AN ALGEBRAIC APPROACH TO THE BAND STRUCTURE OF PERIODIC POTENTIALS

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ABSTRACT

AN ALGEBRAIC APPROACH TO THE BAND STRUCTURE OF PERIODIC POTENTIALS

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A general method based on Lie algebra with three generators is proposed in order to successfully produce physically significant periodic potentials. Some potentials in one dimension are solved in algebraic framework using the Lie algebra. A novel Kronig-Penney model is developed to obtain energy band structure of Kronig-Penney type and Hyperbolic periodic potentials. Our approach can be applied to the other periodic systems with some modifications. In addition, generalized Kronig-Penney model is formulated in one dimension for contact interactions. Here, eigenvalue equations are obtained by using transfer matrix formalism.

It has been shown that the method given in this thesis is useful to generate periodic quasi-exactly solvable potentials and to clarify their band structure. The algebraic method presented here leads to a number of physical potentials given in the literature.

Key words: Periodic potentials, Kronig-Penney model, contact interaction, Lie algebra.

ÖZET

PERİYODİK POTANSİYELLERİN BAND YAPISINA CEBİRSEL YAKLAŞIM

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Fizikte önemli uygulamaları olan periyodik potansiyelleri türetmek için Lie cebiri operatörlerine dayalı genel bir yöntem geliştiridi. Bazı potansiyeller tek boyutta Lie cebirinin bir uygulaması olarak çözüldü. Kronig-Penney ve hiperbolik periyodik potansiyellerin enerji band yapısını elde etmek için yeni bir Kronig-Penney modeli geliştirildi. Sözkonusu model gerekli uyarlamalarla diğer periyodik potansiyellere uygulanabilir. Ayrıca, kontak etkileşimler için genelleştirilmiş Kronig-Penney model denklemleri çıkartıldı. İlgili özdeğer denklemleri transfer matris yöntemi kullanılarak elde edildi.

Tezde verilen metodun aynı zamanda periyodik "quasi-exactly" çözülebilen potansiyellerin türetilmesinde ve band yapılarının açıklanmasında geçerli olduğu gösterildi. Buruda sunulan cebirsel yöntemle literatürde verilen fiziksel potansiyeller elde edilebilir.

Anahtar Kelimeler: Periyodik potansiyeller, Kronig-Penney modeli, kontak etkileşimler, Lie cebiri.

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LIST OF SYMBOLS

Symbols

$J_{\pm,0}$: Ladder operators

J^2 : Casimir operator

l : Periodicity of the lattice

V(x) : Crystal potential

Vo : Interatomic potential barrier

a : Width of the potential well around an atom

b : Width of the interatomic potential barrier

l : Periodicity of the lattice

$u(x)$: Arbitrary functions

A : Arbitrary constants

T : Kinetic energy operator

σ_i : Pauli matrices

j(x) : Current operator

$\psi(x)$: Arbitrary functions

H : Hamiltonian operator

μ : Quantum number

γ_i : Arbitrary constants

n : Positive numbers

α : Arbitrary constant

β : Arbitrary constant

δ : Periodic potential

$c_{\pm\pm}$: Arbitrary constants

$\chi(z)$: Polynomial of degree at most n.

$\mu(z)$: Gauge factor

$P^{(n)}$: Polynomials of degree at most n

$\rho_{n,i}$: Multiplier representation

γ_{μ}^{2} : Reduced width of the level μ.

CHAPTER 1

INTRODUCTION

The study of periodic potentials is of both physical and mathematical interest. For instance, in condensed matter physics, knowledge of the existence and locations of band edges and band gaps of periodic potential is very important for determining many physical properties. Unfortunately, even in one dimension, there are very few analytically solvable potential problems in condensed matter physics.

One of the most fundamental problems in solid state physics is that of an electron in a periodic potential. . The energy band structure of electrons in a periodic potential is essential to an understanding of many basic properties of the solid state of matter. Kronig and Penney [1,2] introduced the one dimensional periodic square well potential which is known as the *Kronig-Penney* model. Exact solution of the Hamiltonian can be obtained by this model

Also, the band structure of semiconductor superlattices can be discussed in terms of the standard Kronig-Penney model. The energy bands of electrons in one-dimension periodic potential for more complex superlattices that consisting of two different rectangular bands and wells per period are calculated by H. X. Jiang and Y. J. Lin [3]. The variation of the energy and band structure as a function of the size of the wells in each period is presented in this paper.

The case of perfectly periodic potentials has discussed by Hubert M. James et al. [4]. Solutions for the entire range of x are constructed by joining together "cell solutions"- solutions defined for a single period of the potential. (The range of x can be divided into periods or *cells* of length a(period). The potential has then the same form in each cell). The concept of "self-matching cell solutions" leads to a simple demonstration of the band structure of permitted energy levels. Several types of cell solution are discussed in their paper to give a particularly clear and elementary demonstration of the band structure of permitted energy levels.

The weak- and tight-binding approximation to the periodic Scarf potential is discussed by Frederic L. Scarf [5]. It has shown that the wave functions have intermediate forms even when $m^* \cong m$, $m^* \cong \infty$, where m^* is the effective mass. This suggests that these approximations, respectively, should be valid in these region, but it is actually found that they are not appropriate. The wave functions have complex intermediate form for wide ranges of parameter. The results illustrates Slater's conjecture that the wave function may be quite complicated even when m^* and $E(k)$ have values which indicate that the particle is almost free or that it is tightly bound.

The application of group theoretical techniques to physical problem has along and fruitful history. Spectrum generating algebra (SGA) and dynamical symmetry techniques are applied to Hamiltonians with periodic potentials, and band structure can arise naturally from representation theory [6,7]. Hamiltonians such as Scarf's are reduced to problem as simple as solving by reducing the Hamiltonian in the form $H = J_z^2$, using representation with multi-valued wave functions. Further, both compact and non-compact Lie algebras are shown that they play a role in the band edges-$su(1,1)$ for the Scarf and extended Scarf potentials, and $su(2)$ for the Lamé equations [6]. And they constructed dynamical symmetries Hamiltonians in $so(2,1)$ and $so(2,2)$ [7] which can be expressed as Schrödinger operators with periodic potential allowing the calculation of dispersion relations and transfer matrices. One-dimensional potentials within the R matrix theory are described algebraicly with $su(1,1)$ Lie algebra [8]. A. Gonzalez-Lopez and their collaborators et al [9] showed the recent work on quasi-exactly Schrödinger operators and Lie algebras of differential operators.

One of very successful methods in numerous applications in physics for periodic potentials is the semi-classical approach. Sukhatme and Sergeenko derived the semi-classical WKB quantization condition for obtaining the energy band edges of periodic potentials [10]. They applied successfully their semi-classical approach with considering applications to the well-studied class of Lamé potential $V(x) = ma(a+1)sn^2(x,m)$ where *sn(x,m)* is a Jacobi elliptic function of real elliptic modulus parameter $m(0 \le m \le 1)$ with period *4K(m)*.

Alternatively, using the formalism of supersymmetric quantum mechanics, A. Khare and U. Sukhatme [11] have obtained a large number of new analytically solvable one-dimensional periodic potentials and studied their properties. More specially, the supersymmetric partners of the Lamé potential $ma(a+1)sn^2(x,m)$ are derived and they discussed the energy band edges of the associated Lamé potentials $pmsn^2(x,m) + qmcn^2(x,m)/dn^2(x,m)$ which constitute a much richer class of periodic problems. In particular, Dunne and Feinberg [12] defined the concept of self-isospectral periodic potentials in detail, which are "self-isospectral" in the sense that the potentials have identical shape, but are translated by one half period relative to one another. Recently, two solvable, real and shape invariant Pösch-Teller I and Pösch-Teller II potentials on the half-axis are obtained [13].

In addition, several authors have recently investigated the eigenstates of periodic complex-potentials [14,15], especially those with PT symmetry and real spectra. In addition, the eigenstates of periodic complex Pösch-Teller I and Pösch-Teller II like potentials are found explicitly [16].

Many authors classified the potentials in physics in three classes such as exactly-solvable potentials, quasi-exactly solvable potentials, and conditionally-exactly solvable potentials . It is well known that the Natanzon potentials [17] are exactly solvable in non-relativistic quantum mechanics. These are of two types corresponding to whether the Schrödinger equation can be reduced to either a hypergeometric or confluent hypergeometric equation. Chapters 4 and 5 are devoted to eactly- and quasi exactly solvable potentials.

1.1 Outline Of The Study

This thesis consists of two parts. In the first part, we have solved the Kronig-Penney model for periodic potentials, in chapter 2, and the application of Kronig-Penney model to the contact interactions are given in chapter 3. In chapter 2, the eigenvalue problem for periodic potentials is solved exactly and we have shown that electrons in that periodic potential are arranged in energy bands separated by forbidden gaps. In addition, Kronig-Penney model is written as a Mathematica program to do some simplification in the calculations. The Schrödinger equation is written in the form of summation of two functions such as even and odd function solutions. The accuracy of the calculations are checked out for two examples.

In chapter 3, one example of the application of the Kronig-Penney model is given with periodic δ potentials to the cases with generalized contact interaction. By applying Bloch theorem, the eigenvalue equation is deduced within the framework of the transfer matrix formalism.

The second part of this thesis, chapters 4 and 5 are devoted to the applications of the Lie algebra. In chapter 4, exactly solvable potentials are classified in two classes depending on whether the Schrödinger equation can be reduced to hypergeometric or a confluent hypergeometric functions. Then, quasi-exactly solvable Hamiltonian are written in algebraic framework to produce quasi-exactly solvable potentials by using canonical transforms. Through the developed expressions, potentials corresponding to some canonical forms are discussed by considering exactly-solvable cases.

In chapter 5, the eigenstates of a particle in a rectangular-well potential with appropriate boundary conditions are proved to be standard basis of an irreducible representation of the $su(1,1)$ Lie algebra. And trigonometric-like potentials are written in algebraic framework of operators of $su(1,1)$ Lie algebra. Finally, the last section contains the conclusion of the thesis.

CHAPTER 2

THE KRONIG-PENNEY MODEL OF AN INFINITE ONE-DIMENSIONAL CRYSTAL

2.1 Introduction

The free-electron theory of metals is based upon the notion that the conduction electrons within a metallic substance act like the classical free particles of a gas, subject only to the limitations of the Fermi-Dirac statistics. It is not immediately obvious, from the quantum mechanical point of view, why this should be the case. It is also not clear why some substances have large numbers of free electrons and are thus very good conductors, while others have hardly any and behave as insulators.

The simplest quantum mechanical view of an electron in a crystal is that of a single electron in a perfectly periodic potential which has the periodicity of the lattice. In this *one-electron* model of solid, the periodic potential may be thought of as arising from the periodic charge distribution associated with the ion cores situated on the lattice sites, *plus* the (constant) average "smeared out" potential contribution due to all the other free electrons belonging to the crystal, so that the interaction of the single electron with all the others is accounted for in an average sense. The solution of Schrödinger's equation for the single electron in this potential then provides a set of "one-electron" states which the single electron may occupy, and in

fact which may be occupied (subject to the limitations of the Pauli principle) by the all electrons of the crystal, since the single electron which is considered initially may be regarded as typical of all electrons of the system.

We shall find that one-electron wave functions (called Bloch functions) calculated by the above prescription always have certain properties closely related to the lattice periodicity, and that the allowed electronic energies occur in bands of permitted states separated by forbidden energy regions. Within the allowed energy bands, the dynamical behavior of electrons will be found to be in many ways similar to that of free particles, and the question of whether a crystal is a conductor or an insulator will depend upon whether the electronic states within a given allowed band or set of bands is completely filled or partially empty. In addition, we shall see that the collective behavior of electrons in an *almost* filled band of allowed states is very much like that of a few *positive* charge carriers in an almost energy empty band! The one-electron picture will thus serve to justify the free-electron model form a fundamental point of view, and also to answer certain rather puzzling questions which the free- electron theory, of itself, could not even attempt to explain. It should be remembered, however, that the one-electron treatment is an approximation in which the *details* of electron-electron interactions are completely overlooked.

