decrease with increasing energy, but such a behaviour is rare and confined to small energy intervals because of (26).

3. The characteristic exponent and the band structure

Since $Q(x)$ in (3) is T-periodic, it follows from Floquet's theorem that there exists a so-called Floquet solution of the form

$$F_+(x)=\mathrm{e}^{+\mathrm{i}\nu x}p(+x) \tag{27}$$

where $p(x)$ is a periodic function with period T and ν a complex number known as the characteristic exponent. Since $Q(x)$ satisfies the symmetry condition (5),

$$F_-(x)=F_+(-x)=\mathrm{e}^{-\mathrm{i}\nu x}p(-x) \tag{28}$$

is another solution of (3), not necessarily independent of $F_+(x)$. Using (27) one obtains the following relations between F_+ and F_-:

$$F_\pm(x)=\mathrm{e}^{\mp\mathrm{i}\nu T}F_\pm(x+T) \tag{29}$$

$$F_\pm\left(\frac{T}{2}\right)=\mathrm{e}^{\pm\mathrm{i}\nu T}F_\pm\left(-\frac{T}{2}\right) \tag{30}$$

$$F_\pm\left(-\frac{T}{2}\right)F'_\pm\left(\frac{T}{2}\right)=F_\pm\left(\frac{T}{2}\right)F'_\pm\left(-\frac{T}{2}\right). \tag{31}$$

Because of the symmetry $Q(x)=Q(-x)$ we will in the following choose a symmetric Milne solution denoted here as $\rho_s(x)$. The general solution of (3) is now (compare to (8))

$$y(x)=a\rho_s(x)(\mathrm{e}^{\mathrm{i}\varphi_s(x)}+\alpha\,\mathrm{e}^{-\mathrm{i}\varphi_s(x)}) \tag{32}$$

where a and α are arbitrary constants related to the initial conditions. From (31) and (32) one obtains after a little algebra an expression for α:

$$\alpha^2+2\alpha g+1=0 \tag{33}$$

where the g-function is defined as

$$g(E)=\cos\Phi-\frac{1}{\Delta}\sin\Phi \tag{34}$$

with

$$\Phi(E)=2\int_0^{T/2}\frac{dx}{\rho_s^2(x)}=2\varphi_s\left(\frac{T}{2}\right) \tag{35}$$

and

$$\Delta=\rho_s'\left(\frac{T}{2}\right)\rho_s\left(\frac{T}{2}\right) \tag{36}$$

(compare (14) and (20)). Defining furthermore the function

$$\mu(E)=\cos\Phi+\Delta\sin\Phi \tag{37}$$

we find from (30) the Floquet exponent ν, related to μ by

$$\cos(\nu T)=\mu(E). \tag{38}$$

The function μ is an oscillating function of the energy E. The characteristic exponent ν takes real values only if μ satisfies the condition $|\mu|\leqslant 1$. In other cases ν is a complex number. According to Floquet's theory real values of ν are associated with bounded (stable) solutions and complex νs with unstable ones. Hence the range of the μ-function indicates stability and instability zones. The g-function is related to μ by

$$\mu^2=1+(1-\Delta^2)g^2. \tag{39}$$

and has a reverse behaviour, in fact ν is real if $|g|>1$.

In spite of the fact that Φ and Δ are in general dependent on the initial condition for ρ_s, the μ-function is independent of it as expected (see appendix 1). We conclude the μ and g allow an immediate characterization of zones with stable and unstable solutions in the following way:

$$\begin{array}{lll} \nu\in\mathbb{R} & |\mu|<1\leftrightarrow|g|>1 & \text{stability zone ('band')} \\ \nu\in\mathbb{C} & |\mu|>1\leftrightarrow|g|<1 & \text{instability zone ('gap').} \end{array} \tag{40}$$

The conditions $|\mu|=1$ or $|g|=1$ can be easily used to calculate the band edges numerically.

Figure 3 shows the behaviour of μ and g as a function of E calculated for the case of the Mathieu equation (22) with $q=-4$. Solving the equation $|\mu|=1$ numerically, the band edges of the lowest three bands as shown in figure 3 are obtained in agreement with the results given in [19].

