A New Simple Method of Simulating One Dimensional Quantum Problem Based on Lattice Point Concepts

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Abstract. One-dimensional quantum problems have always been an important issue in various branches of quantum mechanics fields, and many quantum models can be idealized as one-dimensional potential profiles. Therefore, it is necessary to investigates the way to deal with and calculate the problems. This paper proposes a new and simple method for simulation and calculation of one-dimensional quantum problems. To be specific, by representing continuous X values by a series of discrete lattice points, the Hamiltonian matrix is constructed for the system in the way of dealing with monomer and many-body problems, so as to simply calculate the energy level distribution and draw the wave function image. In terms of simulating one-dimensional infinite deep potential well, one-dimensional finite deep potential well, one-dimensional multi-potential well and other one-dimensional quantum systems with this method, this paper shows that the method is accurate and practical. Compared with other methods for one-dimensional quantum problems, this paper also presents the superiority of this method. To deal with the problem based on such a method can save the computation cost and time cost, which is more convenient to study the one-dimensional quantum problem in the future. These results shed light on studying complex one-dimensional quantum problems conveniently.

Keywords: One-dimensional quantum problems; Lattice points; Simulation.

1. Introduction

One-dimensional quantum problems have always attracted scholars since many directions will involve dealing with a one-dimensional quantum problem in the field of quantum research. As early as 1973, Tsu and Esaki treated the potential profile of a one-dimensional finite superlattice problem into a one-dimensional multi-barrier problem [1]. In 1980, Holonyak et al. also found that the use of multiple-Quantum-well heterostructure overcomes some defects while studying the properties of Quantum-well Semiconductor lasers [2]. During 2005-2006, some researches on new materials (e.g., Silicon-Germanium structures, InGaN⁄GaN, or HgTe) and analyzed the impacts brought by one-dimensional multi-quantum Wells [3-5]. Recently, a study pointed out that changing the width of quantum Wells can modulate the conductance in graphene nanoribbons [6].

The way to solve a relatively complex one-dimensional quantum problem has also been investigated. Previously scholars use a phase-integral method to deal with a one-dimensional quantum problem. By obtaining the phase-Integral quantization condition, the energy eigenvalues of a system can be calculated with an accuracy relative to the chosen order of the phase-integral approximation [7]. In another study, researchers proposed to use transfer matrix method to solve the Schrödinger equation in arbitrary quantum-well potential profiles and pointed out the superiority of the method [8]. Contemporarily, some new and easier methods have emerged. For example, in A Simple Approach to solve the Time Independent Schrödinger Equation for 1D Systems, the author uses Angular Momentum SU (2) Algebra to describe 1D systems [9]. Apparently, there are also some articles with similar concepts to method proposed in this paper, e.g., An Exact Analytical Scheme using a new potential to solve one-dimensional quantum systems. In this paper, the study used collection of short-width potential to denote an arbitrary potential to achieve simplified calculation [10]. In addition, the approach proposed in this paper is one step further than his. Other articles used filter operator selects the eigenfunction from wave packet at the rate comparable to δ function [11, 12].

When studying quantum one-body problems, Aubry-Andre Model and quantum many-body problems (e.g., Hubbard Model). It has been noticed that the advantages of dealing with such problems through quadratic quantization. Since the generation operator, annihilation operator, and particle number operator are introduced into processing the problem, it becomes very easy to construct the Hamiltonian matrix of these problems. On this basis, it is relatively convenient to obtain the energy levels and corresponding wave functions of the system by solving the Hamiltonian matrix. If the same method could be applied to general one-dimensional quantum problems (e.g., one-dimensional potential well problems), it would greatly simplify the process of solving these problems. The reason is that this approach does not contain the steps for solving the Hamiltonian by performing a complex mathematical transformation of the Schrodinger equation for these problems. Obviously, there is clear difference between the Hamiltonian described by the quadratic quantized system and the Hamiltonian described by the Schrodinger equation system. To be specific, the position of the particle is described by the separated lattice points in the quadratic quantized system, while the position of the particle is described by the variable X that can be continuously varied in the Schrodinger equation system. So, in this article, the idea of how to simulate the continuous variable X with separate variables like lattice points will first be elaborated on. Then, the paper will show the process of adjusting the parameters of the matrix, thus the simulated values are close to the theoretical values by taking the one-dimensional infinite depth potential well and the one-dimensional finite depth potential well as examples. Finally, this new simulation method is used to simulate some one-dimensional quantum problems, such as the one-dimensional multi-potential well problem, and the simulation results obtained by the method proposed in this paper are compared with the simulation results obtained by other methods, so as to obtain the superiority and accuracy of this new method.