2.2 The Bloch Theorem

The Bloch theorem [19] is a mathematical statement regarding the form of the one-electron wave functions for a perfectly periodic potential. Consider a differential equation of the form

$$\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = 0 \tag{2.1}$$

where $V(x)$ is a given function which is *periodic* with a period l so that

$$V(x+l)=V(x) \tag{2.2}$$

If the potential function $V(x)$ for one-dimensional Schrödinger equation is periodic, then Schrödinger's equation will be a special case of equation (2.1). Since (2.1) is a linear second-order differential equation, any solution $\psi(x)$ may be represented as a linear combination of two linearly independent solutions [18] $\psi_1(x)$ and $\psi_2(x)$

$$\psi(x)=c_1\psi_1(x)+c_2\psi_2(x) \tag{2.3}$$

Now $\psi_1(x+l)$ and $\psi_2(x+l)$ are also solution of (2.1), and hence may be represented as linear combinations of $\psi_1(x)$ and $\psi_2(x)$

$$\begin{aligned}\psi_1(x+l)&=a_{11}\psi_1(x)+a_{12}\psi_2(x)\\ \psi_2(x+l)&=a_{21}\psi_1(x)+a_{22}\psi_2(x)\end{aligned} \tag{2.4}$$

Thus, using (2.3), (2.4) and the fact that $\psi(x+l)$ is also a solution, we may write

$$\begin{aligned}\psi(x+l)&=(c_1a_{11}+c_2a_{21})\psi_1(x)+(c_1a_{12}+c_2a_{22})\psi_2(x)\\ \psi(x+l)&=d_1\psi_1(x)+d_2\psi_2(x)\end{aligned} \tag{2.5}$$

The relation between the coefficients (c_1,c_2) and (d_1,d_2) clearly involves the matrix multiplication

$$\begin{pmatrix}d_1\\ d_2\end{pmatrix}=\begin{pmatrix}a_{11} & a_{21}\\ a_{12} & a_{22}\end{pmatrix}\begin{pmatrix}c_1\\ c_2\end{pmatrix} \tag{2.6}$$

Let us see what happens if we diagonalise the 2x2 matrix in this equation to solve the corresponding eigenvalue. This system of homogeneous equations in c_1 and c_2 has solutions other than $c_1=c_2=0$ only if

$$\begin{vmatrix} a_{11}-\lambda & a_{21} \\ a_{12} & a_{22}-\lambda \end{vmatrix} = \lambda^2 - (a_{11}+a_{22})\lambda + (a_{11}a_{22}-a_{12}a_{21}) = 0 \tag{2.7}$$

which is a quadratic equation for λ having two solutions λ_1 and λ_2. If (c_1, c_2) is an eigenvector corresponding to one of the eigenvalues $\lambda = \lambda_i (i = 1,2)$. We have $d_1 = \lambda c_1$ and $d_2 = \lambda c_2$. The solution of this quadratic equation in λ serves to determine the two possible values of λ having the property

$$\psi(x+l) = \lambda\psi(x) \tag{2.8}$$

where λ is a constant vector. This results is known as *Floquent's theorem.* Of course, Eq. (2.8) can be written as [2] by designating them λ_1 and λ_2,

$$\begin{aligned} \psi(x+l) &= \lambda_1\psi(x) \\ \psi(x+l) &= \lambda_2\psi(x) \end{aligned} \tag{2.9}$$

If we now define k_1 and k_2 such that

$$\begin{aligned} \lambda_1 &= e^{ik_1 l} \\ \lambda_2 &= e^{ik_2 l}, \end{aligned} \tag{2.10}$$

and define $u_{k_1}(x)$ and $u_{k_2}(x)$ as

$$\begin{aligned} u_{k_1}(x) &= e^{-ik_1 x}\psi(x) \\ u_{k_2}(x) &= e^{-ik_2 x}\psi(x), \end{aligned} \tag{2.11}$$

then, using (2.11), (2.9), and (2.10) it is clear that

$$\begin{aligned} u_{k_1}(x+l) &= e^{-ik_1(x+l)}\psi(x+l) = e^{-ik_1(x+l)}\lambda_1\psi(x) \\ u_{k_1}(x+l) &= e^{-ik_1(x+l)}e^{ik_1 l}\psi(x) = e^{-ik_1 x}\psi(x) = u_{k_1}(x) \end{aligned} \tag{2.12}$$

where * denotes the complex conjugate. The function $u_{k_1}(x)$ is thus *periodic* with period l; the same is found to be true for $u_{k_2}(x)$ in a similar way. According to (2.11), then $\psi(x)$ can then always be written in the form

$$\psi_k(x) = e^{ikx} u_k(x) \tag{2.13}$$

where $u_k(x)$ is a *periodic* function of period l, and where k represents either k_1 or k_2 as determined above. This is Bloch's theorem; all one-electron wave functions for periodic potentials can be written in this way. In three dimensions Bloch's theorem becomes

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}\, u_{\mathbf{k}}(\mathbf{r}) \tag{2.14}$$

The wave functions (2.13) and (2.14) clearly have the form of plane waves with propagation vector **k** modulated by a function whose periodicity is that of the crystal lattice.

The Bloch functions (2.13) can be thought of as the most general way of writing a solution of Schrödinger's equation which leads to the same probability density $\psi^*\psi$ in each unit cell of the crystal. From (2.13) it is apparent that in the nth unit cell, due to the periodicity of u_k,

$$\begin{aligned} \psi(x+nl) &= e^{ik(x+nl)} u_k(x+nl) = e^{ik(x+nl)} u_k(x) \\ \psi(x+nl) &= e^{iknl}\psi(x) \end{aligned} \tag{2.15}$$

Likewise,

$$\psi^*(x+nl) = e^{-iknl}\psi^*(x) \tag{2.16}$$

and,

$$\psi^*(x+nl)\psi(x+nl) = \psi^*(x)\psi(x) \tag{2.17}$$

where * denotes the complex conjugate.

The 3-dimensional wave function (2.14) exhibits the same sort of behavior. In the one-dimensional case, for an *infinite* crystal, one can find a formal solution to Schrödinger's equation for every value of the E within certain ranges, and corresponding to each such value of E, by (2.8) and (2.10), are two values of k. The allowed energy eigenvalues for such a system within these range are continuos. If the crystal is of finite extent, however, in which case appropriate physical boundary conditions must be satisfied at the surfaces, then solutions which satisfy Schrödinger's equation *and* the boundary conditions can be found only for certain discrete energy eigenvalues. Since for each energy eigenvalue there are only two related values of k, the allowed values of k also form a discrete set. Of course when the number of atoms in the crystal becomes very large, the allowed values of E and k, although still discrete, crowd very closely together and in most cases can be regarded as quasi-continuous bands of allowed values. The same qualitative behavior is found for three-dimensional crystals, except that in this case there are more than two allowed values of **k** for each energy eigenvalue.

For example, if periodic boundary conditions are imposed in a one-dimensional crystal of N atoms (or if the lattice is assumed to have form of a closed ring of N atoms), then if the wave function ψ is to be single-valued, we must have (using (2.15))

$$\psi(x+Nl) = e^{ikNl}\psi(x) = \psi(x) \tag{2.18}$$

whereby

$$e^{ikNl} = 1$$

or

$$e^{ikl} = (1)^{1/N} = e^{\frac{2\pi in}{N}} \qquad (n=0,1,2,.....N-1) \tag{2.19}$$

recalling the form of the Nth roots of unity. Taking the logarithm of both sides of this equation and solving for k, we find that the possible values for k under these boundary conditions are

$$k_n = \frac{2\pi n}{Nl} \qquad (n=0,1,2,.....N-1) \tag{2.20}$$

If N is large, there will be very many allowed values of k as given by (2.20), and in this case they may be regarded as forming a quasi-continuous range of values. Of course the N distinct values of k allowed by (2.20) do not correspond to the same value of energy. For each constant value of E, there are only *two* allowed values of k given by (2.10).

2.3 The Kronig-Penney Model

This model was first investigated by Kronig and Penney (1930) [1], and is concerned with the solution of Schrödinger's equation, assuming a certain potential distribution inside the solid [5]. According to the free-electron model the potential inside the solid is uniform: the Kronig-Penney model goes one step further by taking into account the variation of potential due to the presence of immobile lattice ions. Considering a one-dimensional case for simplicity, the potential energy of an electron is shown in Fig. 2.1. The highest potential is halfway between the ions and the potential tends to minus infinity as the position of the ions is approached. This potential distribution is still very complicated for a straightforward mathematical solution. We shall therefore replace it by a simpler one that still displays the essential features of the function, namely

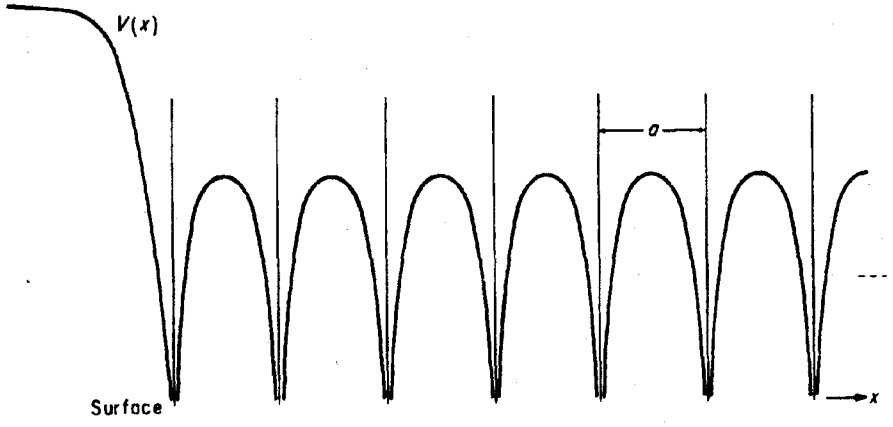

Figure 2.1 The variation of the electrons potential energy in one-dimensional crystal. [2]

i) it has the same period as the lattice;

ii) the potential is lower in the vicinity of the lattice ion and higher between the ions.

We shall consider the motion of a particle in a periodic potential of period l, so that

$$V(x+l) = V(x) \tag{2.21}$$

As an illustration we show in Fig. 2.2 a periodic potential with rectangular sections, called the *Kronig-Penney* potential, which can be used as a model of the interaction to which an electron is subjected in a crystal lattice consisting of a rectangular array of single atoms separated by the distance l.

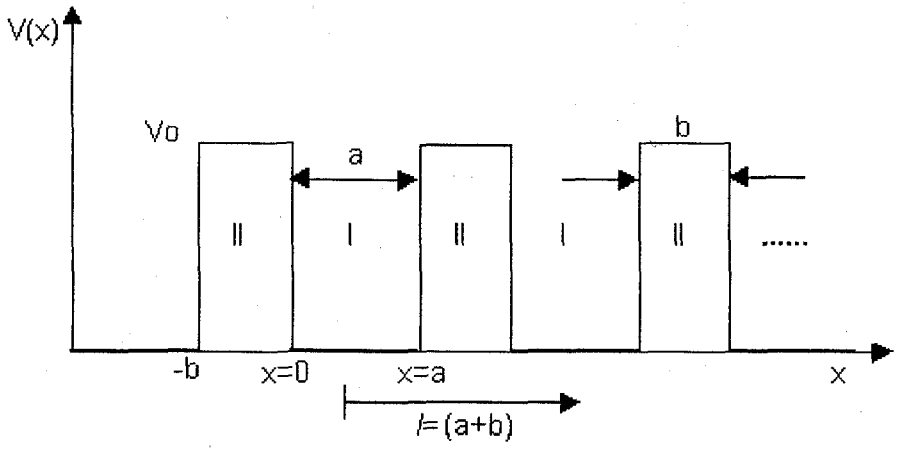

Figure 2.2 A periodic potential with rectangular sections, called the Kronig-Penney potential.

The period has length *l*. The wells represent schematically the attraction exerted by the atoms (ions) of the crystal lattice on the electrons.

where;

Table 2.1 The parameters and boundary conditions in Kronig-Penney model

V(x) :	is the crystal potential
Vo :	is the interatomic potential barrier
a :	is the width of the potential well around an atom
b :	is the width of the interatomic potential barrier
a+b :	Periodicity of the lattice
Region I :	$0 \leq x \leq a$ Boundary condition: V(x) = 0, electron is in the well
Region II :	$-b \leq x \leq 0$ Boundary condition: V(x) = Vo, electron is in the barrier

The Kronig-Penney Model can predict energy bands for a string of atoms subject to a periodic potential, Vo. We are interested in knowing about the E(k) relationship for electrons moving in the crystal potential, V(x).

