Finite Square Well and its Applications

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Abstract. The relation between finite square well and laser is paramount in quantum mechanics. This paper focuses on establishing the relationship between finite square well and laser through the most fundamental theory of quantum mechanics. This paper first introduced the importance of finite square well and the Kronig-Penney model in the development of the theory of laser and Quantum mechanics briefly. Then, this paper gives a detailed derivation of energy level finite square well through the Schrodinger equation. In the application section, we first introduced Bloch's Law, a vital theorem for the following subsection. It describes the form of wave function under periodic potential. Then, the energy level of the finite square well is put into the application of the Kronig-Penney model, which is an infinite repetition of the finite square well. This part focus on the derivation of the energy level of the Kronig-Penney model. It applies both the energy level of the finite square well and Bloch's Law. In the end, we note that the energy level of the Kronig-Penny model exhibits a band gap. It is an important phenomenon for lasers.

Keywords: Quantum mechanics, Kronig-Penney model, laser, finite square well

1. Introduction

Quantum mechanics is a useful subject in the current world, and Finite Square well is the most fundamental model of quantum mechanics and its applications. All the following topics of quantum mechanics depend on the idea of energy level, which was first established in the finite square well [2]. Harmonic Oscillator, Zeeman Effect, and hydrogen atom are all famous models branches of finite square well. Besides theory, Finite Square well also has profound application in real life. Laser technology, such as semiconductor laser and quantum cascade laser, implements finite square well [3]. An important model in laser technology is the Kronig-Penney model. Kronig-Penney model is an infinite repetition of finite square well. It is an extended theory of finite square well and the simplest model that exhibits band gap [4]. Band gap allows atoms to radiate high energy photons when atoms jump from one band to another. It is the principle of laser. Besides laser technology, Finite Square well could also apply in radiation, Phonon and so on. More applications can be found in reference [5], in which Cohen-Tannoudji introduced theories, cutting-edge research, and classical as well as the newest applications in Quantum mechanics. Therefore, it is important to derive the energy level of the Kronig-Penney model. In this paper, we first explore the general theory of finite square well and then introduces Bloch's theorem, a necessary theorem to calculate the energy gap of the Kronig-Penney model. At last, I will give a detailed derivation of the energy gap of the Kronig-Penney model and relate it to the laser.

There are several ways to develop the solution of finite square well. As mentioned in reference [6], we can develop a series solution of finite square well. This solution is useful to approximate local maxima. We can also use the method provided by Griffiths [2], in which we can plug in the Schrodinger equation. Then we can use the partial differential equation to solve the Schrodinger equation. There are two possible situations for the Schrodinger equation: bound state and unbounded state. Bound state means that the total energy of the particle was smaller than the well. So, the particle would be mostly trapped inside the well. An unbounded state means that the energy of the particle is higher than the well. So it can move above the well. We will show that the unbounded state is exactly the same as the classical situation. So, we should not pay too much attention to it. We are more interested in the bounded state. Because the potential is symmetric, we can safely assume that the wave function is an even or odd function. Notice that we need to consider both situations, for there is no evidence that wave function is only an odd function or only an even function. In this way, the

wave function could be much easier to solve. When we are solving the partial differential equations for the wave function, we need to assume integers $\boldsymbol{l}$ and$\boldsymbol{k}$. We can use these integers to represent total energy$\boldsymbol{E}$. This should be the equation for the energy level of$\boldsymbol{E}$. However, energy level is not our primary concern here. We are focus on the form of the wave function. The result should be a combination of $\boldsymbol{sin}$ and $\boldsymbol{cos}$ functions. Following their process, the energy level of wave function well should be easy to solve.