2. Principle, procedure and setups of simulation

2.1. The Rationality of Using This Method

It should be noted there will not cover the part of the mathematical argument of this method, i.e., there will not present the specific equation describing the physical system and the discretization of the equation. Because the main purpose of this paper is to propose this new and simple simulation method, and it can be seen in the later part of the paper that the method is effective and accurate. Primarily, it is known that hopping strength occurs in the quadratic quantization description, which describes the process by which a particle hops from one lattice point to another. In this method of simulating one-dimensional quantum system, particle hop is also adopted to describe the motion of particles in the X direction. Imagine one tiny distance x, treating the x as a string of lattice points, if the lattice sites get big enough, the range of x is small enough. Subsequently, from a physical point of view, it is reasonable to describe the movement of the particle on this x range as the hop of the particle in the corresponding separation lattice points. Obviously, specific hopping strength value is needed to be determined.

2.2. Basic Theory for Choosing the Number of Lattice Points

In theory, the more points the better, but for this simulation, 1000 points is chosen to represent the x length of 10^{-7} m. It is a value that comes from physical common sense, because an instinctive thought is that one point represents something on the scale of an atom, and since the diameter of an atom is about 10^{-10} m, hence 1000 points represent 10^{-7} m of x length. After determining the simulation method, it is only needed to add the potential energy value on the corresponding lattice points according to the specific barrier or potential well distribution of the one-dimensional quantum system to complete the construction of the model. Taking the following as an example, one supposes that it is needed to simulate a five-barrier quantum system, where each barrier is 10^{-7} m wide, V high, and the spacing between the barriers is 2×10^{-7} m. Afterwards, it is needed to construct a model of 13,000 lattice points, where the lattice points 0 to 1000,3001 to 4000,6001 to 7000, 9001 to 10000

and 12001 to 13000 should have potential energy V, while the lattice points between them as barrier spacing have no potential energy distribution.

2.3. Basic Theory for Determination of Hopping Strength

Finally, it is also necessary to determine the hopping strength of the particle before finishing writing the Hamiltonian matrix of the system completely according to this method. Just as the momentum of different particles in the potential well is different, the hopping strength of different particles in the model should also be different. In the experiment, by simulating a one-dimensional infinite deep potential well and constantly adjusting the value of hopping Strength, the energy level distribution curve obtained after the diagonalization of the Hamiltonian matrix is compared with the theoretical calculation. The hopping strength of an electron in the 1D infinite deep potential well is obtained by matching the energy level curve obtained by the method with theoretical energy level curve. After obtaining this value, it is applied to simulate the energy level distribution of electron in a one-dimensional finite deep potential well and found that it was in good agreement with the theoretical value, thus verifying its correctness. Measuring the hopping strength of other particles can adopt the same method. After completing the above steps, the Hamiltonian matrix of the system can be constructed in the same way as the one-body problem (e.g., AA Model), and diagonalized by mathematical processing tools. The eigenvalue matrix (energy levels) and eigenfunction matrix (wave functions) of the Hamiltonian matrix are obtained.