For the case of the infinite periodic one-dimensional square-well potential shown in Figure 2.2, it is possible to arrive at an exact solution of the Schrödinger equation. This solution was first investigated by Kronig and Penney [1], and although it is related to a somewhat idealized periodic potential which is only a crude approximation to that found in the actual crystal, it is nevertheless very useful

because it serves to illustrate in a most explicit way many of the important characteristic features of the quantum behavior of electrons in periodic lattices. The wave functions associated with this model may be calculated in the one-electron approximation by solving Schrödinger's equation

$$\frac{d^2\psi(x)}{dx^2}+\frac{2m}{\hbar}(E-V(x))\psi(x)=0 \tag{2.21}$$

for a single electron in the periodic potential $V(x)$ as given by Figure 2.2. Since, the wave functions must have the Bloch form, we may expect that

$$\psi_k(x)=e^{ikx}u_k(x) \tag{2.22}$$

2.3.1 Energy Bands

Let us now discuss the energy spectrum. For simplicity, we shall focus our attention on the Kronig-Penney potential (see Fig. 2.2) which exhibits the basic features of the interaction felt by an electron in a crystal and leads to a readily solvable problem. We choose the zero of the energy scale to coincide with the top of the wells, and consider successively the two cases for which the electron energy E is such that $Vo<E<\infty$ and $0<E<Vo$.

2.3.1.1 Case1. Vo<E<∞

Substituting (2.22) into (2.21), it is found that the functions $u(x)$ must satisfy

$$\frac{d^2u}{dx^2}+2ik\frac{du}{dx}-\left(k^2-\alpha^2+\frac{2mV(x)}{\hbar^2}\right)u(x)=0 \tag{2.23}$$

where

$$\alpha=(2mE/\hbar^2)^{1/2} \tag{2.24}$$

For the potential of Figure 2.2, then, we shall find that

$$\frac{d^2u_1}{dx^2} + 2ik\frac{du_1}{dx} - \left(k^2 - \alpha^2\right)u_1(x) = 0 \qquad (0<x<a) \tag{2.25}$$

and

$$\frac{d^2u_2}{dx^2} + 2ik\frac{du_2}{dx} - \left(k^2 - \beta^2\right)u_2(x) = 0 \qquad (-b<x<0) \tag{2.26}$$

where $u_1(x)$ represents the value of $u(x)$ in the interval $(0<x<a)$ and $u_2(x)$ represents the value of $u(x)$ in $(-b<x<0)$, and where

$$\beta = (2m(E - Vo)/\hbar^2)^{1/2} \tag{2.27}$$

The differential equations (2.25) and (2.26) are easily solved by standard procedures to give

$$u_1(x) = Ae^{i(\alpha-k)x} + Be^{-i(\alpha+k)x} \qquad (0<x<a) \tag{2.28}$$

$$u_2(x) = Ce^{i(\beta-k)x} + De^{-i(\beta+k)x} \qquad (-b<x<0) \tag{2.29}$$

where A, B, C, and D are arbitrary constants. Note that the quantity β is a purely imaginary one for $0<E<Vo$.

The requirement of continuity for the wave functions ψ and its derivative at $x=a$ and $x=-b$ demands that the function $u(x)$ satisfy these same conditions, since in (2.22) e^{ikx} is a well-behaved function. Applying these boundary conditions (and recalling that since $u(x)$ has the periodicity of the lattice, $u_1(a) = u_2(-b)$), we find that

$$A + B = C + D$$

$$i(\alpha - k)A - i(\alpha + k)B = i(\beta - k)C - i(\beta + k)D$$

$$Ae^{i(\alpha-k)a} + Be^{-i(\alpha+k)a} = Ce^{-i(\beta-k)b} + De^{i(\beta+k)b} \tag{2.30}$$

$$i(\alpha - k)Ae^{i(\alpha-k)a} - i(\alpha + k)Be^{-i(\alpha+k)a} = i(\beta - k)Ce^{-i(\beta-k)b} - i(\beta + k)De^{i(\beta+k)b}$$

The coefficients *A, B, C,* and *D* can thus be determined as the solution of a set of four simultaneous linear homogeneous equations in those quantities. There is no solution other than $A = B = C = D = 0$, of course, unless the determinant of the coefficients vanishes. This requires that

$$\begin{vmatrix} 1 & 1 & -1 & -1 \\ \alpha - k & -(\alpha + k) & -(\beta - k) & (\beta + k) \\ e^{i(\alpha-k)a} & e^{-i(\alpha+k)a} & -e^{-i(\beta-k)b} & -e^{i(\beta+k)b} \\ (\alpha - k)e^{i(\alpha-k)a} & -(\alpha + k)e^{-i(\alpha+k)a} & -(\beta - k)e^{-i(\beta-k)b} & (\beta + k)e^{i(\beta+k)b} \end{vmatrix} = 0 \tag{2.31}$$

Expanding the determinant, one can show after a quite a lot of tedious but straight-forward algebra that (2.31) can be expressed as

$$-\frac{\alpha^2 + \beta^2}{2\alpha\beta}\sin \alpha a \sin \beta b + \cos \alpha a \cos \beta b = \cos k(a + b) \tag{2.32}$$

Since in the range $(0 < E < Vo)$, β as defined by (2.27) is imaginary, for these values of energy it is most convenient to express (2.32) in a slightly different form. Letting

$$\beta = i\gamma \tag{2.33}$$

in this region, and noting that $\cos ix = \cosh x$ and $\sin ix = i \sinh x$, Equation (2.32) can be written as

$$\frac{\gamma^2-\alpha^2}{2\alpha\gamma}\sinh\gamma b\sin\alpha a+\cos\alpha a\cosh\gamma b=\cos k(a+b) \qquad (2.34)$$

which is an implicit equation for the energy E. Here γ is a real positive quantity in the interval *(0<E<Vo)*, just as β is in the interval *(Vo<E<∞)*. We may thus use (2.32) most conveniently when *(Vo<E<∞)* and (2.34) when *(0<E<Vo)*.

2.3.1.2 Case 2. 0<E<Vo

The modifications required to threat the case *E>0* are very simple. We see from (2.24) and (2.27) that when the energy E is positive the quantity γ becomes imaginary. We shall therefore set $\gamma = i\,k'$, with $k'=(2mE/\hbar^2)^{1/2}$. Since no assumption about the reality of γ has been made in deriving (2.34), we may at once rewrite this equation for the case *E>0* as

$$-\frac{\alpha^2+k'^2}{2\alpha k'}\sin k'b\sin\alpha a+\cos\alpha a\cos k'b=\cos k(a+b) \qquad (2.35)$$

and we see that this is again an implicit equation for the energy *E*.

The wave functions (2.22) must, like all wave functions, be well-behaved functions as x approaches $\pm\infty$. Since $u(x)$ is a periodic function whose values are the same in each unit cell, no difficulties arise on its account, provided that the factor e^{ikx} in (2.22) is well behaved under these conditions. But e^{ikx} is well behaved at *both* $+\infty$ and $-\infty$ only if k is real, whereby e^{ikx} is oscillatory. If k were imaginary, e^{ikx} would diverge to infinity either at $+\infty$ or $-\infty$, and the resulting expression for $\psi(x)$ would not behave properly as a wave function. We must therefore accept only the functions of the form (2.22) with *real* values for k. The above expression (2.32) and (2.33) have, on the left-hand side, a function of the form $K_1\sin\alpha a+K_2\cos\alpha a$ which must equal to $\cos k(a+b)$. If for a given value of energy function on the left-hand side of equations should have a value in the range between +1 and –1, then the required value for $\cos k(a+b)$ is obtained with a *real* value for argument *k(a+b)*. On

the other hand, if the value of the function on the left-hand side of (2.32) or (2.34) should lie outside this range, it would mean that $\cos k(a+b)$ would have to be greater than +1 or less than –1, which would, in turn, require that the argument *k(a+b)* be a *complex* number with an imaginary part other than zero. Under these circumstances the solutions (2.22) would not behave properly at infinity and would not satisfy the physical requirement for wave functions of the system. The energies associated with such values of *k* would simply be forbidden to the electron.

The equations (2.32) and (2.34) can be transformed into another useful form through some trigonometric identities. One can always write,

$$K_1 \sin(\alpha a) + K_2 \cos(\alpha a) = K_3 \cos(k(a+b) - \delta),$$

where

$$K_3 = (K_1^2 + K_2^2)^{1/2} \qquad \text{and} \qquad \tan\delta = \frac{K_1}{K_2} \tag{2.36}$$

The identity $\cos(A-B) = \cos A \cos B + \sin A \sin B$ has been used to obtain (2.36). Now, in this way (2.32) and (2.34) can be written as

$$\left[1 + \frac{(\alpha^2 - \beta^2)^2}{4\alpha^2\beta^2} \sin^2 \beta b\right]^{1/2} \cos(\alpha a - \delta) = \cos k(a+b) \tag{2.37}$$

where

$$\tan\delta = -\frac{\alpha^2 + \beta^2}{2\alpha\beta} \tan\beta b \qquad (Vo<E<\infty)$$

$$\left[1 + \frac{(\alpha^2 + \gamma^2)^2}{4\alpha^2\gamma^2} \sin^2 \gamma b\right]^{1/2} \cos(\alpha a - \delta) = \cos k(a+b) \tag{2.38}$$

where

$$\tan\delta = \frac{\alpha^2+\delta^2}{2\alpha\delta}\tan\gamma b \qquad (0<E<Vo)$$

From these expressions it is clear that in both cases the left-hand side has the form of cosine function times a modulating factor whose amplitude is *invariably* grater than unity. The value of this modulating factor is actually a maximum for $\alpha = 0$ (hence for $E = 0$) and approaches unity in the limit of large energies, where $\alpha \cong \beta$.

When the left-hand sides of (2.37) and (2.38) are plotted as a function of energy $F(E)$, in which connection one should note from (2.24) and (2.27) that

$$\alpha^2 - \beta^2 = \alpha^2 + \gamma^2 = 2mVo/\hbar^2 = const., \qquad (2.39)$$

The results are as illustrated in Figure 2.3. In this figure the left-hand side of (2.37) or (2.38) is plotted as a function of energy.

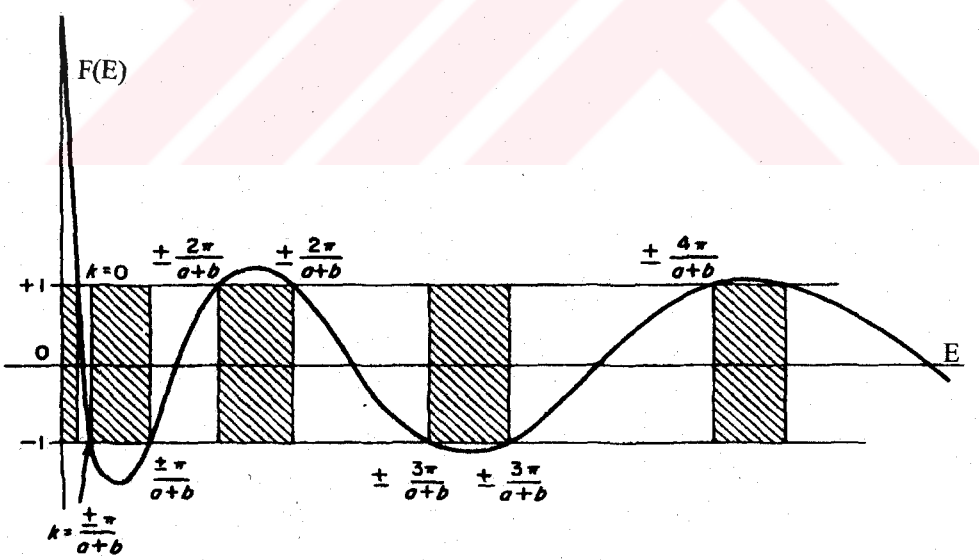

Figure 2.3. A plot of the functions on the left-hand side of (2.37) and (2.38) *versus* energy. The shaded regions show forbidden energy bands where the value of k is complex, the unshaded regions allowed energy bands corresponding to real values of k [2].

The dispersion relation expresses the relationship between energy and crystal momentum for the electron. Since the energy is given in terms of the parameter α by (2.24), assuming a value for α allows one to determine *both* the energy and crystal

momentum (solve for k in equation (2.38)). Each such assumed value gives a point on the dispersion curve, and by assuming a sufficient number of α values, the entire dispersion curve can be constructed. The results are shown in Figure 2.4 below.

