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Solvable Hill equation

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A second-order linear differential equation with continuous periodic coefficients is solved exactly in terms of elementary functions. Equations of this type arise commonly in several areas of physics, and the solutions may find practical applications. As an illustration, the results are applied to the problem of an electron in a one-dimensional periodic potential.

I. INTRODUCTION

The mathematical formulations of many problems in physics are reducible to ordinary differential equations with nonconstant coefficients. Often the coefficients are periodic functions of the independent variable, and the equations may be considered to be special cases of the Hill equation

$$\frac{d^2y}{dx^2}+f(x)y=0 \ , \tag{1}$$

where $f(x)$ is a periodic function of x. This type of equation was first investigated by Hill in connection with the theory of the moon's motion.[1] Such equations are also well known in the quantum theory of metals and semiconductors, since the Schrödinger equation for an electron in a periodic lattice has the form of Eq. (1).[2] More recently, various superlattice structures have been fabricated and similar principles apply.[3] Hill equations also arise in the theory of particle orbits in linear accelerators and alternating gradient synchrotrons, because the field structures are periodic.[4,5] The same equations govern the propagation of electromagnetic waves in periodically loaded transmission lines,[6] distributed feedback lasers,[7] fiber-optic waveguides,[8] and the numerous other circumstances in which a wave pheonomenon interacts with a periodic structure.

Hill equations are, in general, difficult to solve analytically, and therefore much attention has been focused on a few special cases. Approximate solutions are always possible if the periodic terms in $f(x)$ are small, but our main interest here is in solutions which are exact. Most previous investigations of exact solutions to the Hill equation have emphasized one or the other of two basic forms for the periodic function $f(x)$. The simplest general class of equations is obtained when $f(x)$ is a rectangular function having the value f_1 for one portion of each period and the value f_2 for the remainder. In this case, the equation may be easily solved for the exponential or sinusoidal wave functions in each region, and the general solution can be obtained by matching the wave functions at the boundaries between regions. Such solutions are the basis of, for example, the Kronig-Penney model, which is widely used in discussions of electrons in crystal lattices.[9]

For some applications, a composite function, like the rectangle wave mentioned above, is an unsatisfactory representation of $f(x)$, and there would be value in finding Hill equations with continuous $f(x)$ which could also be solved analytically. The simplest appearing equation of this type is the Mathieu equation, in which $f(x)$ varies sinusoidally:

$$\frac{d^2y}{dx^2}+(a-2q\cos 2x)y=0 \ . \tag{2}$$

This equation was introduced by Mathieu in his study of the vibrational modes of a stretched membrane having an elliptical boundary.[10] The same equation has been investigated extensively since the time of Mathieu, but the solutions must still be obtained numerically or from the various published graphs and tables.[11] The Hill equation with a composite periodic function $f(x)$, as described above, is the only Hill equation that has previously been solved in terms of elementary functions.[12] The purpose of this paper is to report that another Hill equation having a two-parameter continuous periodic function is also solvable analytically, and as an illustration the results are applied to the problem of an electron in a one-dimensional periodic potential.

II. THEORY

The periodic function of interest here is

$$f(x)=\frac{F}{(1+G\cos 2x)^4}+\frac{4G\cos 2x}{1+G\cos 2x} \ . \tag{3}$$

Therefore, the Hill equation from Eq. (1) is

$$\frac{d^2y}{dx^2}+\left[\frac{F}{(1+G\cos 2x)^4}+\frac{4G\cos 2x}{1+G\cos 2x}\right]y=0 \ . \tag{4}$$

This equation has been chosen in such a way that it has several features in common with the Mathieu equation given in Eq. (2). Obviously, it could as well have been written with different trigonometric functions or a different oscillation frequency. If x is replaced by ix, one obtains

$$\frac{d^2y}{dx^2}-\left[\frac{F}{(1+G\cosh 2x)^4}+\frac{4G\cosh 2x}{1+G\cosh 2x}\right]y=0 \ , \tag{5}$$

which is analogous to the modified Mathieu equation.

The solution of Eq. (4) can be written

$$\begin{aligned} y(x)={}&a\left[\frac{1+G\cos 2x}{1+G}\right]\cos\left\{\frac{F^{1/2}}{2(1-G^2)}\left[\frac{G\sin 2x}{1+G\sin 2x}-\frac{2}{(1-G^2)^{1/2}}\tan^{-1}\left[\frac{(1-G^2)^{1/2}\tan x}{1+G}\right]\right]\right\}\\ &+b\left[\frac{1+G\cos 2x}{1+G}\right]\sin\left\{\frac{F^{1/2}}{2(1-G^2)}\left[\frac{G\sin 2x}{1+G\sin 2x}-\frac{2}{(1-G^2)^{1/2}}\tan^{-1}\left[\frac{(1-G^2)^{1/2}\tan x}{1+G}\right]\right]\right\} \ , \end{aligned} \tag{6}$$