3. Results & Discussion

3.1. Determination of Hopping Strength in Hamiltonian Matrix

The procedure of determining the hopping Strength and verifying the correctness of the proposed method based on one-dimensional infinite and one-dimensional finite deep potential wells is showed. In the process of simulating these two systems, 3000 lattice points are used to simulate, among which points 1 to 1000 and 2001 to 3000 have potential energy V, while points 1001 to 2000 have no potential energy, representing the part of the potential well.

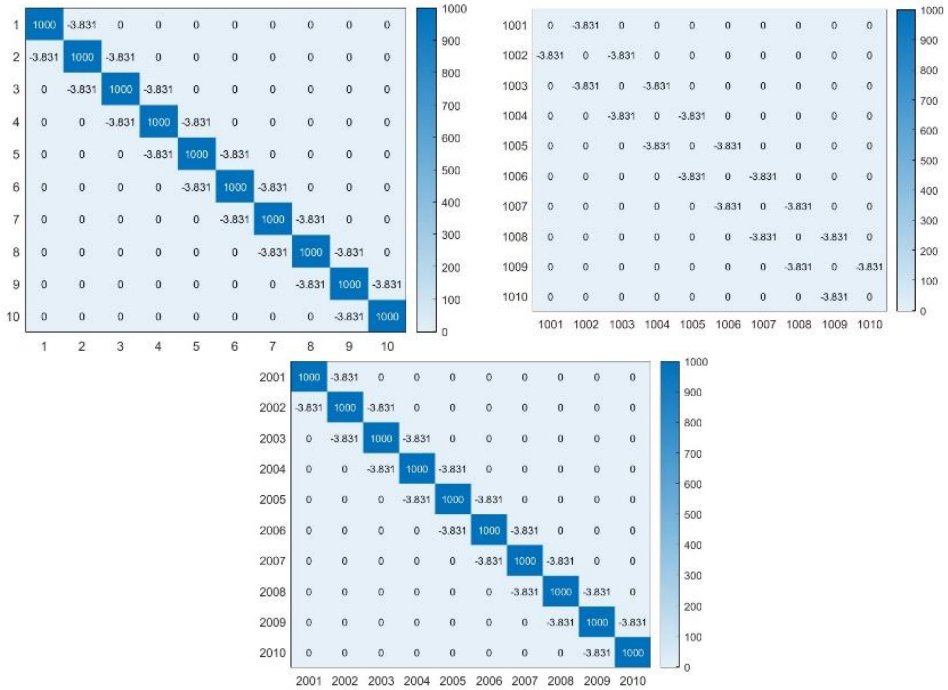


Fig. 1 Appearance of part of the matrix in the form of heat map. Left: The appearance of diagonal elements 1-10 and their surrounding elements. Middle: The appearance of diagonal elements 1001-1010 and their surrounding elements. Right: The appearance of diagonal elements 2001-2010 and their surrounding elements.

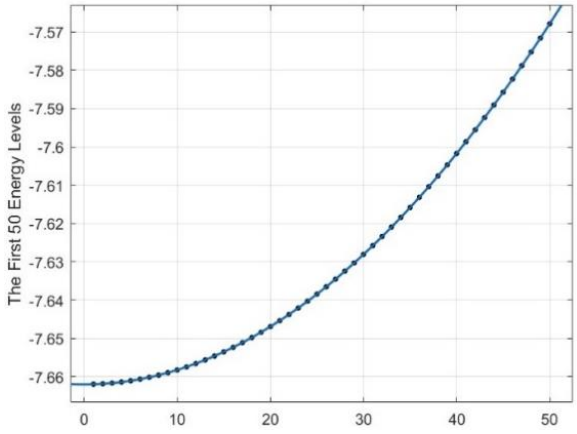


Fig. 2 The first 50 energy levels and the fitted curve got by simulating with the new method. Where V=1000, Hopping strength=3.831.