In the remainder of this section we will discuss the band/gap structure in terms of the Milne solutions. Adopting the notation of Magnus and Winkler [1], the stability boundaries are denoted as

$$E_0^+<E_1^-\leqslant E_2^-<E_1^+\leqslant E_2^+<E_3^-\leqslant E_4^-\leqslant E_3^+\leqslant\ldots \tag{41}$$

and the nth stability band is given by the closed interval

$$\begin{array}{ll} [E_{2k}^+, E_{2k+1}^-] & \text{for } n=2k \\ [E_{2k+2}^-, E_{2k+1}^+] & \text{for } n=2k+1. \end{array} \tag{42}$$

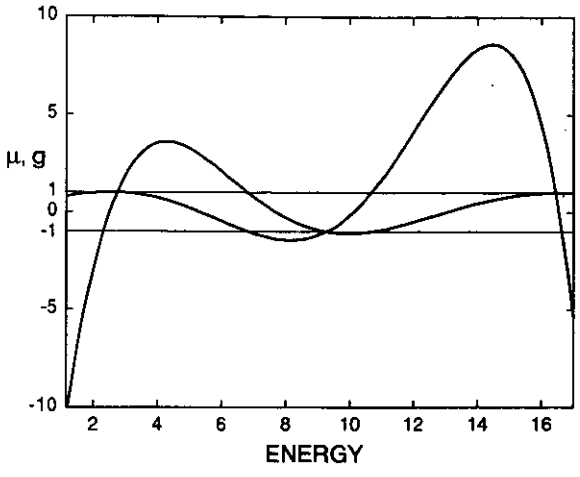

Figure 3. The figure shows a typical behaviour of μ and g as functions of E for the Mathieu potential with $q=-4$. Classical initial conditions are used.

These boundaries depend on the parameters of the system and only the gaps can shrink to zero. In our case the boundaries are determined by the conditions $|\mu|=|g|=1$. Rewriting μ and g as

$$\begin{aligned}\mu(E)&=\sqrt{1+\Delta^2}\cos(\Phi-\beta)\\ g(E)&=\sqrt{1+\Delta^{-2}}\sin(\Phi-\beta)\end{aligned}\tag{43}$$

with $\beta=\tan^{-1}\Delta$, we see that the values of $|\mu|$ at the maximum are bounded by $\sqrt{1+\Delta^2}$ from above and by 1 from below, consequently the gaps ($|\mu|>1$) can shrink to zero only when $\Delta=0$. The bands ($|g|\geqslant 1$) can never disappear because the maximum of $|g|$ exceeds $\sqrt{1+\Delta^2}$ and Δ^{-2} is always different from zero. Note that for a finite potential $V(x)$ both ρ and ρ', and hence also Δ, are finite. These findings are of course in agreement with the results at (41), (42). In addition it should be noted, that $\Delta=0$ implies $|\mu|\leqslant 1$, and a diverging g. Therefore Δ can only vanish inside the bands or at their boundaries.

From (14) we conclude that at the eigenvalues ε_n^- of the unit box we have

$$\mu_n^+=\mu(\varepsilon_n^+)=g(\varepsilon_n^+)=-(-1)^n\tag{44}$$

i.e. these energies appear at the gap boundaries and vice versa $g(E)=\mu(E)$ implies $E=\varepsilon_n^+$. In addition we find

$$\mu_n^{+\prime}=\left.\frac{\mathrm{d}\mu}{\mathrm{d}E}\right|_{\varepsilon_n^+}=-(-1)^n\Delta_n\left.\frac{\mathrm{d}\Phi}{\mathrm{d}E}\right|_{\varepsilon_n^+}\tag{45}$$

with $\Delta_n=\Delta(\varepsilon_n^+)$ and

$$\mu_n^{+\prime}\mu_n^+=\Delta_n\left.\frac{\mathrm{d}\Phi}{\mathrm{d}E}\right|_{\varepsilon_n^+}.\tag{46}$$

Because of $\mathrm{d}\Phi/\mathrm{d}E|_{\varepsilon_n^+}>0$ (see (26)) the sign of (46) is determined by Δ_n. For $\Delta_n>0$ the ε_n^+ constitute an upper band boundary and for $\Delta_n<0$ a lower boundary.

