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Eigenvalues of the Schrödinger Equation for a Periodic Potential

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Abstract: By studying the application of the asymptotic iteration method, we found a new numerical results of the eigenvalues for non-quasi-exactly solvable periodic potential. In addition to that, the results we get for quasi-exactly solvable solution are typical to the results achieved by Qiong-Tao Xie [J. Phys. A: Math. Theor. 44 (2011) 285302].

Keywords: Periodic Potential, Asymptotic Iteration Method, Eigenvalues E_n

1. Introduction

Recently, periodic potential gained considerable interests among physicists**.** The periodic potential is a particularly important as it is applied to crystalline solids. The Schrödinger equation with a periodic potential is an important model in solid state physics [1]. It describes the motion of electrons in a crystal with a lattice structure. Several studies in periodic potentials have already been performed to illustrate Bloch waves and energy bands for a spatially periodic potential [2-4].

In this paper, we will study model of quasi-exactly solvable (QES) periodic potential introduced by Qiong-Tao Xie [J. Phys. A: Math. Theor. 44 (2011) 285302]. The obtained potential is classes of QES periodic potentials. QES periodic potentials are closely related to exact solvability. If all the eigenvalues of a quantum mechanical system are known together with the corresponding eigenfunctions the system is exactly solvable. In contrast a system QES if only a finite number (usually the lowest lying ones) of exact eigenvalues and eigenfunctions are known. QES periodic potentials hold an intermediate place between exactly solvable and non-solvable potentials. However, an exactly solvable periodic potential is still not found [5]. This situation partly leads to a considerable interest in the quasi-exactly solvable (QES) periodic potentials. In the past decades, based on different methods, a number of QES singular and non-singular periodic potentials have been found [7-9].

Razavy potential is an important study of QES non-singular periodic potential which Schrödinger equation with this potential can be reduced to the Heun confluent equation [10-14]. Recently, a new type of periodic potential has been generated in the photonic lattices [15–16]. This motivates us to consider such a new type of periodic potential, for this new type of periodic potential can be transformed into the Heun general equation. The analytical solution can be constructed in terms of the Heun functions. By making use of the properties of the Heun functions, it has been shown that for special values of the potential parameters, the lowest energy levels and associated eigen-functions can be found exactly in closed form [17].

In this paper, we construct a type of one-dimensional QES periodic potential which is introduced by Qiong-Tao Xie [18] in a new form in order to calculate the eigenvalues for this potential.

In recent years, a simple technique called the asymptotic iteration method (AIM) has taken much attention to obtain energy eigenvalues and eigenfunctions of the class of differential equations [19–23]. By using this technique, one can reproduce exact solutions to many differential equations which are important in applications to many problems in physics, such as the equations of Hermite, Laguerre, Legendre and Bessel. In the case of most solvable potentials, the AIM has reproduced the exact spectrum [10] while for non exactly solvable potentials, it leads reasonably good approximate values [21–23]. The purpose of the present work is to apply the AIM to the QES periodic potential which is introduced by Qiong-Tao Xie [18].

The organization of the paper is as follows: In Sec 2, we

present the periodic potential and introduced the eigenvalues for QES case. In Sec 3, we briefly introduce the AIM, while in Sec. 4 eigenvalues of periodic potential is presented by using AIM. In Sec. 5, we conclude our paper and remark our results.

2. QES Periodic Potential

For one-dimensional systems, the Schrödinger equation in atomic units ($\hbar = 2\mu = 1$) is given by,

$$-\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \tag{1}$$

where $V(x)$ is a periodic potential of the form,

$$V(x) = \frac{V_0}{1 + I_0 \cos^2(x)} + \frac{V_1}{[1 + I_0 \cos^2(x)]^2} \tag{2}$$

The Schrödinger equation is formally similar to the non-dimensionalized model equation for the probe beam in the one-dimensional photonic lattices, where V_0, V_1 are the applied DC field and I_0 is the peak intensity of the uniform photonic lattice. If $I_0 = 0$, the resulting singular potential is just a special case of the trigonometric Pöschl–Teller potentials [18]. By making the transformation to equation (1), it is found that $\psi(x)$ satisfies the Heun general equation. One can obtain a terminated polynomial of degree $N, N = 1, 2, 3, ...$

Qiong-Tao Xie listed some of the analytical QES eigenvalues E in a closed form for the simplest nontrivial two cases,