The whole model describes a potential well with a width of 10^{-7} m. In the simulation of the infinite well, V is set to be 1000 eV, which is a large enough value to approximate the infinite depth of the well. The constructed Hamiltonian matrix should be a matrix of 3000×3000 elements. Fig. 1 shows the general appearance of part of the matrix in the form of heat map, where the darker the blue color is, the larger the value of the element at this position of the matrix. On the main diagonal of the matrix are the potential values, while on either side of the main diagonal are the hopping strength values. After obtaining the energy levels by matrix diagonalization, the first 50 energy levels are selected and are used to fit curve. The first 50 energy levels and the fitted curve is illustrated in the Fig. 2.

The equation of the curve can be expressed in the following form:

$$f(x) = p_1x^2 + p_2x + p_3 \tag{1}$$

It can also be simplified as:

$$f(x) = p_1\left(x + \frac{p_2}{p_1}\right)^2 + p_3 - \left(\frac{p_2}{p_1}\right)^2 \tag{2}$$

This is an equation for a standard quadratic function that the vertex is shifted from the origin point. By theoretical calculation, the energy level of an electron moving in a potential well with a trap width of 10^{-7} m should be:

$$En(Theory) = \frac{\hbar^2\pi^2}{2ma^2}n^2 \approx 3.76 \times 10^{-5}n^2(eV) \tag{3}$$

Since in this simulation the only need is to consider the quadratic coefficient, it is a need to adjust the hopping strength so that:

$$p_1 = 3.76 \times 10^{-5} \tag{4}$$

By repeatedly adjusting, it is finally found that P1 of the fitted curve conforms to the above equation when hopping strength ≈3.831. At the same time, it has also been observed that the value of P3 is actually -2×hopping strength. Therefore, the simulated energy level value by this method should have the following relationship with the theoretical energy level value:

$$En(Theory) = En(Simulation) + 2 \times \text{hopping strength} \tag{5}$$

By the same means, the hopping strength of the system described by this method when a proton is moving in the infinitely deep potential well is also measured, and it is ≈0.0020867. In order to find out the value of hopping strength when different particles moving in a one-dimensional quantum problem are treated with this method, an empirical formula describing the hopping strength and particle mass in this method is found:

$$Hopping\ Strength = \frac{\hbar^2\pi^2}{2ma^2e \cdot 9.814 \cdot 10^{-6}} \tag{6}$$

Here, m is the mass of the particle in the system that need to be simulated, a is 10-7 m, e is the elementary charge. There is e in the formula because this paper takes the unit of all the energy as eV.

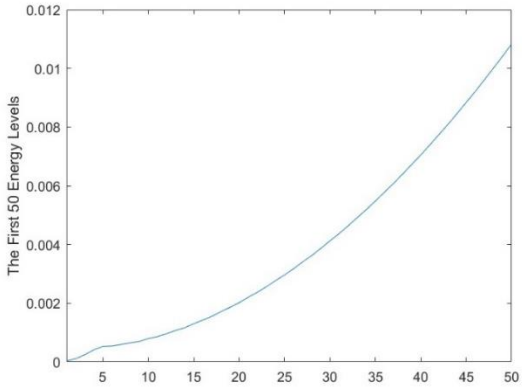


Fig. 3 The curve formed by the first 50 energy levels of the one-dimensional finite potential well, where $V=5\times10^{-4}$ eV, Hopping strength=3.831.

3.2. Simulation & Comparison of 1-D Finite Potential Well

Subseuqently, the electron motion in a one-dimensional finite deep potential well is simulated in a similar way and the energy level is solved. The potential energy V is 5×10^{-4} eV. For finite deep potential well problems, it is generally needed to find the bound state energy levels. In this method, in addition to directly observing the parts of the solved energy levels whose values are less than the set barrier height V to find the bound state energy, there is a more interesting and maybe a more meaningful method.