As is well known, the one-dimensional bound state energies are strictly non-degenerate and hence the ε_n^+ can never cross if parameters are varied. They thus constitute the basic skeleton of the band/gap structure. On the other hand we have

$$\mu_n^- = \mu(\varepsilon_n^-) = -g(\varepsilon_n^-) = (-1)^n \tag{47}$$

for energies ε_n^- satisfying conditions (18) or (19), i.e. there exist solutions $y_n^{(-)}(x)$ with n nodes and vanishing derivatives at the box ends. These are the only energies satisfying $\mu(E) = -g(E) = 1$. For many cases the $\varepsilon_n^-(\varepsilon_n^+)$ form the lower (upper) boundaries of the bands (compare (42), see also the discussion of the band structure by Harrell [3]). If a parameter of the system is varied, Δ can change sign and the band structure changes. A numerical example is given in figure 4 for the potential

$$V(x, \delta) = 2q(\cos\delta \cos 2x + \sin\delta \cos x) \tag{48}$$

for $q = -4$. Here the band/gap structure is shown as a function of the parameter δ, varying from 0 to π (a similar study for this potential has been published almost 50 years ago [20]). For all values of δ the potential is 2π-periodic. In fact (48) can be regarded as the first two terms of a Fourier expansion of a general 2π-periodic potential. For $\delta = 0$ and π it agrees with the π-periodic Mathieu potential (22) and the spectra are identical. For $\delta = \pi/2$ we also have a Mathieu potential, but with doubled period. Between these values the potential shows a more complicated behaviour with more than one minimum per period for $|\tan\delta| < 4$. Some representative examples are shown in figure 5. The basic features of the band/gap structure shown in figure 4 can be understood as follows. Increasing δ from 0 destroys the π-symmetry and the degeneracy of ε_{2k}^+ and ε_{2k-1}^-, thus opening a new gap inside the bands. This band splitting is analogous to the level splitting in a double-well potential. The new gap region grows with increasing δ, whereas the higher gaps of the $V(x, 0)$-potential decrease until they shrink to zero close to $\delta = \pi/4$, where the band/gap edges cross (Δ vanishes). More such crossings are observed for higher energies and increasing values of δ. Note that only band edges satisfying $\varepsilon_n^- = \varepsilon_{n-1}^-$ can cross, as discussed in section 2.

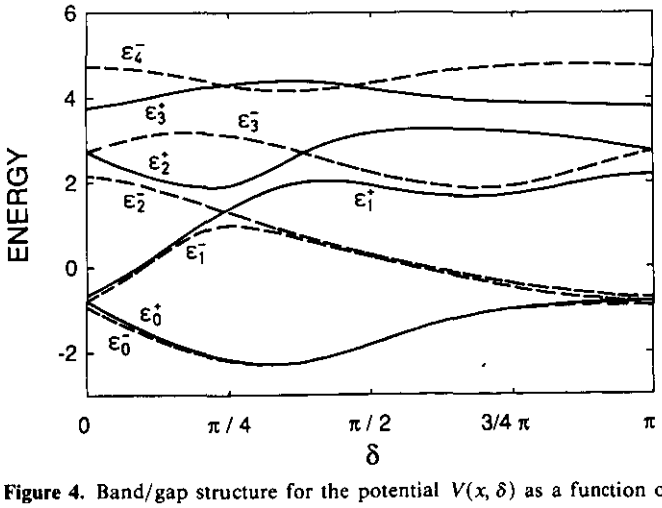

Figure 4. Band/gap structure for the potential $V(x, \delta)$ as a function of the parameter δ for $q = -4$.