For the Kronig-Penney model, we already know that it is an extension of finite square well. But this does not mean it is an easy job to solve its energy level. As mentioned in source [4], we need first derive Bloch's law and then use Bloch's law's conclusion to express wave function at the periodic potential. After that, an approximation is needed, in which we need to consider the infinite periodic potential as a perturbation. We expand the perturbation until the second order. Then we use the perturbation theory to calculate the energy level. More specifically, we could approximate the energy level by adding the unperturbed energy plus the perturbation term. We do this to solve the matrix element$|< \boldsymbol{k}|\boldsymbol{V}|\boldsymbol{k}' >|^{\boldsymbol{2}}$. Once we solved it, we can get the energy level. We can first expand the potential in the form ofthe Fourier series. Then we can calculate the amplitude of the Fourier expansion. We then plug in the Fourier expansion back into the equation of perturbation theory. Now the term $|< \boldsymbol{k}|\boldsymbol{V}|\boldsymbol{k}' >|^{\boldsymbol{2}}$ is an expression of integers and $\boldsymbol{sin}$ functions. We can immediately read out the energy band gap from the perturbation equation. Another way to solve the Kronig Penny model was mentioned in reference [9], in which we use the techniques called formalism. This method is easier to use than considering the boundary condition of the Kronig-Penney model.

We have mentioned Bloch's law several times, and we have already noticed the importance of this law. The prove of this law was mentioned in reference [10]. To prove this law, we first need to define the translational operator$\widehat{\boldsymbol{T}}$. As its name has been told, the physical meaning of this operator is to move the wave function for a certain unit. If we put this operator on a wave function of two consecutive times, we would get an equation that suggests the form of the translational operator. The only function that conforms to this equation is the exponential function. Then, we normalize the wave function and hence get the exact form of the exponential function. At this point, we have already known the form of translational operator. The periodic potential requires that the wave function is also periodic. So, we use the translational operator to move the wave for exactly one period length, and hence we should get the exactly same function. Following this process, we should be able to prove Bloch's law. In reference [11], people republished the original paper of Bloch's law. This paper is too old for our derivation, so we will not use it here. Those who are more interested in history, they can refer to this paper.

An interesting application of Kronig-Penney model was mentioned in the source [12]. In this paper, the author uses the Kronig-Penney model to solve the Fibonacci lattice. Readers could refer to this paper for further application.

At the end of the introduction, I would like to refer to the book introduction to Quantum Mechanics written by Griffiths and Quantum mechanics written by Cohen-Tanoudji. These two books contain more application on quantum mechanics.

2. Methodology

We first derive the energy level of quantum square well. Apparently, there are two possible scenarios: $E < V_0$ and$E > V_0$, we will derive them separately. The Schrodinger equation is always equal to

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi. \tag{1}$$

2.1. $E < V_0$

2.1.1. Region II

In Region II,$V_0 = 0$ The Schrodinger equation reduces to

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \tag{2}$$

And hence

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi. \tag{3}$$

It is an ordinary differential equation. Let

$$k^2 = \frac{2mE}{\hbar^2} \tag{4}$$

The solution is

$$\psi = Acos(kx) + Bsin(kx) \tag{5}$$

2.1.2. Region I&III

Region I and III look symmetric, so they should have similar solutions. We shall solve Region I as an example. In Region one,$V = V_0$ The Schrodinger equation reduces to

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_0\psi = E\psi. \tag{6}$$

Rewrite this equation in the form

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}(E - V_0)\psi. \tag{7}$$

Since$E < V_0$,$-\frac{2m}{\hbar^2}(E - V_0) > 0$ we define

$$l^2 = \frac{2m}{\hbar^2}(V_0 - E) \tag{8}$$

The solution of this ordinary differential equation is

$$\psi = Ce^{lx} + De^{-lx}, x < 0. \tag{9}$$

For$x > 0$, we have similar solution

$$\psi = Ee^{lx} + Fe^{-lx}, x > 0. \tag{10}$$

We want the wave function to be square integrable, which means wave function should be a limited number as x approaches to ∞ and $-\infty$. For$x > 0$, we notice that $\lim_{x\to\infty} Ee^{lx} \to \infty$. Hence we let$E = 0$. Similarly, for$x < 0$, let$D = 0$.