As depicted in Fig. 3, in which shows the curve formed by the first 50 energy levels of the one-dimensional finite depth potential well, there is an obvious turning point. In fact, all the energy levels below this turning point are bound state energy levels. With this image pointer, bound state energy levels can be found more intuitively and conveniently when simulating more complex one-dimensional quantum problems using this method. Fig. 4 exhibits the four bound State energy levels of the one-dimensional finite deep potential well, and the Y-coordinate value of the label in the figure is the value of the energy level (in eV). By calculating the theoretical value of Bound State energy level of electron under the condition that the well width is 10^{-7} m and the potential barrier on both sides of the well is 5×10^{-4} eV, the comparison of four energy levels is summarized in Table 1. Apparently, the theoretical values are in good agreement with the simulated values obtained by this method, which also proves the correctness and accuracy of this method.

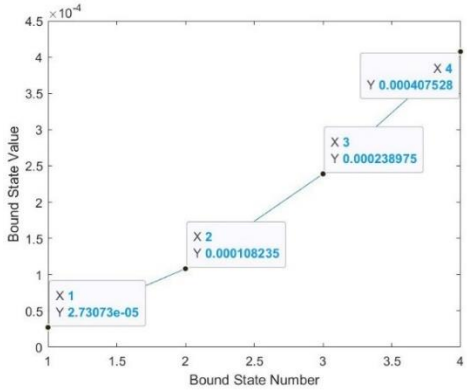


Fig. 4. The four bound state energy levels of the one-dimensional finite potential well, and the Y-coordinate value of the label in the figure is the value of the energy level in eV.

Table 1. Comparison between the four bound energy levels of new method and theoretical value.

Level	New Method(eV)	Theory(eV)
1	0.0000273073	0.00002717984
2	0.000108235	0.0001077378
3	0.000238975	0.0002379163
4	0.000407528	0.0004059276

3.3. Simulation & Comparison of Kronig-Penney Model

In this part, this paper mainly reproduces the content of paper Implementation of filter method to solve the Kronig-Penney model. The band distributions calculated by their method are compared with those calculated by theoretical analysis. It should be mentioned that since Hartree Atomic units were used in the paper, for the convenience of simulation, the results are converted back to SI when reproducing, and 100 lattice points is used to simulate 1 a.u. length. Therefore, the hopping Strength that got earlier needs to be changed. And new value is 136827.8. Fig. 5 and Fig. 6 shows the eigenfunction of Kronig-Penney model calculated with the new method proposed in this paper at the energy of 0.0316 a.u., the modulus square of this eigenfunction, the potential energy distribution of the Kronig-Penney model and the corresponding results in paper Implementation of filter method to solve the Kronig-Penney model. The calculation results of left panel of Fig. 5 and Fig. 6 are slightly different, but the trend and shape of the two functions are completely consistent, while others are basically the same. The difference between the Y values comes from the difference in the normalization of the function and it could be neglected. The correctness of the method proposed in this paper is self-evident. At the same time, this method does not involve complex mathematical operations when obtaining the results shown in Fig. 5, which is superior to the method provided in paper Implementation of filter method to solve the Kronig-Penney model.