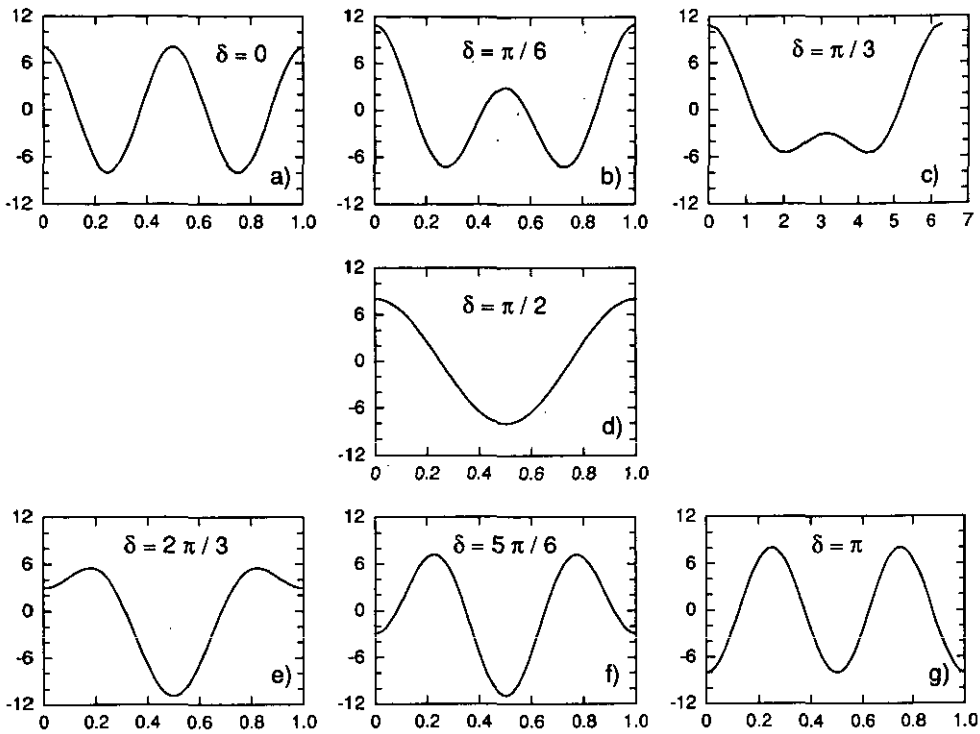

Figure 5. Potential $V(x, \delta)$ inside the period $-\pi < x < \pi$ for various values of the parameter δ, namely $\delta = k\pi/6$, $k = 0, 1, \ldots, 6$.

4. Periodic solutions of the Milne equation

Properties such as the zeros and the number of zeros of the solution of the Hill equation or the characteristic exponent in the Floquet representation can be easily derived if we know explicitly periodic solutions of the Milne equation.

In this section we will construct the periodic and symmetric Milne solution in terms of an arbitrary real symmetric one. To do this we choose two independent Hill solutions defined as

$$\begin{aligned} y_1(x) &= \rho_s(x) \sin \varphi_s(x) \\ y_2(x) &= \rho_s(x) \cos \varphi_s(x) \end{aligned} \tag{49}$$

and by (10) the general solution of the Milne equation can be written as

$$\tilde{\rho}(x) = (A \sin^2 \varphi_s(x) + B \cos^2 \varphi_s(x) + 2C \sin \varphi_s(x) \cos \varphi_s(x))^{1/2} \rho_s(x). \tag{50}$$

The general symmetric solution is obtained by requiring symmetric conditions, i.e. $C = 0$. Then $AB - C^2 = W^{-2} = 1$ implies $A = 1/B$ and (50) now reads

$$\tilde{\rho}(x) = \left(\frac{(1 - A^2) \cos(2\varphi_s(x)) + 1 + A^2}{2A} \right)^{1/2} \rho_s(x) \tag{51}$$

where A is related to the initial condition $\tilde{\rho}(0)$.

Now fixing $A=\sqrt{(g+1)/(g-1)}$, where g depends on $\rho_s(x)$ by (34), (51) satisfies $\tilde{\rho}(T/2)=0$, that is, $\tilde{\rho}(x)$ is a T-periodic function. With this value of A we get

$$\rho_p(x)=\left(\pm\frac{1}{\sqrt{g^2-1}}[\cos(2\varphi_s(x))-g]\right)^{1/2}\rho_s(x). \tag{52}$$

This constitutes the symmetric and periodic solution of Milne's equation in terms of an arbitrary symmetric one, and we find that $\rho_p(x)$ is: (i) a real or pure imaginary function if $|g|>1$ ('band'); (ii) a complex function if $|g|<1$ ('gap').