First case when $N = 1, \quad V_1 = 0$,

$$\begin{aligned} V_0 &= 2I_0 + 4, \quad \Rightarrow \quad E = 4 \\ V_0 &= 6I_0 + 12, \quad \Rightarrow \quad E = 16 \\ V_0 &= 6I_0 + 8, \quad \Rightarrow \quad E = 9 \\ V_0 &= 2I_0 + 8, \quad \Rightarrow \quad E = 9 \end{aligned} \tag{3}$$

Second case when $N = 1, \quad V_0 = 0$,

$$\begin{aligned} V_1 &= -3I_0 - 3, \quad \Rightarrow \quad E = 1 \\ V_1 &= -8I_0 - 8, \quad \Rightarrow \quad E = 1 \end{aligned} \tag{4}$$

From above equations (3) and (4), it is clear that there is a relationship between V_0, V_1 and I_0. The QES eigenvalues are restricted to the potential parameters V_0, V_1 and I_0. This works only under certain conditions on the parameters V_0, V_1 and I_0 of the potential under the above consideration, where the obtained numbers of the QES eigenvalues are limited. Hence, in this work, the asymptotic iteration method is used to calculate the eigenenergies E_n for the periodic potential (2) without any constraints on the parameters of the potential.

3. Brief Introduction of the Solution Method

The asymptotic iteration method was introduced by [19] to obtain exact and approximate solutions of eigenvalues equations. The first step in applying this method for solving Schrödinger eigenvalues differential equation is to transform this equation, with the aid of appropriate asymptotic forms, to second-order homogeneous linear differential equation of the general form,

$$y''(x) = k_0(x)y'(x) + z_0(x)y(x), \tag{5}$$

where $y'(x)$ and $y''(x)$ are the first and the second derivatives with respect to x, $k_0(x)$ and $z_0(x)$ are functions in $C_\infty(a,b)$. A key feature of AIM is to denote the invariant structure of the right-hand side of (5) under further differentiation. Indeed, if we differentiate (5) with respect to x, we find that,

$$y'''(x) = k_1(x)y'(x) + z_1(x)y(x), \tag{6}$$

where,

$$\begin{aligned} k_1(x) &= k_0'(x) + z_0(x) + k_0^2(x) \\ z_1(x) &= z_0'(x) + z_0(x)k_0(x) \end{aligned} \tag{7}$$

Meanwhile, the second derivative of (5) yields to,

$$y^{(4)}(x) = k_2(x)y'(x) + z_2(x)y(x), \tag{8}$$

for which,

$$\begin{aligned} k_2(x) &= k_1'(x) + z_1(x) + k_0(x)\,k_1(x) \\ z_2(x) &= z_0'(x) + z_0(x)k_1(x) \end{aligned} \tag{9}$$

To find a general solution to this equation, it can be iterated up $(j+1)^{th}$ and to $(j+2)^{th}$ derivatives, $j = 1, 2, 3, ...$. Thus, one obtains,

$$\begin{aligned} y^{(j+1)}(x) &= k_{j-1}(x)y'(x) + z_{j-1}(x)y(x), \\ y^{(j+2)}(x) &= k_j(x)y'(x) + z_j(x)y(x) \end{aligned} \tag{10}$$

respectively, where,

$$\begin{aligned} k_j(x) &= k_{j-1}'(x) + z_{j-1}(x) + k_0(x)k_{j-1}(x) \\ z_j(x) &= z_{j-1}'(x) + z_0(x)k_{j-1}(x) \end{aligned} \tag{11}$$

which are called as the recurrence relation of the Eq. (5). The ratio of the $(j+2)^{th}$ and $(j+1)^{th}$ derivatives can be expressed as,

$$\frac{d}{dx}\ln(y^{j+1}(x)) = \frac{y^{j+2}(x)}{y^{j+1}(x)} = \frac{k_j(x)[y^{/}(x) + \frac{z_j(x)}{k_j(x)}y(x)]}{k_{j-1}(x)[y^{/}(x) + \frac{z_{j-1}(x)}{k_{j-1}(x)}y(x)]} \quad (12)$$

Now, we introduce the asymptotic aspect of the method. If we have, for sufficiently large j ,

$$\frac{z_j(x)}{k_j(x)} = \frac{z_{j-1}(x)}{k_{j-1}(x)} = \phi(x) \quad (13)$$

with a quantization condition,

$$\Delta_j(x) = \begin{vmatrix} k_j(x) & z_j(x) \\ k_{j-1}(x) & z_{j-1}(x) \end{vmatrix} \quad (14)$$