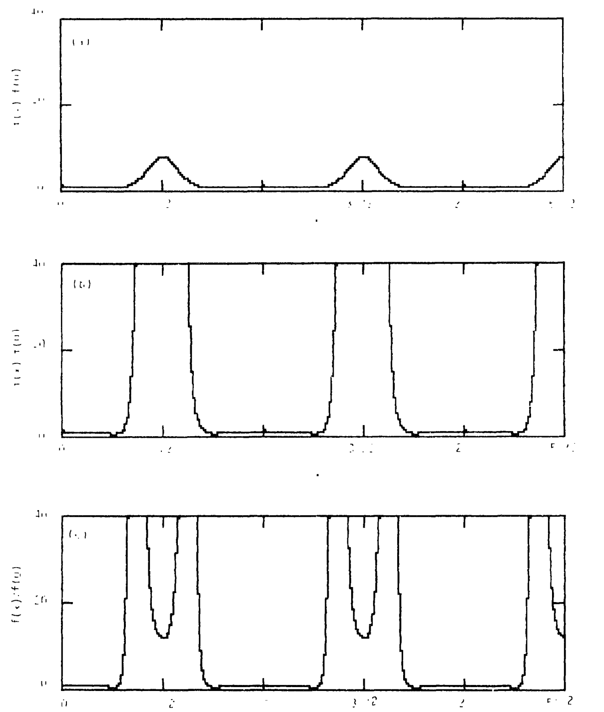

FIG. 1. Periodic functions for analytically solvable Hill equations. These examples are for $F=1$ and (a) $G=0.5$, (b) $G=1.0$, and (c) $G=1.5$. The possibility of single or double positive singularities is illustrated in parts (b) and (c), respectively.

where a and b are arbitrary constants, and this result can be verified by direct substitution into Eq. (1) using $f(x)$ from Eq. (3).[13] The first half of this solution corresponds to the even cosine-type Mathieu functions ce_n, and the second half corresponds to the sine-type functions se_n. The various extensions and special cases of Eq. (6) may be easily derived by the reader.

While the results, indicated above, may be mathematically interesting, they only have practical value to the extent that the function $f(x)$ can approximate the periodic potentials encountered in the real world. Therefore, it is appropriate to plot $f(x)$ to see what forms it can take. In doing this, one discovers that $f(x)$ can be nearly sinusoidal, or it can have narrow minima or maxima depending on the values of F and G. Figure 1 shows a plot of $f(x)$ for $F=1$ and various values of G. In this case, $f(x)$ has one rounded maximum per period for $G<1$, one infinitely sharp maximum for $G=1$, and two infinite maxima for $G>1$. If Eq. (2) were taken to represent Schrödinger's equation for an electron in a one-dimensional lattice, the curves in Fig. 1 could be interpreted as the potential functions corresponding to a periodic distribution of single or double potential wells.

The application of these new solutions of the Hill equation can perhaps be best illustrated by means of a specific example. The time-independent Schrödinger equation for an electron in a one-dimensional potential $V(x)$ is written

$$-\frac{\hbar^2}{2m}\frac{d^2y}{dx^2}+V(x)y=Ey \ . \tag{7}$$

This equation is identical to Eq. (1) if the function $f(x)$ is

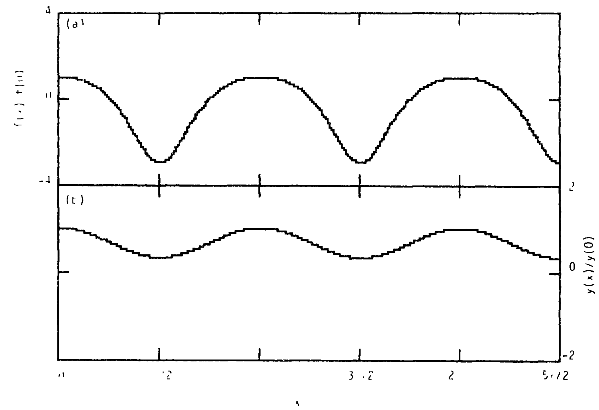

FIG. 2. Plot (a), the periodic function with $F=0$ and $G=0.5$ together with (b), the corresponding solution of the Hill equation.

recognized as

$$f(x)=\frac{2m}{\hbar^2}[E-V(x)] \ . \tag{8}$$

To be specific, it will be postulated that the coefficient F in Eq. (3) is equal to zero. Therefore, the periodic potential is

$$V(X)=E-\frac{\hbar^2}{2m}\frac{4G\cos 2x}{1+G\cos 2x} \ . \tag{9}$$

If the coefficient G is chosen to be 0.5 and the potential maximum is chosen to be zero, it follows from Eq. (9) that the energy of the eigenstate is $E=-2\hbar^2/m$. The wave function for this example is given by Eq. (6) as

$$y(x)=\frac{2a}{3}(1+0.5\cos 2x) \ . \tag{10}$$

The constant a in front of this result could, of course, be obtained by an appropriate normalization of the wave function. The periodic function $f(x)$ and the wave function for this example are plotted in Fig. 2. It is apparent from the figure that the potential "seen" by the electron has rather broad minima with sharper maxima separating adjacent wells. As mentioned above and shown in Fig. 1, potentials having sharp minima or maxima are also obtainable with this model.

III. CONCLUSION

Hill equations arise in many areas of physics. It is commonly assumed that one must either approximate the periodic function by a rectangle wave or else be content with numerical or tabular results. It has been shown here that for a class of two-parameter continuous (or sometimes singular) periodic functions, the Hill equation can be solved analytically.

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[13]An intermediate relationship is

$$\int_0^x \frac{dx'}{(1+G\cos 2x')^2} = \frac{1}{2(1-G)^2}\left[\frac{G\sin 2x}{1+G\sin 2x} - \frac{2}{(1-G^2)^{1/2}}\tan^{-1}\left(\frac{(1-G^2)^{1/2}\tan x}{1+G}\right)\right].$$