When the ordinate of the curve lies between +1 and –1, there exists a real value for k corresponding to physically possible wave functions. Outside these limits, however, k must be complex with a nonzero imaginary part. Such values for k can never lead to physically well-behaved wave functions; the corresponding ranges of energy are forbidden and shown in Figure 2.3 as shaded regions. There are thus formed alternate regions of allowed energy eigenvalues and forbidden regions. These regions are usually referred to as allowed and forbidden *energy bands,* and the grouping of the permitted energy values into these bands is one of the most important and characteristic features of the behavior of electrons in periodic lattices. It can be shown that energy bands having the same qualitative aspects as those shown in Figure 2.3 are formed no matter what the detailed form of the potential is, so long as it is periodic.

It is clear from Figure 2.3 that energies close to zero are forbidden, a fact that it also seen in Figure 2.4. The allowed band of lowest energy is obtained when the crystal momentum k is in the interval $(-\pi/(a+b) < k < \pi/(a+b)$. The values of $k = \frac{\pm n\pi}{a+b}$ defines the *band edges,* where two allowed bands are separated by an energy gap. The Bragg condition is clearly satisfied at these points. One may visualize the electron as being *internally diffracted* by the crystal lattice for these values of crystal momentum. The region of the k-axis associated with the lowest allowed band is the first Brillouin zone of the lattice, the regions associated with the second-lowest allowed band is the second Brillouin zone, and so on. The zone boundaries are always points at which internal Bragg reflections occur.

Using (2.37), (2.38), (2.24), and (2.27) it is possible to plot a curve showing the energy E as a function of k *E(k).*The result is illustrated schematically in Figure 2.4. The forbidden energy bands and the relationship of E *vs.* k within the various allowed bands have been assigned in accord with the scheme shown in Figure 2.3.

Since $\cos^{-1} k(a+b)$ is not a single valued function this assignment is necessity somewhat arbitrary. For large energies, it is apparent that the function *E(k)* approaches the free-electron relation $E = \hbar^2 k^2 / 2m$ (shown as a dotted curve in Figure 2.4) quite closely within the allowed bands. Also, for large energies it is found that the allowed bands become very broad and the forbidden regions quite narrow. Nevertheless, the curve *E(k)* always has *zero* slope at the edges of the allowed bands, that is, at $k = \pm n\pi/(a+b)$, where *n* is an integer. This result can be proved by direct differentiation of (2.37) and (2.38), but we shall not go through the details of the calculation. This feature of the *E(k)* curve is quite general, and can be shown to occur even in the three-dimensional case independent of the precise mathematical form of the potential function.

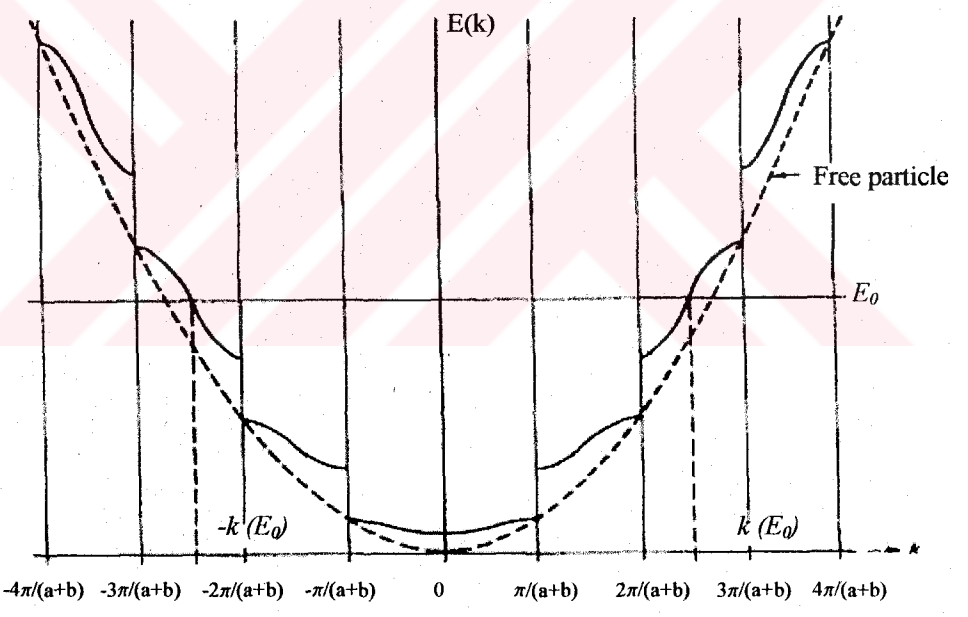

Figure 2.4. This feature of the *E(k)* curve is quite general, and can be shown to occur even in the three-dimensional case independent of the precise mathematical form of the potential function [2].

2.4 A Mathematical Approach

We have shown the general solution of the Kronig-Penney model of an infinite one-dimensional crystal for the rectangular potential. In this part, we have developed a Mathematica code to avoid from the tedious algebra which, produces dispersion relation easily.

Assume that, the solution of the Schrödinger equation with the periodic potential for two regions are in the form ϕ_1 and ϕ_2. One can, of course, express these two solutions in terms of $g_1(x), u_1(x), g_2(x),$ and $u_2(x)$, such that

$$\begin{aligned} \phi_1 &= Ag_1(x) + Bu_1(x) \\ \phi_2 &= Cg_2(x) + Du_2(x) \end{aligned} \tag{2.40}$$

They are four arbitrary linearly independent solutions of the Schrödinger equation with energy E. $u_1(x)$ and $u_2(x)$ are odd functions and $g_1(x), g_2(x)$ are even functions.

When the potential is symmetric about the center of each period, it is convenient to consider these even and odd solutions such that;

$$\begin{aligned} g_1(0) &= 1 \qquad g_1'(0) = 0 \\ g_2(0) &= 1 \qquad g_2'(0) = 0 \\ u_1(0) &= 0 \qquad u_1'(0) = 1 \\ u_2(0) &= 0 \qquad u_2'(0) = 1 \end{aligned} \tag{2.41}$$

Now, the step is to write ϕ_1 and ϕ_2 by using Bloch's theorem in the form such that;

$$\begin{aligned} \phi_1(x) &= e^{-ikx}(Ag_1(x) + Bu_1(x)) \\ \phi_2(x) &= e^{-ikx}(Cg_2(x) + Du_2(x)) \end{aligned} \tag{2.42}$$

The functions $\phi_1(x)$ is thus *periodic* with *l=(a+b),* the same is found to be true for $\phi_2(x)$ in a similar way.

The next step is to impose the same periodic boundary conditions that the both functions in Eq. (2.42) and their first derivatives must be equal to each other at each points *x=0* and $x = a = -b$ (see Appendix)

$$\begin{vmatrix} P_{11} & P_{12} & P_{13} & P_{14} \\ P_{21} & P_{22} & P_{23} & P_{24} \\ P_{31} & P_{32} & P_{33} & P_{34} \\ P_{41} & P_{42} & P_{43} & P_{44} \end{vmatrix} = 0 \qquad (2.43)$$

where

$$P_{11} = g_1[0] \qquad P_{12} = u_1[0]$$

$$P_{21} = -ikg_1[0] + g_1'[0] \qquad P_{22} = -iku_1[0] + u_1'[0]$$

$$P_{31} = e^{-iak} g_1[a] \qquad P_{32} = e^{-iak} u_1[a]$$

$$P_{41} = -ie^{-iak} kg_1[a] + e^{-iak} g_1'[a] \qquad P_{42} = -ie^{-iak} ku_1[a] + e^{-iak} u_1'[a]$$

$$P_{13} = -g_2[0] \qquad P_{14} = -u_2[0]$$

$$P_{23} = ikg_2[0] - g_2'[0] \qquad P_{24} = iku_2[0] - u_2'[0]$$

$$P_{33} = -e^{-ibk} g_2[-b] \qquad P_{34} = -e^{ibk} u_2[-b]$$

$$P_{43} = ie^{ibk} kg_2[-b] - e^{ibk} g_2'[-b] \qquad P_{44} = ie^{ibk} ku_2[-b] - e^{-ibk} u_2'[-b]$$

The equation (2.43) is the desired equation to find the dispersion relation of an infinite one-dimensional crystal for the rectangular potential. Using the boundary conditions given in (2.41), Eq.(2.43) can be reduced to the,

$$P_{11} = g_1[0] \qquad P_{12} = 0$$

$$P_{21} = -ikg_1[0] \qquad P_{22} = u_1'[0]$$

$$P_{31} = e^{-iak} g_1[a] \qquad P_{32} = e^{-iak} u_1[a]$$

$$P_{41} = -ie^{-iak} kg_1[a] + e^{-iak} g_1'[a] \qquad P_{42} = -ie^{-iak} ku_1[a] + e^{-iak} u_1'[a]$$

$$P_{13} = -g_2[0] \qquad P_{14} = 0$$

$$P_{23} = ikg_2[0] \qquad P_{24} = u_2'[0]$$

$$P_{33} = -e^{-ibk} g_2[-b] \qquad P_{34} = -e^{ibk} u_2[-b]$$

$$P_{43} = ie^{ibk} kg_2[-b] - e^{ibk} g_2'[-b] \qquad P_{44} = ie^{ibk} ku_2[-b] - e^{-ibk} u_2'[-b]$$

When these determinant coefficients are reduced to these form, some boundary conditions in Eq. (2.41) are equal to one are not used. Since for rectangular potential barrier, the wave functions have some quantities such as α ,and β.

The dispersion relation is found by solving Eq. (2.43). This generalized solution determines the band structure of the crystal.

2.4.1 Examples

In this part we will show the application of Mathematica program which is developed for the Kronig-Penney model. By assuming some odd and even functions solutions such as

$$\begin{aligned} g_1[x] &= A_1 \cos[\alpha x] & u_1[x] &= C_1 \sin[\alpha x] \\ g_2[x] &= B_1 \cos[\beta x] & u_2[x] &= D_1 \sin[\beta x] \end{aligned} \qquad (2.44)$$

Substituting these even and odd functions into the Mathematica program, Eq. (2.43) becomes to

$$A_1 B_1 C_1 D_1 e^{-i(a-b)k}$$
$$(-2\alpha\beta(-\cos[ak]\cos[bk]+\cos[a\alpha]\cos[b\beta]+\sin[ak]\sin[bj])+(\alpha^2+\beta^2)\sin[a\alpha]\sin[b\beta])=0$$

and with doing some mathematical calculations, it reduces to

$$-\frac{\alpha^2+\beta^2}{2\alpha\beta}\sin[\alpha a]\sin[\beta b]+\cos[\alpha a]\cos[\beta b]=\cos[k(a+b)] \qquad (2.45)$$

which is same with the solution of the Kronig-Penney model (eq. (2.42)).

If we assume another even and odd solutions like,

$$g_1[x]=A_1\cos[\alpha x] \qquad u_1[x]=C_1\sin[\alpha x]$$
$$g_2[x]=B_1\cosh[\beta x] \qquad u_2[x]=D_1\sinh[\beta x]$$

The equation (2.43) which gives the dispersion relations of the system becomes,

$$A_1 B_1 C_1 D_1 e^{-i(a-b)k}(2\alpha\beta(\cos[(a+b)k]-\cos[a\alpha]\cosh[b\beta])+(\alpha-\beta)(\alpha+\beta)\sin[a\alpha]\sinh[b\beta])=0$$

and by simplifying, it is reduced to

$$-\frac{\alpha^2+\beta^2}{2\alpha\beta}\sin[\alpha a]\sinh[\beta b]+\cos[\alpha a]\cosh[\beta]b=\cos[k(a+b)] \qquad (2.46)$$

From equations (2.45) and (2.46), we can see easily the coefficients of each functions can not affected the general solution, also the combinations of each functions can satisfy equation (2.43).

We can easily see that, the dispersion relations obtained by this method in Eq. (2.45) and (2.46) are same as with the dispersion relations obtained in Eq. (2.32) and Eq. (2.34) [1].

In this chapter, Kronig-Penney model is solved for periodic potentials. And the solution of the Schrödinger equation is rearranged as the summation of odd and even

functions to obtain energy band structure of electrons in the Kronig-Penney type potentials. A Mathematica code is written for this model involving odd and even solutions, and the accuracy of our calculations are checked. The dispersion relations obtained are compared with those exist in the literature and satisfactory agreements are observed.