Thus, Eq. (12) can be reduced to,

$$\frac{d}{dx}\ln(y^{j+1}(x)) = \frac{k_j(x)}{k_{j-1}(x)} \quad (15)$$

which yields to,

$$y^{j+1}(x) = C_1 \exp(\int \frac{k_j(x)}{k_{j-1}(x)}dx) = C_1 k_{j-1}(x) \exp[\int \{\phi(x) + k_0(x)\}dx] \quad (16)$$

where C_1 is the integration constant, and the right-hand side of Eq. (16) follows from Eq. (13) and the definition of $\phi(x)$. Substituting Eq. (16) into Eq. (15), we obtain a first-order differential equation,

$$y^{/}(x) + \phi(x)y(x) = C_1 \exp[\int \{\phi(x) + k_0(x)\}dx] \quad (17)$$

which, in turn, yields the general solution to Eq. (5),

$$y(x) = \exp(-\int \phi(x)dx)\,[C_2 + C_1 \int (\exp[\int \{k_0(x) + 2\phi(x)\}dx])] \quad (18)$$

For a given potential, the procedure constructed first to convert the Schrödinger equation into the form of equation (5). Then, $k_0(x)$ and $z_0(x)$ are determined, while $k_j(x)$ and $z_j(x)$ are calculated via the recurrence relations given by equation (11). The energy eigenvalues are then obtained by imposing the condition shown in Eq. (14) if the problem is exactly solvable. If not, for a specific principal quantum number j , we choose a suitable x_0 point, generally determined as the maximum value of the asymptotic wave function or the minimum value of the potential. The approximate energy eigenvalues are determined from the roots of the quantization condition (14). We now present the application of the method to the periodic potential introduced by Qiong-Tao Xie [18].

4. Application

In [18], the author introduces periodic potentials (2) and shows that, when the parameters I_0 , V0 and V1 in the periodic potentials satisfy a certain condition, some of the Bloch waves and associated energies can be found exactly and in closed form at either the center or the edge of the first Brillouin zone. Two fundamental sets of solutions have been constructed to calculate all the Blochwaves and energy bands.

In this work, we rewrite the periodic potentials (2) in a new form,

$$V(x) = \frac{V_\xi}{[1 + I_0 \cos^2(x)]^\sigma} \quad (19)$$

where $\xi = 0,1$, $\sigma = 1,2$. This new form enables us to follow the result obtained by Qiong-Tao Xie [18]. By applying the AIM we show that the potential (19) can be used to calculate the eigenvalues of the potentials (2).

In most applications of AIM, the Schrödinger eigenvalues differential equation (1) must be transferred into the form of equation (5). By making this transformation, one should apply possible change of coordinate if it is necessary and then performing a change to the wave function in the form $\psi(x) = g(x)\,y(x)$ where the function $g(x)$ is the asymptotic behavior of the system, and the function $y(x)$ is obtained in the polynomial form by using equation (19). The wave function is to be substituted into equation (1) to obtain the second-order homogeneous linear differential equation as in equation (5).

In the recent work, we transform the equation (1) to the form of equation (5) without defining the form of a wave function. Instead of this technique, we transform the Schrödinger equation (1) to an amenable form for AIM by using the change of variables as:

$$r = \cos(x) \quad (20)$$

If we make this change of variables to equation (1) with $V(x)$ as in (20), this will transform equation (1) into the form of equation (5) as

$$y^{//}(r) = k_0(r)\,y^{/}(r) + z_0(r)\,y(r), \quad (21)$$

where,

$$k_0(r) = -\frac{r}{r^2 - 1} \quad (22)$$

and,

$$z_0(r) = -\frac{V\xi}{(r^2-1)(1+I_0\, r^2)^{\sigma}} + \frac{E}{r^2-1} \tag{23}$$

with the help of equation (11), it is possible now to compute the sequences $k_j(r)$ and $z_j(r)$, $j = 1,2,3....$ In order to calculate the eigenvalues E_n , $n = 0,1,2....$, we need to iterate the expansion,

$$\phi_j(r) = k_{j-1}(r) z_j(r) - z_{j-1}(r) k_j(r) \tag{24}$$

For each iteration, the expansion depends on two variables, E and r. The calculated eigenvalues En by the means of the condition $\phi(r) = 0$ should, however, be independent of selecting r . Selecting r is observed to be critical only to the speed of the convergence to the eigenvalues E_n , as well as for the stability of the process. In our work, it has been observed that best value of r must be equals to zero. Therefore, at the end of the iterations, we substitute $r = 0$. In order to improve the energy eigenvalues, the iteration number has to be increased until the convergence for E_n takes place.