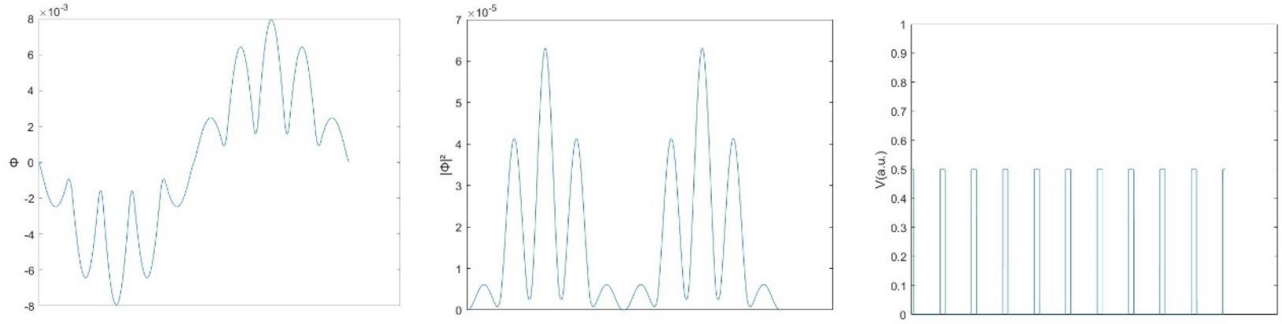


Fig. 5 The wave function of Kronig-Penney model calculated with the new method proposed in this paper at the energy of 0.0316 a.u., the modulus square of the wave function and the potential energy distribution of the Kronig-Penney model (from left to right panel). The figure is based on data from lattice points24,000-36,000.

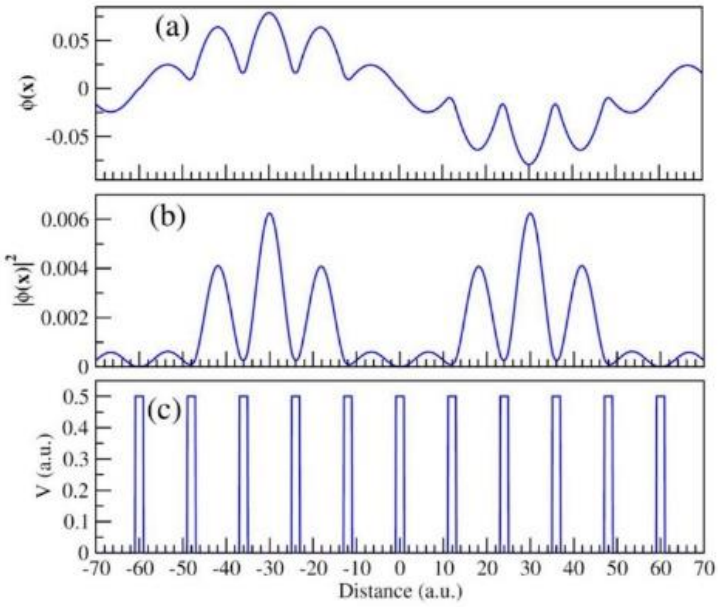


Fig. 6 Implementation of filter method to solve the Kronig-Penney model for results in Fig. 5.

Fig. 7 and Fig. 8 display the comparison between the energy band range calculated by the new method proposed in this paper, the energy band range calculated by the reproduced paper and the energy band range calculated by the theory. Table 2 lists the range of each energy band in more details.

The energy band distribution calculated by this method is very close to the theoretical value, and some energy band values are even more consistent with the theoretical value than the energy band values calculated in the reproduced paper. This also shows the superiority of the new method.

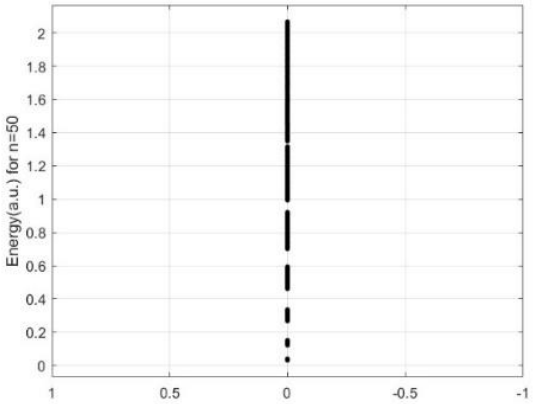


Fig. 7 The energy band ranges calculated by the new method proposed in this paper. Where n=50.