It also follows that for a periodic solution $\rho_p(x)$ the boundary term Δ defined in (20) vanishes, i.e. $\Delta_p=0$. comparing (37) and (38) immediately gives the desired result

$$\nu=\frac{1}{T}\int_{-T/2}^{T/2}\frac{dx}{\rho_p^2(x)}+\frac{2n\pi}{T} \tag{53}$$

and again we find that $\nu\in\mathbb{R}$ if $|g|>1$ ('band') and $\nu\in\mathbb{C}$ if $|g|<1$ ('gap'). Inserting $\rho_p(x)$ into (53) we obtain

$$\nu=\pm\frac{2}{T}\tan^{-1}\left[\sqrt{\frac{g+1}{g-1}}\tan\left(\int_0^{T/2}\frac{dx}{\rho_s^2(x)}\right)\right]. \tag{54}$$

But by (34) and (38)

$$\sqrt{\frac{g-1}{g+1}}=\sqrt{\frac{1+\mu}{1-\mu}}\tan\left(\int_0^{T/2}\frac{dx}{\rho_s^2(x)}\right) \tag{55}$$

then one can rewrite ν as

$$\nu=\pm\frac{2}{T}\tan^{-1}\sqrt{\frac{1-\mu}{1+\mu}} \tag{56}$$

which is equivalent to (38).

One interesting point for analysing the following is related to the zeros of the periodic Milne's solution. Denoting the zeros of ρ_p by $\tilde{x}$, one sees from (52) that

$$\cos 2\varphi_s(\tilde{x})=g \tag{57}$$

because $\rho_s(x)$ itself cannot vanish as is proven in appendix 2.

In principle, (57) allows two kinds of solutions: (i) real solutions if $|g|\leqslant 1$, i.e. in the energy gaps, and (ii) imaginary solutions if $|g|>1$, i.e. in the energy bands. But since ρ_s and φ_s are both real only the first case is realized, i.e. $\rho_p(x)$ has zeros in the gaps.

Let $\{\varepsilon_n^+\}_{n=1,\ldots,\infty}$ be the set of energy values defined by (44) and $N(E)$ the quantum number function defined by (see [12, 14])

$$N(E)=\frac{2}{\pi}\varphi_s\left(\frac{T}{2},E\right)=\frac{\Phi(E)}{\pi}. \tag{58}$$

Assuming $\Delta>0$ the ε_n^+ constitute an upper band boundary (see section 3) then $N(\varepsilon_n^+)$ takes integer values and since $\varphi_s(x,\varepsilon_n^+)\leqslant\varphi_s(T/2,\varepsilon_n^+)$ the inequality

$$\varphi_s(\tilde{x},\varepsilon_n^+)\leqslant n\frac{\pi}{2} \tag{59}$$

holds and similarly

$$\varphi_s(\tilde{x},\varepsilon_n^-)\leqslant n\frac{\pi}{2}. \tag{60}$$

Equations (57), (59) and (60) define the number of zeros on the band edges $N_{u.b.} = [n/2]+1$ and $N_{l.b.} = [n/2]$ with $n = 1, \ldots$, for the upper and lower band respectively, where $[f]$ denotes the integer part of f. If Δ_n changes sign this behaviour is inverted, as was already mentioned in section 3.

The $\varphi_s(x)$ function satisfies the relation (see (59))

$$0 \leq \varphi_s(x, \varepsilon_n^+) \leq n\frac{\pi}{2} \tag{61}$$

then (57) is satisfied once for $n = 1$, twice for $n = 2$ and so on. In other words, the number of zeros of $\rho_p(x)$ or $y(x)$ is given by the band number n.

5. Concluding remarks

In the present article we tried to show the usefulness of the Milne approach for treating a well-known and well-studied problem: the Hill equation or, equivalently, the periodic Schrödinger equation. We restricted ourselves to a few points of general interest and investigated in some more detail the question of periodic Milne solutions, which are of basic importance for our current work on the quasienergy spectrum of time-periodically driven quantum oscillators [15]. The Milne method has, however, a much broader range of applications, for instance:

(i) The Milne method can be used in a straightforward way to analyse and compute the spectrum of a long but finite chain of identical box potentials.

(ii) The same technique can also be used to study chains with different box potentials, e.g. one-dimensional binary alloys and ordered or random crystals.

(iii) In various articles semiclassical approximations to the band spectrum have been derived [19, 21-24]. The Milne method offers a very convenient way to introduce semiclassical approximations for the band spectrum (for previous semiclassical approximations in context with the Milne equation see [12]).

Work along these lines is in progress.