We present the numerical eigenvalues determined by AIM in Table 1. The AIM results are presented up to 10 digits.

Table 1. *The eigenvalues E_n of the potential (19) with $\xi = 0, \sigma = 1, I_0 = -\frac{1}{4}$ and for different parameter V_0.*

state	$V_0 = 2I_0 + 4$	$V_0 = 6I_0 + 8$	$V_0 = 6I_0 + 12$
0	4	7.366419531	11.77902951
1	5.319088249	9	13.87476085
2	8.096536427	11.65839645	16
3	13.05017052	16.53444561	21.20105685
4	20.04452446	23.51612084	28.15229365

The eigenvalues in Table 1 are obtained for several different values of the parameter V_0 while $I_0 = \frac{-1}{4}$. In each case the results include QES and non- QES eigenvalues. The QES eigenvalues are consistent with Qiong-Tao Xie results, while the non-QES eigenvalues are considered as new results. It is interesting to note that for V0=2I0+4, the QES eigenvalues are the ground state, while for $V_0 = 6I_0 + 8$ and $V_0 = 6I_0 + 12$ the QES eigenvalues are the first excited state and the second excited state.

Table 2. *The eigenvalues E_n of the potential (19) with $\xi = 1, \sigma = 2, I_0 = -\frac{2}{10}$ and for different parameter V_0.*

state	$V_1 = -3I_0 - 3$	$V_1 = -8I_0 - 8$
0	-3.074942011	-8.429993592
1	-2.370002998	-8.049950370
2	1	-3.811729591
3	5.988044213	1
4	12.98504990	7.976878537

In table 2, the eigenvalues for two different values of the parameter V_1 and for $I_0 = -\frac{1}{4}$ are presented, the results for QES eigenvalues are identical like the results in [18]. The non-QES eigenvalues that we gained also are considered new results.

In Table 3, we present the results for $V_0 = 2I_0 + 4$, and for three values of I_0. One can note that the QES eigenvalues are fixed and do not depend on changes for the I_0 values, while the non-QES eigenvalues depend on the values of I_0.

Table 3. *The eigenvalues E_n of the potential (19) with $\xi = 0, \sigma = 1, V_0 = 2I_0 + 4$ and for different parameter I_0.*

state	$I_0 = -\frac{1}{5}$	$I_0 = \frac{1}{5}$	$I_0 = \frac{1}{3}$
0	4	4	4
1	5.242017667	4.829953673	4.742542287
2	8.058085957	8.038778834	8.096536427
3	13.02966616	13.01788162	13.04341627
4	20.02669531	20.01779047	20.04452446

In Table 4, we present our new results where the AIM is valid for arbitrarily values of parameters I_0 and V_0 , we present results for non-QES eigenenergies.

Table 4. *The eigenvalues E_n of the potential (19) with $\xi = 1, \sigma = 2,$ and for different parameter I_0, V_1.*

state	$I_0 = \frac{1}{4}, V_1 = -\frac{29}{4}$	$I_0 = \frac{1}{2}, V_1 = 3$	$I_0 = \frac{1}{2}, V_1 = \frac{19}{2}$
0	-6.041761114	1.960715439	5.776439758
1	-4.235833646	2.618661149	6.042908383
2	-1.720175852	6.168109178	11.18683632
3	5.189626653	11.03670714	15.46003216
4	10.17793782	18.04903621	22.54085543

5. Conclusion

We have applied the AIM for obtaining the eigenvalues E_n for the periodic potential which is introduced by Qiong-Tao Xie [18] over the full range of parameters I_0 and V_0 . Our results are in comply with those of Qiong-Tao Xie [18] as a QES case. The accuracy of the results for higher excited state (non-QES case) can be increased if the number of iterations is increased. This is not valid for infinity, but, in our experiments we reached values of convergence where the values are not changes even if we increase the iterations. We hope that the new results presented in this paper attracts the interest of scientists active in this field, and will lead to further researches and applications.

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