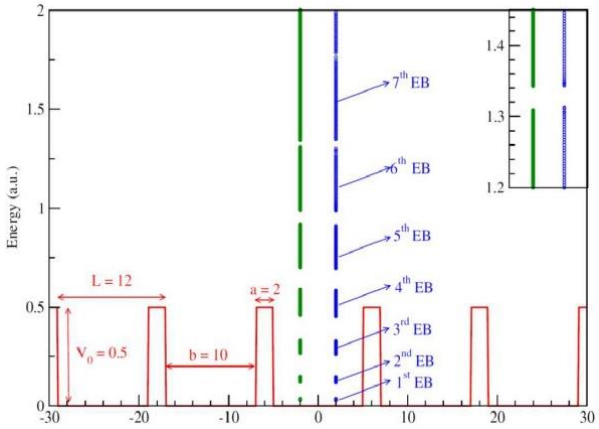


Fig. 8 The energy band ranges calculated by the paper Implementation of filter method to solve the Kronig-Penney model and the energy band ranges calculated by the theory with n=50.

Table 2. The range of each energy band got from three ways. The data in column 3 and column 4 of the table are from paper Implementation of filter method to solve the Kronig-Penney model.

Energy band	Results of new method in this paper	Numerical results from reproduced paper	Analytic results calculated theoretically
1	0.0309269-0.0373472	0.030007-0.036291	0.030796-0.037141
2	0.121819-0.149113	0.120179-0.146878	0.121302-0.148295
3	0.267489-0.33447	0.260877-0.329653	0.266337-0.332651
4	0.461765-0.59204	0.453034-0.584022	0.459674-0.588875
5	0.702436-0.919887	0.693768-0.908540	0.698950-0.915166
6	0.995193-1.3152	0.988431-1.301516	0.989655-1.309390
7	1.35084-1.76852	1.347481-1.761236	1.342598-1.767130

4. Limitation & Prospects

As mentioned earlier, this paper only presents a novel and simple simulation method in this way, and describes how to apply the method to simulate, as well as the advantages and accuracy of using the method, but it does not involve the demonstration of the method at the mathematical level. Secondly, using this method to solve one-dimensional quantum problems obviously does not involve solving the Schrodinger equation from a mathematical point of view, so the expression of the wave function cannot be got mathematically. Although it is feasible to use this method to draw the wave function corresponding to different energy levels, and to use the fitting method to get the equation

expression. In addition, it may not get all the required bound state energy levels when using this method to analyze one-dimensional quantum problems. The reason is that it is limited by the number of lattice points. If it is a need to get more energy levels, it can be realized by increasing the number of points, say increasing from simulating 10-7 m with 1000 points to with 2000 points. It should also be noted that if the method is successfully demonstrated mathematically, the empirical relation which has been obtained describing the hopping strength and the mass of the particle should be derivable.

With the development of computer technology, now simulating very complex quantum systems using traditional computational methods is possible. However, if the desired result can be got in a simpler way, with less computational time and less computational cost, it is certainly better. Moreover, the method proposed in this paper is very intuitive in physics. It is necessary to study some kinds of one-dimensional quantum system, which can be simulated only by setting the corresponding potential energy distribution on a series of lattice points. Therefore, this method is promising.

5. Conclusion

In summary, this paper proposes an easier and more efficient way to deal with one-dimensional quantum problems (e.g., one-dimensional single-well or multi-well problems) by latticing the X-value. To be specific, the one-dimensional problem of finite depth and infinite depth potential well, as well as the one-dimensional problem, are analyzed by this method, and the corresponding energy level distribution and wave function images are calculated for comparison with conventional method. The correctness and superiority of the new method are verified by comparison with the calculated values of theory and other simulation methods. According to the analysis, this method is effective in the simulation. Nevertheless, the proposed method lacks further mathematical proof, which is limited in the number of energy levels that can be obtained. Besides, it cannot directly derive wave function expressions. In the future study of one-dimensional quantum system, it can be used as a very effective processing tools, saving the cost of computing and computing time. Overall, these results offer a guideline for more conveniently studying complex one-dimensional quantum problems.

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