Acknowledgments

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Appendix 1

Let $\rho(x)$ be a solution for Milne's equation given in (9)

$$\rho(x) = [Ay_1^2(x) + By_2^2(x) + 2Cy_1(x)y_2(x))^{1/2}. \tag{A1.1}$$

We need only the symmetric solutions for constructing the μ-function, i.e. $\rho(x)$ must satisfy the condition

$$\rho'(0) = 0. \tag{A1.2}$$

Using (A1.1) and (A1.2) we get $C=0$ and

$$\begin{aligned} y_1(x) &= y_1(-x) \\ y_2(x) &= -y_2(-x) \end{aligned} \tag{A1.3}$$

and using the restriction (A1.3) we get, for Δ and Φ,

$$\Delta = \rho'\left(\frac{T}{2}\right)\rho\left(\frac{T}{2}\right) = Ay_1\left(\frac{T}{2}\right)y_1'\left(\frac{T}{2}\right) + By_2\left(\frac{T}{2}\right)y_2'\left(\frac{T}{2}\right) \tag{A1.4}$$

$$\Phi = -2\tan^{-1}\left(WA\frac{y_1(T/2)}{y_2(T/2)}\right). \tag{A1.5}$$

The Wronskian evaluated at $T/2$ is

$$W = y_1\left(\frac{T}{2}\right)y_2'\left(\frac{T}{2}\right) - y_1\left(\frac{T}{2}\right)y_2'\left(\frac{T}{2}\right) \tag{A1.6}$$

and inserting (A1.4)–(A1.6) into (36) we can rewrite the μ-function as

$$\mu = \frac{y_1(T/2)y_2'(T/2) + y_1(T/2)y_2'(T/2)}{y_1(T/2)y_2'(T/2) - y_1(T/2)y_2'(T/2)} \tag{A1.7}$$

which is independent of the initial conditions for $\rho_s(x)$. Furthermore, μ is shown to be identical with the so-called Floquet determinant (up to a factor of 2).

Appendix 2

Let y_1, y_2 be two real linear independent solutions of

$$y''(x) + Q(x)y(x) = 0. \tag{A2.1}$$

Then the Wronskian W of y_i and y_2 is real and different from zero. In particular, one can choose solutions satisfying

$$\begin{aligned} y_1(x_0) &= 1 \qquad & y_2(x_0) &= 0 \\ y_1'(x_0) &= 0 \qquad & y_2'(x_0) &= 1 \end{aligned} \tag{A2.2}$$

with $W=1$. Then the general real solution of the Milne equation (7) can be written as

$$\rho(x) = (Ay_1^2(x) + By_2^2(x) + 2Cy_1(x)y_2(x))^{1/2} \tag{A2.3}$$

where the three real constants A, B, C coupled by

$$AB - C^2 = W^{-2} \tag{A2.4}$$

are determined by the initial conditions of ρ.

Lemma. A real solution of the Milne equation (7) has no zeros.

Proof. Assume ρ has a root at $\tilde{x}$, i.e.

$$Ay_1^2(\tilde{x}) + By_2^2(\tilde{x}) + 2Cy_1(\tilde{x})y_2(\tilde{x}) = 0 \tag{A2.5}$$

or

$$(Ay_1^2(\tilde{x}) + By_2^2(\tilde{x}))^2 = 4C^2y_1^2(\tilde{x})y_2^2(\tilde{x}). \tag{A2.6}$$

Using (A2.4) this gives

$$(Ay_1^2(\tilde{x}) - By_2^2(\tilde{x}))^2 + 4W^{-2}y_1^2(\tilde{x})y_2^2(\tilde{x}) = 0. \tag{A2.7}$$

Since both terms in (A2.7) are squares of real numbers they both must vanish. Because $W \neq 0$, $y_1(\tilde{x})$ and $y_2(\tilde{x})$ cannot both be zero. Let us assume that $y_1(\tilde{x}) = 0$ and $y_2(\tilde{x}) \neq 0$, then $(-By_2^2(\tilde{x}))^2 = 0$, and $B = 0$. Now, because $W^2 > 0$ this implies $C^2 < 0$ in contradiction to C being real. Similar for the case $y_2(\tilde{x}) = 0$. Therefore the assumption $\rho^2(\tilde{x}) = 0$ cannot be correct, which proves the lemma.

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