CHAPTER 3

A MODEL TO INVESTIGATE THE BAND STRUCTURE OF A GENERALIZED CONTACT INTERACTION

In the previous chapter, we have explained the Kronig-Penney model in detail for periodic potentials in detail. Now, we extend the standard Kronig-Penney model with periodic δ potentials to the cases with generalized contact interactions under the assumption that the system has time-reversal symmetry. And by applying Bloch theorem, the eigenvalue equation which determines the dispersion relation for one-dimensional periodic array of the generalized contact interactions is deduced within the framework of the transfer matrix formalism.

The contact interaction occupies a special position in both mathematical and practical quantum mechanics. The system with contact interaction is not only rigorously solvable in most cases, but also gives useful information of the effect small obstacle on particle motion. The first influential work on contact interactions was done by Kronig and Penney [1]. The model, which has potential consisting of periodic array of δ functions, has been widely regarded as a standard reference model in the solid-state physics for more than half a century.

In spite of the seeming simplicity of contact interactions, there are several non-trival aspects which are largely left unexplored. Even in the simplest setting of one dimension, there has been historically longstanding problem of realizing the generalized contact interaction in the small-size limit of a local self-adjoint interaction. In one dimension, there are a four-parameter family of generalized

contact interactions which conserve the current at both sides of interaction [21]. This corresponds to the fact that one-dimensional kinetic energy operator $T = -\frac{d^2}{dx^2}$. In non-relativistic formalism, the current operator is given by

$$j(x) = \Psi^{\dagger}(x)\,\Psi(x).$$

Since we are dealing with contact interaction, in this case the current operator may be defined as,

$$j(x) = \Psi^{\dagger}(x)\,\sigma_2\,\Psi(x), \tag{3.1}$$

where the matrix σ_2 is the second component of Pauli matrices;

$$\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{3.2}$$

In Eq. (3.1), it is convenient to introduce Ψ in terms of the wave function ψ and its space derivative which gives the solution of the Schrödinger equation as

$$\Psi(x) = \begin{pmatrix} \psi(x) \\ \frac{1}{2m}\psi'(x) \end{pmatrix} \tag{3.3}$$

In Eq.(3.3), m is the mass of a particle. If we put a contact interaction at $x = 0$, the connection of Ψ between both sides of the origin can be characterized by

$$\Psi(+0) = \upsilon\Psi(-0) \tag{3.4}$$

If we substitute Eq. (3.3) into (3.4), we obtain

$$\begin{pmatrix} \psi(0_+) \\ \frac{1}{2m}\psi'(0_+) \end{pmatrix} = \upsilon \begin{pmatrix} \psi(0_-) \\ \frac{1}{2m}\psi'(0_-) \end{pmatrix}$$

where the current conservation $j(+0)=j(-0)$ requires

$$\upsilon^{\dagger}\sigma_2\upsilon=\sigma_2 \tag{3.5}$$

The generic solution of Eq.(3.5) is given by

$$\upsilon=e^{i\theta}\begin{pmatrix}\gamma & \delta\\ \beta & \alpha\end{pmatrix} \tag{3.6}$$

where $\theta\in R$ and $\alpha\gamma-\beta\delta=1$. The condition (3.6) covers a four-parameter family. The case $\gamma-1=\alpha-1=\delta=0$, and $e^{i\theta}=0$ and gives the usual function δ potential of strength β as,

$$\upsilon_{\delta}(\nu)=\begin{pmatrix}1 & 0\\ \nu & 1\end{pmatrix}, \tag{3.7}$$

corresponds to the δ potential of strength ν.

This family includes so-called ε potential (also known by a misnomer, δ' potential.). The case $\gamma-1=\alpha-1=\beta=0$, and $e^{i\theta}=0$ and gives the usual function ε potential of strength δ. The ε potential induces such a boundary condition that the wave function has continuous first derivative on the right and left, but it has a jump proportional to the first derivative ;

$$\upsilon_{\varepsilon}(u)=\begin{pmatrix}1 & u\\ 0 & 1\end{pmatrix}, \tag{3.8}$$

corresponds to the ε potential of strength u.

Keeping in mind the establishment of realistic approximation for generic contact interactions as well as the recent amazing progress of mesoscopic technology, it is quite interesting to examine the nature of "exotic solid" which has a periodic array of generalized contact interactions. For this purpose, we generalize the

Kronig-Penney model to the cases of generalized interactions [20]. We assume that the system has time-reversal symmetry. In this case, we have $\theta = 0$ in Eq. (3.6), hence

$$\upsilon = \begin{pmatrix} \gamma & \delta \\ \beta & \alpha \end{pmatrix} \in SL(2,R). \tag{3.9}$$

Now, we will formulate the generalized Kronig-Penney model with generic contact interactions.

3.1 Formalism of Generalized Contact Interaction

We consider a one-dimensional periodic array of a generalized contact interaction, the connection condition of which is described by υ in eq. (3.9). We assume that the interactions are located at $x = na$, $(n = 0,\pm1,\pm2,.....)$ [20]. Here we denote the lattice interval by a. The assumed potential is shown in Figure 3.1.

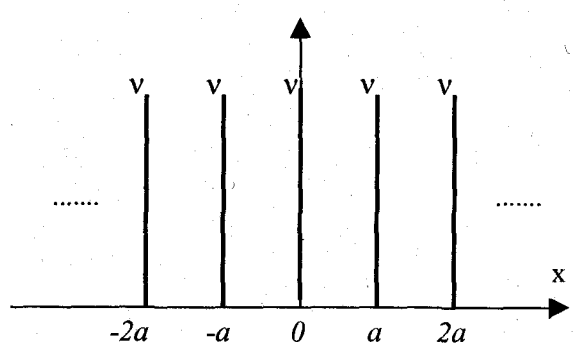

Figure 3.1: Periodic potential of Kronig-Penney model with generalized contact interaction. The two-by-two matrix $\upsilon \in SL(2,R)$ represents the connection condition at each interaction in the transfer formalism.

Schrödinger equation is given by

$$-\frac{1}{2m}\psi''(x) = E\psi(x) \tag{3.10}$$

with the boundary condition

$$\Psi(na+0) = \upsilon\Psi(na-0) \tag{3.11}$$

at $x = na$. In the transfer matrix formalism, Eq. (3.10) is written as the first-order coupled equation;

$$\Psi'(x) = H\Psi(x), \qquad (x \neq na) \tag{3.12}$$

where we define

$$H = \begin{pmatrix} 0 & 2m \\ -\dfrac{k_0^2}{2m} & 0 \end{pmatrix} \tag{3.13}$$

with $k_0 = \sqrt{2mE}$. The solution of Eq. (3.12) is written in terms of Green function

$$\Psi(x) = G(x - x_0)\Psi(x) \tag{3.14}$$

by using the exponential function of Hx which is the solution of Eq. (3.12) and with expanding the exponential function we can obtain ;

$$G(x) \equiv e^{Hx} = \cos(k_0 x)I_2 + \frac{\sin(k_0 x)}{k_0} H \tag{3.15}$$

Here we assume $na \notin [x_0, x]$ in Eq. (3.14). In Eq. (3.15), I_2 is the two-by-two identity matrix. Note that $\det G(x) = 1$ because of $TrH = 0$.

Now we can set the solution of the Schrödinger equation by using Bloch theorem to find the dispersion relation of the generalized contact interaction as;

$$\psi(x) = e^{ikx}u(x), \qquad (k \in R) \tag{3.16}$$

where the function u(x) has a period a;

$$u(x+a) = u(x). \tag{3.17}$$

Since

$$\psi'(x) = e^{ikx}\left(u'(x) + iku(x)\right) \tag{3.18}$$

$$\psi''(x) = e^{ikx}\left(u''(x) + 2iku'(x) - k^2u(x)\right) \tag{3.19}$$

we obtain the equation for u;

$$-u''(x) - 2iku'(x) + k^2u(x) = k_0^2u(x) \tag{3.20}$$

$\left(x \neq na\right)$. In the vector notation

$$\overline{\Psi}(x) = \begin{pmatrix} u(x) \\ \frac{1}{2m}u'(x) \end{pmatrix} \tag{3.21}$$

we rewrite Eq. (3.20) in matrix form as

$$\overline{\Psi}'(x) = \overline{H}\,\Psi(x), \qquad \left(x \neq na\right) \tag{3.22}$$

with

$$\overline{H} = \begin{pmatrix} 0 & 2m \\ \frac{k^2 - k_0^2}{2m} & -2ik \end{pmatrix} \tag{3.23}$$

It is clear from Eqns. (3.16) and (3.18) that two vectors $\Psi(x)$ and $\overline{\Psi}(x)$ are related by

$$\Psi(x) = M\,\overline{\Psi}(x) \tag{3.24}$$

with

$$M = e^{ikx}\begin{pmatrix} 1 & 0 \\ \dfrac{ik}{2m} & 1 \end{pmatrix} \tag{3.25}$$

The solution of Eq. (3.22) is given by

$$\overline{\Psi}(x) = \overline{G}(x - x_0)\overline{\Psi}(x_0) \tag{3.26}$$

where $\overline{G}(x)$ is the exponential function of $\overline{H}x$;

$$\begin{aligned} \overline{G}(x) &= e^{\overline{H}x} \\ &= e^{-ikx}\left(\cos(k_0 x) I_2 + \frac{\sin(k_0 x)}{k_0}\begin{pmatrix} ik & 2m \\ \dfrac{k^2 - k_0^2}{2m} & -ik \end{pmatrix}\right) \end{aligned} \tag{3.27}$$

Here we assume that $na \notin [x_0, x]$. Since $Tr\overline{H} = -2ik$, we have get $\det \overline{G}(x) = e^{(Tr\overline{H})x} = e^{-2ikx}$. It is realized from Eqs. (3.11) and (3.24) that the connection condition for $\overline{\Psi}$ at $x = na$ is given by

$$\overline{\Psi}(na + 0) = \overline{\upsilon}\overline{\Psi}(na - 0) \tag{3.28}$$

with

$$\begin{aligned} \overline{\upsilon} &= M^{-1}\upsilon M \\ &= \begin{pmatrix} 1 & 0 \\ -\dfrac{ik}{2m} & 1 \end{pmatrix}\upsilon\begin{pmatrix} 1 & 0 \\ \dfrac{ik}{2m} & 1 \end{pmatrix} \end{aligned} \tag{3.29}$$

Note that $\det\bar{\upsilon} = \det\upsilon = 1$. The periodicity for u in Eq. (3.17) is equivalent to

$$\bar{\Psi}(x+a) = \bar{\Psi}(x) \tag{3.30}$$

In particular, with $x = na - 0$, we have

$$\bar{G}(a)\bar{\upsilon}\bar{\Psi}(na-0) = \bar{\Psi}(na-0) \tag{3.31}$$

Since

$$\begin{aligned}\bar{\Psi}((n+1)a-0) &= \bar{G}(0)\bar{\Psi}((na+0) \\ &= \bar{G}(a)\bar{\upsilon}\bar{\Psi}(na-0)\end{aligned} \tag{3.32}$$

Eq. (3.31) requires the two-by-two matrix $\bar{G}(a)\bar{\upsilon}$ has eigenvalue 1:

$$\det\left(I_2 - \bar{G}(a)\bar{\upsilon}\right) = 0 \tag{3.33}$$

Since $\det\left(\bar{G}(a)\bar{\upsilon}\right) = \det\bar{G}(a) = e^{-2ika}$, the other eigenvalue of the matrix $\bar{G}(a)\bar{\upsilon}$ should be e^{-2ika}. This indicates

$$Tr\left(\bar{G}(a)\bar{\upsilon}\right) = 1 + e^{-2ika} \tag{3.34}$$

A simple matrix calculation shows

$$M\bar{H}M^{-1} = -ikI_2 + H \tag{3.35}$$

which gives relation between $\bar{G}(x)$ and $G(x)$;

$$M\bar{G}(x)M^{-1} = e^{M\bar{H}M^{-1}x} = e^{-ikx}G(x) \tag{3.36}$$

From Eq. (3.36), we obtain

$$\overline{G}(a)\overline{\upsilon} = e^{-ka}M^{-1}G(x)\upsilon M \tag{3.37}$$

Thus we conclude that the condition (3.34) is equivalent to

$$Tr\left(G(a)\upsilon\right) = 2\cos(ka) \tag{3.38}$$

Eq. (3.38) determines the dispersion relation for a periodic array of the generalized contact interaction characterized by the connection condition (3.9). Inserting Eqs. (3.9) and (3.15) into Eq. (3.38), we obtain the eigenvalue equation

$$(\alpha+\gamma)\cos(k_0a)+\sin(k_0a)\left(\frac{2m}{k_0}\beta-\frac{k_0}{2m}\delta\right)=2\cos(ka) \tag{3.39}$$

Lets take the mass of particle $m=1/2$ and the lattice interval $a=1$ for periodic δ potentials. From Eq. (3.39) together Eq. (3.7), we obtain the eigenvalue equation for δ array;

$$\cos(k_0)+\frac{\nu\sin(k_0a)}{2k_0}=\cos(k) \tag{3.40}$$

where ν is the strength of each δ. Eq. (3.40) is the well known result in the standard Kronig-Penney model. Similarly for ε potential of strength u, we obtain

$$\cos(k_0)-\frac{uk_0\sin(k_0a)}{2}=\cos(k) \tag{3.41}$$

And these equations (3.40) and (3.41) are the eigenvalue equations for δ periodic potential and ε periodic potential respectively.