The overall solution would become

$$\psi = \begin{cases} Ce^{lx}, x < -a \\ Acos(kx) + Bsin(kx), -a < x < a \\ Fe^{-lx}, x > a \end{cases} \tag{11}$$

2.1.3. Symmetric

It can be shown that when the potential is symmetric, the wave function should also be symmetric.

We first consider the wave function to be even function, which means, $\psi(x) = \psi(-x)$ and the coefficient in ψ becomes

$$\begin{aligned} C &= F \\ B &= 0 \end{aligned} \tag{12}$$

If the wave function is an odd function, $\psi(x) = -\psi(-x)$ we have

$$\begin{aligned} C &= -F \\ A &= 0 \end{aligned} \tag{13}$$

We shall use even function in the following sections.

2.1.4 Continuous condition

The continuous condition requires that the function and it first derivative is continuous at every boundary. For Finite Square well, it requires that

$$\psi(-a^-) = \psi(-a^+) \tag{14}$$

$$\psi'(-a^-) = \psi'(-a^+) \tag{15}$$

$$\psi(a^-) = \psi(a^+) \tag{16}$$

$$\psi'(a^-) = \psi'^{(a^+)} \tag{17}$$

Take point $-a$ as an example. Equation 14 and 15 requires that

$$Ce^{-la} = Acos(ka) \tag{18}$$

$$Cle^{-la} = Aksin(ka) \tag{19}$$

Equations 16 and 17 would give the same result.
Divide 19 by 18 we can get

$$k \cdot \tan(ka) = l. \tag{20}$$

Plug in $k = \frac{\sqrt{2mE}}{\hbar}$ and $l = \frac{\sqrt{2m(V_0-E)}}{\hbar}$ we get the energy level equation

$$\frac{\sqrt{2mE}}{\hbar} tan\left(\frac{\sqrt{2mE}}{\hbar} a\right) = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \tag{21}$$

Let

$$\begin{aligned} \frac{\sqrt{2mE}}{\hbar} &= z \\ \frac{\sqrt{2mV_0}}{\hbar} &= z_0 \end{aligned} \tag{22}$$

The energy level equation reduces to

$$z \cdot \tan(za) = \sqrt{z_0^2 - z^2} \tag{23}$$

Now the energy level function becomes a function of$z$.
Remember that the above derivation is done based on the assumption that the wave function is even. Following similar derivation, we can find energy level equation when wave function is odd

$$-z \cdot \cot(za) = \sqrt{z_0^2 - z^2} \tag{24}$$

Plotting $\sqrt{z_0^2 - z^2}$ versus $-z\cot(za)$ and $z\tan(za)$ we get Energy level of finite square well

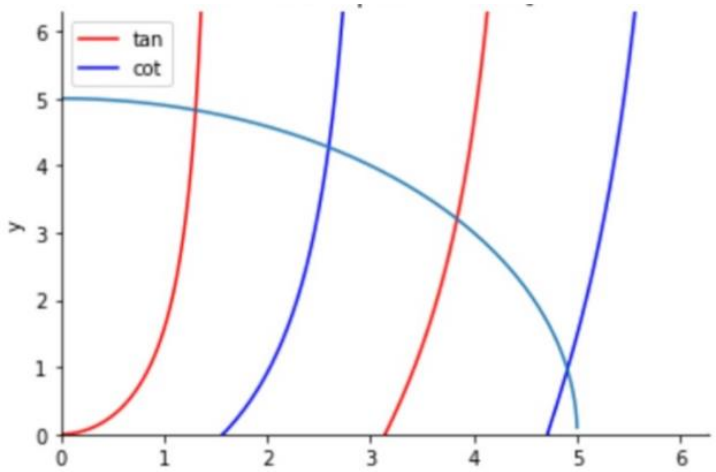


Figure 1. Energy level of finite square well.

2.2. $E > V_0$

Now consider the scenario where $E > V_0$

The solution of Schrodinger equation in Region II should remain the same. In Region I and III, Schrodinger equation would become

$$\frac{d^2\psi}{dx^2} = -\frac{2m(E - V_0)}{\hbar^2}\psi. \tag{25}$$

Let

$$\kappa^2 = \frac{2m(E - V_0)}{\hbar^2} \tag{26}$$

The solution of Region I and III has the form

$$\psi = G\cos(\kappa x) + H\sin(\kappa x) \tag{27}$$

All three regions of wave functions are oscillatory, which means wave function is not square integrable. It means that the energy level is continuous like a classical scenario.

3. Application

For the sake of simplicity, in this section, we redefine all the variables in the previous section.

Now we introduce the application of finite square well in laser.

In lattice, there is an infinite array of finite square well. In an ideal lattice, the material should be identical in all direction. So we only focus on one direction. This model is called the Kronig-Penney model. We know that the result is the same as the classical scenario in the unbounded state, so we only focus on the bounded state.

Kronig-Penney model

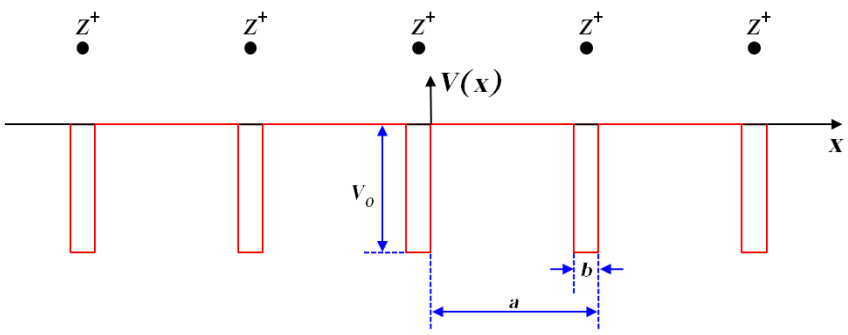


Figure 2. Kronig-Penney model.

We shall try to find the energy level in this case.

3.1. Bloch's Law

We first try to prove Bloch's Law. It stated that wave function in periodic potential could be written in the multiplication of a plane wave and a periodic function, which means

$$\psi(x) = e^{ikx}u(x) \tag{28}$$

Where e^{ikx} represents the plane wave and $u(x)$ is the periodic function.
Prove: First define the translation operator

$$\hat{T}(a)\psi(x) = \psi(x+a) \tag{29}$$

Transnational operator $\hat{T}$ does not vary with time. So

$$i\hbar\frac{d<\hat{T}>}{dt} =< \left[\hat{T},\hat{H}\right] \geq 0. \tag{30}$$

Hence

$$\left[\hat{T},\hat{H}\right] = 0. \tag{31}$$

This means that $\hat{H}$ and $\hat{T}$ have the same eigenvectorψ. So

$$\hat{T}\psi = \lambda\psi. \tag{32}$$

Where λ is the eigenvalue of the operator$\hat{T}$. If we multiple two transnational operator to wave function, we get

$$T_{n1}(a_1)T_{n2}(a_2)\psi(x) = \lambda_1\lambda_2\psi(x) = \psi(x+a_1+a_2) \tag{33}$$

We notice that

$$T_{n3}(a_1+a_2)\psi = T_{n1}(a_1)T_{n2}(a_2)\psi. \tag{34}$$

The function with this property is exponential function. It is natural to define

$$\hat{T}(a) = e^{s\cdot a} \tag{35}$$

Where s is a number that we don't know? We can solve s through normalization of wave function.

$$\int\left|\hat{T}\psi\right|^2 dx = |\lambda|^2\int\psi dx = |\lambda|^2 = 1. \tag{36}$$

It is normal to consider that s is a complex number. Set

$$s = ik. \tag{37}$$

Hence

$$\hat{T}(a)\psi(x) = e^{ika}\psi(x) = \psi(x+a) \tag{38}$$

The wave function in a periodic potential is of course periodic. So

$$\hat{T}(x)\psi(x) = e^{ikx}\psi(x) \tag{39}$$

Let $\psi(x)$ in the above equation equals to$u(x)$. Hence

$$\psi(x) = e^{ikx}u(x) \tag{40}$$

This is the Bloch theorem.