In this chapter, we have formulated the generalized Kronig-Penney model which has a periodic array of generalized interactions in one dimension. The transfer matrix formalism serves to deduce the eigenvalue equation which determines the dispersion relation.

CHAPTER 4

QUASI-EXACTLY SOLVABLE PERIODIC POTENTIALS

The whole family of the exactly solvable potentials are investigated in two classes depending on whether the Schrödinger equation can be reduced to hypergeometric or a confluent hypergeometric equation. Those that lead to a hypergeometric equation (confluent hypergeometric equation) will be called type-I (type-II) potentials [26]. For these class 1 potentials, the eigenfunctions correspond to confluent hypergeometric functions which can be written as Laguerre polynomials. Furthermore, using canonical transformations [27], potentials such as the Rosen-Morse (hyperbolic and trigonometric), Eckart, Pösch-Teller (I and II) etc. can be mapped into the generalized Scarf Potentials [28], and they form a second class. For these class II potentials, the eigenfunctions which can be written as associated Legendre functions.

Type-I potentials can be mapped onto (in case of some limits and redefining parameters) generalized Pösch-Teller, Scarf (hyperbolic and trigonometric), Eckart and Rosen-Morse I potentials. These potentials can be transformed to periodic potentials. However, type II potentials ,Harmonic oscillator, Morse potential, and coulomb potentials, can not be transformed to periodic type. All of these potentials are called exactly solvable shape invariant potentials.

The potential in physics can be classified as type-I, type-II and the classes contain Jacobi elliptic functions. And another classification is exactly-solvable potentials and quasi-exactly solvable potentials corresponding to the some canonical forms.

4.1. Quasi-Exact Solvability Case

A differential operator is said to be *Lie algebraic* if it lies in the universal enveloping algebra U(g) of the Lie algebra *g*, meaning that it can be expressed as a polynomial in the operators J^a. In particular, a second differential operator is Lie algebraic if it can be written as a quadratic combination [9]

$$-H = \sum_{a,b} c_{ab} J^a J^b + \sum_a c_a J^a + c_0 \tag{4.1}$$

for certain constants c_{ab}, c_a, c_0. (The minus sign in front of the Hamiltonian is taken for later convenience).

Consider the Lie algebra g_n spanned by the differential operators

$$J^- = J_n^- = \frac{d}{dz}, J^0 = J_n^0 = z\frac{d}{dz} - \frac{n}{2}, \; J^+ = J_n^+ = z^2\frac{d}{dz} - nz, \tag{4.2}$$

which satisfy the standard *sl*(2) commutation relations. Here n is a nonnegative integer. In this section, we shall use z instead of x for the "canonical coordinate", retaining x for the physical coordinate in which the operator takes Schrödinger form. The Lie algebra $\hat{g}_n$ is merely a central extension (by the constant functions) of the subalgebra g_n, hence $\hat{g}_n$ is isomorphic to the Lie algebra gl(2) of 2 x 2 matrices. Note that since $\hat{g}_n$ and g_n only differ by inclusion of constant functions, in our analysis of Lie algebraic differential operators we can, without loss of generality, concentrate on the Lie algebra g_n, since any Lie algebraic operator (4.1) for the full algebra is automatically a Lie algebraic operator for the subalgebra g_n.

The second order differential equations play exceptionally important role in applications. Thus, the most general second order quasi-exactly solvable Hamiltonian in one space dimension can therefore be written in the form

$$-H = c_{++}(J^+)^2 + c_{+0}[J^+J^0 + J^0J^+] + c_{00}(J^0)^2 + c_{+-}[J^+J^- + J^-J^+] + c_{0-}[J^0J^- + J^-J^0] + c_{--}(J^-)^2 + c_+J^+ + c_0J^0 + c_-J^- + c_* \tag{4.3}$$

Under the conditions $c_{++} = c_{+0} = c_+ = 0$, the operator H becomes exactly-solvable [22] . Substituting the explicit formulas (4.2) for J^+, J^-, J^0 into (4.3), we find that every quasi-exactly solvable operator can be written in the canonical form

$$-H = P(z)\frac{d^2}{dz^2} + \left\{Q(z) - \frac{n-1}{2}P'(z)\right\}\frac{d}{dz} + \left\{R - \frac{n}{2}Q'(z) + \frac{n(n-1)}{12}P''(z)\right\}, \tag{4.4}$$

where

$$P(z) = c_{++}z^4 + 2c_{+0}z^3 + (2c_{+-} + c_{00})z^2 + 2c_{0-}z + c_{--},$$

$$Q(z) = c_+z^2 + c_0z + 2c_-, \tag{4.5}$$

$$R(z) = \frac{n^2+2n}{12}c_{00} - \frac{n^2+2n}{3}c_{+-} + c_*,$$

are (general) polynomials of respective degrees 4,2,0. Since the modulus N is the space $P^{(n)}$ of polynomials of degree at most n, the algebraic eigenfunctions (4.3) will, in the z-coordinates, just be polynomials $\chi_k(z) \in P^{(n)}$. In terms of the standard basis $\chi_k(z) = z^k$, $k = 0,..,n$, the restricted Hamiltonian $H \mid P^{(n)}$ takes the form of a pentadiagonal matrix, or, if $c_{++} = c_{--} = 0$, a tridiagonal matrix. Thus, for a normalizable one-dimensional quasi-exactly solvable operator, there are n+1 algebraic eigenfunctions which, in the canonical z coordinates, are polynomials degree at most n.

Specializing the solution to the equivalence problem given by theorem 3 in [9] to the particular operator (4.4), we find that the change of variables required to place the operator into physical (Schrödinger) form will, in general, be given by an elliptic integral

$$x = \varphi(z) = \int^{z} \frac{dy}{\sqrt{P(y)}} \tag{4.6}$$

The corresponding gauge factor is

$$\mu(z) = |P(z)|^{-n/4} \exp\left\{ \int^{z} \frac{Q(y)}{2P(y)} dy \right\}. \tag{4.7}$$

The potential is given by

$$V(x) = -\frac{n(n+2)(PP''-\frac{3}{4}P'^2) + 3(n+1)(QP'-2PQ') - 3Q^2}{12P} - R \tag{4.8}$$

where the right hand side is evaluated at $z = \varphi^{-1}(x)$. In the physical coordinate, the associated algebraic wave functions will then take the form

$$\psi(x) = \mu(\varphi^{-1}(x))\chi(\varphi^{-1}(x)), \tag{4.9}$$

where $\chi(z)$ is a polynomial of degree at most n.

The canonical form (4.4) of a quasi–exactly solvable differential operator is not unique, since there is a "residual" symmetry group which preserves the Lie algebra g_n. Not surprisingly, this group is GL(2,ℝ), which acts on the (projective) line by linear fractional (Möbius) transformations

$$z \to \omega = \frac{\alpha z + \beta}{\gamma z + \delta}, \qquad A = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}, \qquad \det A = \Delta = \alpha\delta - \beta\lambda \neq 0 \tag{4.10}$$

To describe the induced action of transformations (4.10) on the quasi-exactly solvable operators (4.4), we first recall the basic construction of the finite-dimensional irreducible rational representations of the general linear group GL(2,ℝ).

4.1.1 Definition of the Irreducible Multiplier Representation on the Space Polynomials

Let $n \geq 0$, i be integers. The irreducible multiplier representation $\rho_{n,i}$ of GL(2,ℝ) is defined on the space $P^{(n)}$ of polynomials of degree at most n by the transformation rule $\hat{P} = \rho_{n,i}(P)$, where

$$\hat{P}(z) = (\gamma z + \delta)^n (\alpha\delta - \beta\gamma)^i P(\frac{\alpha z + \beta}{\gamma z + \delta}), \qquad P \in P^{(n)}. \tag{4.11}$$

The multiplier representation $\rho_{n,i}$ has infinitesimal generators given by the differential operators ,which are equivalent if they can be mapped into each other by a combination of change of independent variable $\bar{x} = \varphi(x)$ and gauge transformation $\overline{H} = e^{\sigma(x)}.H.e^{-\sigma(x)}$, combined with the operator of multiplication by i representing the diagonal subalgebra (center) of $\mathfrak{gl}(2,\mathbb{R})$. The action (4.10) induces an automorphism of the Lie algebra g_n, which is isomorphic to the representation $\rho_{2,-1}$, and, consequently, preserves the class of quasi-exactly solvable operators associated with the algebra g_n.Moreover, the corresponding gauge action

$$\hat{H}(z) = (\gamma z + \delta)^n \cdot H \cdot (\gamma z + \delta)^{-n} \tag{4.12}$$

will preserve the space of quasi-exactly solvable Hamiltonians (4.4). Identifying the operator H with the corresponding quartic, quadratic and constant polynomials (4.5), we find that the action (4.12) of GL(2,ℝ) on the space of quasi-exactly solvable operators is isomorphic to the sum of three irreducible representation,

$\rho_{4,-2} \oplus \rho_{2,-1} \oplus \rho_{0,0}$; the quartic *P(z)* transforms according to $\rho_{4,-2}$, the quadratic *Q(z)* according to $\rho_{2,-1}$, while *R* is constant. Finally, the associated module, which is just the space of polynomials $P^{(n)}$, transforms according to the representation $\rho_{n,0}$.

Using the action of GL(2,ℝ), we can place the gauged operator (4.4) into a simpler canonical form, based on the invariant theoretic classification of canonical forms for real quartic polynomials.

4.1.2 Canonical Forms of Space Polynomials

Under the representation $\rho_{4,-2}$ of GL(2,ℝ), every nonzero real quartic polynomial *P(z)* is equivalent to one of the following canonical forms:

$$\nu(1-z^2)(1-k^2z^2), \quad \nu(1-z^2)(1-k^2+k^2z^2), \quad \nu(1+z^2)(1+k^2z^2)$$
$$\nu(z^2-1) \quad ,\nu(z^2+1), \quad \nu z^2, \quad \nu(z^2+1)^2, z, \ 1,$$

where ν and $0< k <1$ are real constants.

The nine cases corresponds to the positions of the complex roots of the quartic, which are, respectively , four simple real roots, two simple roots and two simple complex conjugate roots, four simple complex roots, one double and two simple real roots, one double real and two simple complex roots, two double real roots, two double complex roots, one triple and one simple real roots, and one quadruple real root. Note that we are allowing ∞ to be root, whose order is defined to be 4-*d* where *d* is degree of the polynomial. (This makes the concept of order of a root of a quartic polynomial invariant under the representation $\rho_{4,-2}$).

If *P* has four simple roots, then the Schrödinger equation $H\psi = \lambda\psi$ for the operator (4.4), (4.5), has four regular singularities, and hence, by a *complex* linear fractional transformation, can be mapped to a form of Heun's equation

$$\frac{d^2y}{dz^2}+\left(\frac{\gamma}{z}+\frac{\varepsilon}{z-1}+\frac{\delta}{z-a}\right)\frac{dy}{dz}+\frac{\alpha\beta z+b}{z(z-1)(z-a)}y=0 \qquad (4.13)$$

with $\alpha+\beta-\gamma-\delta-\varepsilon+1=0$, which amounts to placing P into the complex canonical form $P(z)=\nu z(z-1)(z-a)$ with the roots at 0,1,a and ∞. Therefore, the algebraic eigenfunctions can be expressed in terms of Heun polynomials, or, in the case of multiple roots, confluent Heun polynomials.