3.2. Kronig-Penney model

There are two distinct regions in Figure 2

Let's first look at$0 < x < a - b$. Here the Schrodinger equation can be written as

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi. \tag{41}$$

Let

$$\alpha^2 = \frac{2mE}{\hbar^2} \tag{43}$$

The solution of this equation is

$$\psi(0 < x < a - b) = Ae^{i\alpha x} + A'e^{-i\alpha x} \tag{43}$$

Then we focus on $-b < x < 0$ Schrodinger equation in this region can be written as

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - V_0\psi = E\psi. \tag{44}$$

Let

$$\beta^2 = \frac{2m(E + V_0)}{\hbar^2} \tag{45}$$

The solution is

$$\psi(-b < x < 0) = Be^{i\beta x} + B'e^{-i\beta x} \tag{46}$$

We know that, according to Bloch's Law, wave function can be written in a plane wave function and a periodic function. For equation 43,

$$\psi(0 < x < a - b) = e^{ikx}\left(Ae^{i(\alpha-k)x} + A'e^{-i(\alpha+k)x}\right) \tag{47}$$

For equation 46

$$\psi(-b < x < 0) = e^{ikx}\left(Be^{i(\beta-k)x} + B'e^{-i(\beta+k)x}\right) \tag{48}$$

Where the periodic function are defined by

$$u = \begin{cases} Ae^{i(\alpha-k)x} + A'e^{-i(\alpha+k)x}, 0 < x < a - b \\ Be^{i(\beta-k)x} + B'e^{-i(\beta+k)x}, -b < x < 0 \end{cases} \tag{49}$$

Now let us look at boundary condition. Continuous condition of ψ requires ψ and ψ' at point0. So

$$A + A' = B + B' \tag{50}$$

$$A\alpha - A'\alpha = B\beta - B'\beta. \tag{51}$$

u Is a periodic function with period$a$. So

$$u(-b) = u(a - b) \tag{52}$$

$$u'(-b) = u'^{(a-b)} \tag{53}$$

Plug in$u$, we get

$$Ae^{i(\alpha-k)(a-b)} + A'e^{-i(\alpha+k)(a-b)} = Be^{-ib(\beta-k)} + B'e^{ib(\beta+k)} \tag{54}$$

$$A(\alpha - k)e^{i(\alpha-k)(a-b)} - A'(\alpha + k)e^{-i(\alpha+k)(a-b)} = B(\beta - k)e^{-ib(\beta-k)} - B'^{(\beta+k)}e^{ib(\beta+k)} \tag{55}$$

These four equations (eq 50, 51, 54, 55) could be written in the matrix form

$$\begin{bmatrix} 1 & 1 & -1 & -1 \\ \alpha & -\alpha & -\beta & \beta \\ e^{i(\alpha-k)(a-b)} & e^{-i(\alpha+k)(a-b)} & -e^{-ib(\beta-k)} & -e^{ib(\beta+k)} \\ (\alpha-k)e^{i(\alpha-k)(a-b)} & -(\alpha+k)e^{-i(\alpha+k)(a-b)} & -(\beta-k)e^{-ib(\beta-k)} & (\beta+k)e^{ib(\beta+k)} \end{bmatrix} \begin{bmatrix} A \\ A' \\ B \\ B' \end{bmatrix} = 0. \quad (56)$$

The determinant of the square matrix must be 0 if it has nontrivial solutions.
And finally through the determinant we can get the following equation

$$\cos(ka) = \cos(\beta)\cos[\alpha(a-b)] - \frac{\alpha^2+\beta^2}{2\alpha\beta}\sin(\beta b)\sin[\alpha(a-b)] \quad (57)$$

This is the energy level for the Kronig-Penney model. It had profound applications in lasers.
Another important thing about the Kronig Penney model is that it is the simplest model that exhibit band gap.