The solution to the normalizability problem begins with detailed analysis of the elliptic integral (4.6). Consider an interval $z_0<z<z_1$ where $P(z)>0$ is positive and vanishes at the endpoints, $P(z_0)=P(z_1)=0$. Simple asymptotic analysis of (4.6) immediately implies that if both z_0 and z_1 are simple roots, then this equation

$$\bar{x}=\varphi(z)=\int^{x}\frac{dy}{\sqrt{P(y)}}$$

defines z as a periodic function of x; therefore the potential $V(x)$ and the corresponding algebraic eigenfunctions are periodic functions of x, and can not be normalizable. (However, if they have no singularities, they do contribute, albeit minutely, to the continuous spectrum of the operator.). If $P(z)>0$ is everywhere positive and has no real roots including ∞, then the same conclusion of periodicity holds. Therefore, a necessary condition for the quasi- exactly solvable operator (4.4), (4.5), to be normalizable is that the quartic polynomial $P(z)$ have at least one multiple real root, which must lie at the end of an interval of possibility. Thus, the class of quasi-exactly solvable potentials naturally splits into two subclasses-the periodic potentials, which are never normalizable, and the non-periodic potentials, which are sometimes normalizable.

Tedious but direct calculations based on (4.6),(4.7),(4.9), produce the explicit change of variables, the potential, and eigenfunctions for the above normal forms in physical coordinates. Each of classes of potentials is a linear combination of four

elementary and/or elliptic functions, plus a constant which we absorb into the eigenvalue. The potentials naturally divide into two classes, which are listed in the following Tables. In each case, the four coefficients are not arbitrary, but satisfy a single complicated algebraic equation and one or more inequalities.

First, the periodic quasi-exactly solvable potentials correspond to the cases when the roots of P are simple, of which are five cases given in the following Table.

Table 4.1 The periodic quasi-exactly solvable potential cases.

1.	$\nu(1-z^2)$
2.	$\nu(z^2+1)^2$
3.	$\nu(1-z^2)(1-k^2z^2)$
4.	$\nu(1-z^2)(1-k^2+k^2z^2)$
5.	$\nu(1+z^2)(1+(1+k^2)z^2)$

where $\nu>0$, $0<k<1$. The explicit formulas for the corresponding potentials follows. In the first three cases, the corresponding potentials are written in terms of the standard Jacobi elliptic functions of modulus k. Also, as remarked above, the coefficients A,B,C,D are not arbitrary, although the explicit constraints are too complicated to write here.

4.2 Periodic Quasi-Exactly Solvable Potentials

The periodic quasi-exactly solvable potentials can be tabulated as in Table 4.2 below.

Table 4.2. Periodic QES Potentials

1.	$A\sin^2\sqrt{\nu}x + B\sin\sqrt{\nu}x + C\tan\sqrt{\nu}x\sec\sqrt{\nu}x + D\sec^2\sqrt{\nu}x$
2.	$A\cos 4\sqrt{\nu}x + B\cos 2\sqrt{\nu}x + C\sin 2\sqrt{\nu}x + D\sec 4\sqrt{\nu}x$
3.	$dn^{-2}\sqrt{\nu}x(Asn\sqrt{\nu}x + B) + cn^{-2}\sqrt{\nu}x(Csn\sqrt{\nu}x + D)$
4.	$dn^{-2}\sqrt{\nu}x(Acn\sqrt{\nu}x + B) + sn^{-2}\sqrt{\nu}x(Ccn\sqrt{\nu}x + D)$
5.	$Acn\sqrt{\nu}xsn\sqrt{\nu}x + Bcn^2\sqrt{\nu}x + Cdn^{-2}\sqrt{\nu}x\left(cn\sqrt{\nu}xsn\sqrt{\nu}x + Dcn^2\sqrt{\nu}x\right)$

The elliptic functions sn y, cn y, dn y are periodic of period $4K$ (or $2K$ in the case of dn y),where

$$K = \int_0^1 \frac{dz}{\sqrt{(1-z^2)(1-k^2z^2)}},$$

is the complete elliptic integral of modulus k. Moreover, dn y is never zero, cn y vanishes at odd multiplies of K, and sn y vanishes at even multiples of K; also $cn4mK = 1 = sn(4m+1)K$, $cn(4m+2)K = -1 = sn(4m+3)K$. Therefore, the potentials in cases 1,2, and 4 have singularities unless $C = D = 0$. In cases 3 and 5, the potential has no singularities, reflecting the fact that in these cases $P(z)$ has no real roots. Case 3 includes the Lamé equation.

Lamé's potentials is the well studied class of periodic potentials [6] in physics with $V(x) = pmsn^2(x,m)$, $p \equiv a(a+1)$. Here $sn(x,m)$ is a Jacobi elliptic function of real elliptic modulus parameter m with period $4K(m)$. This elliptic function potentials have a period $L = 2K(m)$, and will be referred to as Lamé potentials, since

the corresponding Schrödinger equation is called Lamé's equation. Another much richer class of periodic potentials is given by

$$V(x) = pmsn^2(x) + qm\frac{cn^2(x)}{dn^2(x)}, \qquad p \equiv a(a+1), \quad q \equiv b(b+1),$$

where, like $sn(x)$, the Jacobi elliptic functions $cn(x)$ and $dn(x)$ also have modulus parameter m which, for notational convenience, is not explicitly displayed. These potentials are called associated Lamé potentials, since the corresponding Schrödinger equation is associated called Lamé's equation. Associated Lamé potentials are quasi exactly solvable potentials [6] in contrast to Lamé potentials.

The rest of the canonical forms in the theorem [9] corresponds the non-periodic potentials cases.

In this chapter, the quasi-exactly solvable Hamiltonian is expressed in algebraic framework. This form can be reduced to the exactly-solvable Hamiltonian with choosing appropriate parameters. And the periodic quasi-exactly solvable potentials are constructed by using canonical transformations.

CHAPTER 5

ALGEBRAIC DESCRIPTION OF ONE-DIMENSIONAL POTENTIALS

Exactly solvable quantum mechanical potentials have attracted much attention since early days of quantum mechanics, and the Schrödinger equation has been solved for a large number of potentials by employing a variety of approaches. The fundamental problem of quantum physics is to investigate the Schrödinger equation

$$H\psi_i = E\psi_i$$

where H is a linear Hermitian operator suited to the problem at hand and ψ and E are its eigenfunctions and eigenvalue respectively. The operator H may correspond to any physical observable such as position, momentum, angular momentum (spin or orbital), energy and so on. In general, there are several solutions which satisfy the equation $H\psi_i = E\psi_i$ and which may be denoted by ψ_i (i=1,2,3,.....) with the corresponding eigenvalues E_i. The number of eigenfunctions H in most quantum mechanical problem is in fact infinite. In general, it is very difficult to find the exact eigenfunctions and eigenvalues of an operator, except in some very simple exactly solvable cases. However, the problem can be considerably simplified by using algebraic method.

In our study, we try to find the solutions of the several different Schrödinger equation by using the methods of Lie algebra and by showing how the use of Lie Algebra help in simplifying the eigenvalue problem.

In recent times Lie algebraic techniques have been used to construct complex quasi exactly potentials with real spectrum. The problem of interest can usually be approached in this manner when the Hamiltonian can be expressed in terms of generators of algebra. As a consequence, the solution of Schrödinger equation then becomes an algebraic problem, which can be solved using the tools of Lie algebra. At this point note that, the choice of differential realization of generators becomes important. Because Hamiltonian will take different forms in different realization of generators. On the other word, the solution of Schrödinger equation is greatly simplified if appropriate realization is constructed to express the Hamiltonian as a linear function of generators. To do this we used SU(1,1) group which is most elementary non-compact non-abelian Lie group. It has several series of unitary irreducible representation; discrete, continuous, and supplementary. The Lie algebra corresponding to the *su*(1,1) which has three generators J_+, J_-, J_0 and with the following commutations relations between them,

$$[J_0, J_\pm] = \pm J_\pm$$
$$[J_+, J_-] = -2J_0$$

In the following we introduce this operator for some potentials like rectangular-well potential and trigonometric-like potential.

5.1 Rectangular-Well Potential with Boundary Conditions

We consider the problem of a particle in one-dimensional rectangular-well potential $V(r) = -V_0$ if $r \in [0, a]$ where V_0 is the potential depth and a its radius. The eigenfunctions and the spectrum of Hamiltonian $H_0 = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} - V_0$ with the *R*-matrix boundary conditions [8] such as

$$\Phi(r=0)=0$$
$$\frac{d\Phi}{dr}(r=a)=0 \tag{5.1}$$

are well known. The solution of H_0 given by

$$|\mu\rangle = \Phi_\mu(r) = \sqrt{\frac{2}{a}}\sin\left(\left(\mu+\frac{1}{4}\right)2\pi\frac{r}{a}\right) \tag{5.2}$$

It is obvious that $|\mu\rangle$ is a normalizable function. The eigenvalues of H_0 can be obtained by substituting (5.2) into H_0, yields

$$E_\mu = \frac{h^2}{2m}\left(\frac{2\pi}{a}\right)^2\left(\mu+\frac{1}{4}\right)^2 - V_0 \tag{5.3}$$

where $\mu \in Z$. We would like to note that the second relation in equation (5.1) implies that $\Phi'(a)/\Phi(a) =$ constant or zero, used in the usual R- matrix approaches[23]. When this constant is very small or 0 (in this case, it is zero), the internal eigenstates can be interpreted physically as virtual levels [24]. In fact, the nonzero value of the first derivative of the wave function at $r=0$ implies the fact that the current of probability is zero, as in the case when the function is chosen to be zero.

We will now consider the problem of the R- matrix description of the scattering problem for this potential [23]. The R- matrix is the inverse of the logarithmic derivative of the external channel wave function at the surface. In this approach, the dynamics in the internal region is taken into account through the R-matrix. The R- matrix method is based upon expanding the total wave function for any energy in the interval region in terms of the complete set of eigenfunction. For the potential scattering, the R-matrix reduces to the R-function which can be written in terms of the internal spectrum and the values of the normalized eigenfunctions at the boundary $r=a$

$$R(E) = \sum_{\mu} \frac{\gamma_\mu^2}{E_\mu - E} \tag{5.4}$$

where $\gamma_\mu = \sqrt{\hbar^2 / 2ma}\Phi_\mu(a)$ and γ_μ^2 is the reduced width of the level μ. The R-function together with the logarithmic derivative of the outgoing wave function at $r = a$ allows a complete description of the scattering.

Our aim is to give an algebraic description of the eigenvalue problem for the Hamiltonian

$$H_0 = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} - V_0 \tag{5.5}$$

with the R-matrix boundary condition (5.1).

We introduce the operator T, defined by its action; $Tf(r) = f(a-r)$. The corresponding differential realization of T is given by; $T = e^{-a\partial_r} e^{i\pi r\partial_r}$. Consequently we introduce the operators;

$$\begin{aligned}
J_0 &= \frac{a}{2\pi} T \frac{d}{dr} - \frac{1}{4} \\
J_+ &= \left(\cos\left(2\pi\frac{r}{a}\right) + \sin\left(2\pi\frac{r}{a}\right)T\right)\left(\frac{a}{2\pi}T\frac{d}{dr} - \frac{1}{4} + \frac{1}{2}\right) \\
J_- &= \left(\cos\left(2\pi\frac{r}{a}\right) - \sin\left(2\pi\frac{r}{a}\right)T\right)\left(\frac{a}{2\pi}T\frac{d}{dr} - \frac{1}{4} - \frac{1}{2}\right)
\end{aligned} \tag{5.6}$$

Taking into account the definition of the operators $J_0, J_\pm$ and the obvious relations

$$
\begin{aligned}
T\frac{d}{dr} &= -\frac{d}{dr}T \\
T\cos\left(2\pi\frac{r}{a}\right) &= \cos\left(2\pi\frac{r}{a}\right)T \\
T\sin\left(2\pi\frac{r}{a}\right) &= -\sin\left(2\pi\frac{r}{a}\right)T
\end{aligned}
\tag{5.7}
$$

we establish the following commutation relations

$$
\begin{aligned}
[J_0, J_\pm] &= \pm J_\pm \\
[J_+, J_-] &= -2J_0
\end{aligned}
\tag{5.8}
$$

Also we have Hermiticity properties

$$
J_0^t = J_0 \tag{5.9}
$$

$$
J_+^t = J_- \tag{5.10}
$$

As an example, we prove the relation (5.9). We have

$$
\begin{aligned}
(f_1,(J_0+\frac{1}{4})f_2) &= -\int_0^a f_1^* \frac{a}{2\pi}\frac{df_2(a-r)}{dr}dr \\
&= -\frac{a}{2\pi}f_1^*(r)f_2(a-r)\Big|_0^a + \int_0^a\left(\frac{a}{2\pi}\frac{df_1(r)}{dr}\right)^* f_2(a-r)dr \\
&= \int_0^a\left(\frac{a}{2\pi}\frac{df_1(a-r)}{d(a-r)}\right)^* f_2(r)dr \\
&= ((J_0+\frac{1}{4})f_1, f_2)
\end{aligned}
$$

where we have used the condition $f_{1,2}(r=0)=0$. Relations (5.9) and (5.10) are now obvious. Therefore, the operators $J_0, J_\pm$ are closed under commutation relations (5.8) and express a realization of the Lie algebra $su(1,1)$. It is a straightforward

exercise to prove that the action of operators (5.6) on the eigenfunctions (5.2) can be written

$$J_0|\mu\rangle = \mu|\mu\rangle \qquad (5.11)$$
$$J_\pm|\mu\rangle = (\mu \pm \frac{1}{2})|\mu \pm 1\rangle$$

The *su*(1,1) Casimir operator is

$$C = J_0^2 - J_0 - J_+ J_-,$$

for any irreducible representation is the identity operator times a number

$$J^2 = j(j-1)$$

Thus a representation of the *su*(1,1) is determined by a single number j; for the discrete series this number acquires discrete values j=1/2,1,3/2,2,.....[The corresponding representations of the so-called universal covering group *su*(1,1) are also given by a single number j, but there is goes continuously from zero to infinity.]