3.3. Band gap of Kronig-Penney model

We could consider the potential energy of the Kronig-Penney model imposing a perturbation on the electron. We are interested in the energy of electrons. Hence, we use the equation for the perturbation of electron to the second order.

$$E = \frac{\hbar^2 k^2}{2m} + E_0 + \frac{2m}{\hbar^2}\sum_{k'\neq k}\frac{|< k|V|k' >|^2}{k^2-k'^2} \quad (58)$$

Re call that k is from the expression of $\psi(x) = e^{ikx}u(x)$
The first two terms are unperturbed energy. The third term is the result of perturbation. Our job is to solve third term and get the energy equation.
Notice that $V(x)$ is a periodic function with period$a$.

$$V(x) = \begin{cases} -V_0, & -b+na < x < na \\ 0, & na < x < a-b+na \end{cases} \quad (59)$$

To find the matrix element$< k|V|k' >$, we first use Fourier expansion for$V$.

$$V(x) = \sum_{g=-\infty}^{\infty} A_n\, e^{i\frac{2\pi n}{a}x} \quad (60)$$

And hence we can find A_g

$$\begin{aligned} A_n &= \frac{1}{a}\int_{-b}^{a-b} V(x) e^{-i\frac{2\pi n}{a}x}dx = -\frac{1}{a}\int_{-b}^{0} V_0\, e^{-i\frac{2\pi n}{a}x}dx \\ &= \frac{iV_0}{2\pi n}e^{i\frac{2\pi n}{a}b} \end{aligned} \quad (61)$$

It is the real part of A_n that interest us. So we only left with

$$A_n = -\frac{V_0}{2\pi n}\sin\left(\frac{2\pi n}{a}b\right) \quad (62)$$

Plug A_n into the expression of $V(x)$ and calculate $< k|V(x)|k' >$

$$< k|V(x)|k' \geq -\frac{1}{a}\sum_n A_n \int_{-b}^{0} e^{i\left(\frac{2\pi n}{a}-k+k'\right)x}dx = \sum_n A_n\,\delta_{n,k-k'} = A_{k-k'} \quad (63)$$

Where we have shown $k - k' = n$ Plug it back into eq 58 we get

$$E = \frac{\hbar^2 k^2}{2m} + E_0 + \frac{2m}{\hbar^2}\sum_{k' \neq k}\frac{|A_{k-k'}|^2}{k^2 - k'^2} = \frac{\hbar^2 k^2}{2m} + E_0 + \frac{mV_0^2}{\pi^2\hbar^2}\sum_{n\neq 0}\frac{\sin^2\left(\frac{2\pi n}{a}b\right)}{n^3(2k-n)} \tag{64}$$

This is the energy band equation for Kronig-Penney model.

4. Conclusion

In the above section, we have first shown that the energy level of the bound state of the finite square is discrete. It has the form of equations 23 and 24

$$z \cdot \tan(za) = \sqrt{z_0^2 - z^2} \tag{65}$$

$$-z \cdot cot(za) = \sqrt{z_0^2 - z^2} \tag{66}$$

Where z_0 is a constant and z is the independent variable.

Then we proved Bloch's Law. It claims that in a periodic potential, wave functions can be written as a plane wave times a periodic function (equation 28)

$$\psi(x) = e^{ikx}u(x) \tag{67}$$

And finally, we introduced the Kronig-Penney model and calculated its energy band gap, which reads

$$E = \frac{\hbar^2 k^2}{2m} + E_0 + \frac{mV_0^2}{\pi^2\hbar^2}\sum_{n\neq 0}\frac{\sin^2\left(\frac{2\pi n}{a}b\right)}{n^3(2k-n)} \tag{68}$$

It is an infinite repetition of finite square well. More importantly, it is the basic theory of laser technology.

It could be shown that in other branches of physics, such as condensed matter or high energy physics, the finite square well and Kronig Penney model have important applications. Just as I have mentioned in the Introduction, many other important applications of finite square well have not been recognized or categorized. Further researches on these topics could be helpful to the science community.

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