Casimir operator which commutes with all the generators of a Lie group. According to a theorem due to Racah, the number of independent Casimir operators of a Lie group is equal its rank which is maximum number of mutually commuting generators of a Lie group. It was recognized by Casimir himself that one such operator could always be constructed by taking suitable bilinear combination of the generators. Since the Casimir operators of a Lie group can be diagonalized simultaneously with its generators, the eigenvalues of the Casimir operators may be used to label the irreducible representations of the Lie group.

By Casimir operator we have

$$C|\mu\rangle = -\frac{1}{4}|\mu\rangle \qquad (5.12)$$

Relations (5.11) and (5.12) mean that the internal eigenstates $|\mu\rangle$ can be taken as the standard basis of the irreducible representation of $su(1,1)$ with $j=-\frac{1}{2}$ or $j(j+1)=-\frac{1}{4}$ and $\mu \in Z$. In fact the relations (5.11) are the $j=-\frac{1}{2}$ case of the generator action on the standard basis.

Now, we can write the Hamiltonian (5.5) in the above algebraic framework as

$$H_0=\frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2\left(J_0+\frac{1}{4}\right)^2-V_0 \tag{5.13}$$

Thus, $su(1,1)$ Lie algebra is the dynamical algebra for the internal motion. The appropriate realization is given in terms of a single variable and it is a differential realization,
i.e.

$$T=\sum_0^{\infty}\frac{(a-2r)^n}{n!}\frac{d^n}{dr^n}$$

is an infinite-order differential operator.

The next step is to obtain a purely algebraic relation for the reduced widths for the above case. Since the reduced widths are proportional to the values of the wave function at the boundary, it seems that a purely algebraic description is not possible. Therefore, by taking realization (5.6) in the account, we obtain the asymptotic connection:

$$\lim_{r\to a} J_{\pm}\psi(r)=\lim_{r\to a}(J_0\pm\frac{1}{2})\psi(r) \tag{5.14}$$

where $\psi(r)$ is an arbitrary function of class C^1. If $\psi(r)=\Phi_{\mu}(r)$ and taking into account equation (5.11), we have a simple recurrence relation:

$$(\mu \pm \frac{1}{2})\Phi_{\mu\pm1}(a) = (\mu \pm \frac{1}{2})\Phi_{\mu}(a). \tag{5.15}$$

Consequently the reduced widths do not depend an the quantum number μ as we have $\mu \in Z$. Therefore, all the γ_μ are equal, and we can choose a certain one, e.g. γ_0. Then we can algebraically obtain the *R*-function up to a multiplicative factor in the form:

$$R(E) = \sum_{\mu\in Z} \gamma_0^2 \Bigg/ \left(\frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 \left(\mu + \frac{1}{4}\right) - V_0 - E \right)$$

$$= \frac{a\gamma_0^2}{\hbar} \sqrt{\frac{m}{2(V_0+E)}} \tan\left(\frac{a}{\hbar}\sqrt{2m(V_0+E)}\right).$$

The coefficient γ_0 can be given only by the analytical expression of the state $|0\rangle$. It yields $\gamma_0^2 = \hbar^2/(ma^2)$.

5.2 Algebriazation of Trigonometric-Like Potentials

Now we try to find the *su*(1,1) algebraic description of trigonometric-like potentials. The realization (5.6) allows us to write

$$\cos\left(2\pi\frac{r}{a}\right) = (2J_0 - 1)^{-1} J_+ + (2J_0 + 1)^{-1} J_-$$

$$= J_+ (2J_0 + 1)^{-1} + J_- (2J_0 - 1)^{-1}. \tag{5.16}$$

It is important to note that expression (5.16) is not in the *su*(1,1) universal enveloping algebra, but it can be considered to be well defined on a dense subspace of the *su*(1,1) representation Hilbert space [25]. We can algebraically write

$\cos(n2\pi r/a), n \in N$, by using the expression of $\cos nx$ as an nth-order polynomial in $\cos x$. For example using the particular value of the Casimir operator, we have

$$\cos\left(4\pi\frac{r}{a}\right) = 2(2J_0 - 1)^{-1}(2J_0 - 3)^{-1}J_+^2 + 2(2J_0 + 1)^{-1}(2J_0 + 3)^{-1}J_-^2. \quad (5.17)$$

In order to write algebraically a certain potential which can be written as a Fourier series we also need an expression for $\sin(2\pi r/a)$ in terms of the operators $J_0, J_\pm$. Such an expression seems to be a very complicated one, and we succeeded in obtaining it using the explicit realization of the standard basis (5.2). One can write

$$\sin\left(2\pi\frac{r}{a}\right) = \frac{1}{\pi}\left(2J_0 + \frac{3}{2}\right)^{-1}\left(2J_0 - \frac{1}{2}\right)^{-1} + \frac{1}{\pi}\sum_{n=1}^{\infty}\left(2J_0 + \frac{3}{2} - n\right)^{-1}\left(2J_0 - \frac{1}{2} - n\right)^{-1}$$

$$\times\left[\left(J_0 - \frac{1}{2}\right)^{-1}J_+\right]^n + \frac{1}{\pi}\sum_{n=1}^{\infty}\left(2J_0 + \frac{3}{2} + n\right)^{-1}\left(2J_0 - \frac{1}{2} + n\right)^{-1} \quad (5.18)$$

$$\times\left[\left(J_0 + \frac{1}{2}\right)^{-1}J_-\right].$$

Therefore in principle, every potential developed in a Fourier series can be written in algebraic form. As an example we shall study the Hamiltonian

$$H = H_0 + 2\alpha\cos\left(2\pi\frac{r}{a}\right)$$

$$= -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} - V_0 + 2\alpha\cos\left(2\pi\frac{r}{a}\right)$$

$$= -\frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2(J_0 + \frac{1}{4})^2 - V_0 + 2\alpha\left\{(2J_0 - 1)^{-1}J_+ + (2J_0 + 1)^{-1}J_-\right\} \quad (5.19)$$

where α is a coupling parameter. We would like to obtain the eigenstates of the algebraic Hamiltonian (5.19) in terms of the H_0 eigenstates, i.e. in terms of the *su*(1,1) standard basis (5.11).

We suppose that the eigenstate $|E\rangle$ of H has the eigenvalue of energy E, $H|E\rangle = E|E\rangle$. We can write

$$|E\rangle = \sum_{\mu} C_{\mu}^{E} |\mu\rangle \tag{5.20}$$

We admit that the action of H on the above sum commutes with the sum. When $\alpha = 0$, this assumption gives

$$\left(E - \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 \left(\mu + \frac{1}{4}\right)^2 + V_0 \right) C_{\mu}^{E} = 0$$

for every integer μ, and one obtains that the energy E must be E_{μ}. Therefore, we have reobtained the H_0 spectrum and eigenstates.

In the above assumption concerning the Hamiltonians (5.19) we obtain the following recursion relation

$$\alpha C_{\mu-1}^{E} + \left(\frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 \left(\mu + \frac{1}{4}\right)^2 - (E + V_0) \right) C_{\mu}^{E} + \alpha C_{\mu+1}^{E} = 0 \quad \mu \in Z. \tag{5.21}$$

By writing $C_{\mu+1}^{E} = \xi_{\mu}^{E} C_{\mu}^{E}$, the relation (5.21) read as

$$\alpha \frac{1}{\xi_{\mu-1}^{E}} + \left(\frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 \left(\mu + \frac{1}{4}\right)^2 - (E + V_0) \right) + \alpha \xi_{\mu}^{E} = 0 \tag{5.22}$$

For the convergence of series (5.20) at the boundary, $|\mu\rangle \to$ constant, it is necessary to have $\lim_{\mu\to\infty} \xi_\mu = 0$ and $\lim_{\mu\to-\infty} 1/\xi_\mu = 0$. From equation (5.22), viewed as a defining relation for ξ_μ^E, we can obtain an equation for the unknown eigenvalues, involving continuous fractions. The lowest non-trival order of approximation for these continuous fractions is equivalent to the truncation of the Hilbert space to the first three unperturbed states. It is easy to check that in the second order in α^2 the energy values contain terms corresponding to an order higher than two in the perturbation theory. Following such calculations and by introducing the energy eigenvalues into equation (5.21), one can obtain the normalized eigenstates.

More generally, if H contains, for example, a term $\cos(4\pi r/a)$ in the potential, then a recursion relation similar to (5.21) can be written connecting five coefficients C_μ^E.

Therefore, the rectangular-well potential and trigonometric-like potentials are solved by using *su*(1,1) Lie algebra operators. By using these Lie algebra operators, more complicated periodic potentials can be described algebraicly within *R*-matrix theory.

CHAPTER 6

CONCLUSION

In this thesis, eigenvalue problem for periodic potentials are solved exactly. The periodic potentials have an importance for determining many physical properties. The energy band structure of electrons in a periodic potential is obtained using the Kronig-Penney model, since the Kronig-Penney model can predict energy bands for a string of atoms subject to a periodic potential V_0. To simplify the tedious algebraic calculation, a Mathematica program is written. Here the solution of the Schrödinger equation is written in terms of odd and even functions.

And, we have formulated the generalized Kronig-Penney model with δ periodic potential has a periodic array of generalized contact interactions in one dimension. δ potential has a specific nature in the energy dependence of band structure [20]. The transfer matrix formalism has been used to find the eigenvalue equation which determines the dispersion relation.

We have written the general second order quasi-exactly solvable Hamiltonian in one space dimension in an algebraic framework. This quasi-exactly solvable form can be reduced to the exactly solvable case by the restriction of potential parameters. Hamiltonian can be expressed as a linear function of the generator of Lie algebra.

Quasi-exactly solvable operator is written in a canonical form. With appropriate transformations the related Schrödinger equations are mapped onto Heun's equations. Therefore, the algebraic eigenfunctions are expressed in terms of Heun's polynomials, or, in the case of multiple roots, confluent Heun polynomials.

We have described two particular one-dimensional problems using Lie algebra. The Hamiltonians of rectangular-well potential and trigonometric-like potential are written in the framework of the Lie algebra. More complicated trigonometric potentials can be described in terms of $J_{\pm}$, J_0 operators with the generalization of the equations (5.16) and (5.18).

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APPENDIX

A MATHEMATICA PROGRAM TO CONSTRUCT THE DISPERSION RELATION OF KRONIG-PENNEY MODEL

Assume different wave functions for two examples.

```
Exp1 = {g1[x] → A1 Cos[α x], g2[x] → A1 Cos[β x], u1[x] → C1 Sin[α x], u2[x] → D1 Sin[β x]};
Exp2 = {g1[x] → A1 Cos[α x], g2[x] → A1 Cosh[β x], u1[x] → C1 Sin[α x], u2[x] → D1 Sinh[β x]};
```

Form the wave functions.

```
Ψ11[x_] = (A g1[x] + B u1[x]) e^(-i k x) /. Exp1
Ψ12[x_] = (C g2[x] + D u2[x]) e^(-i k x) /. Exp1
Ψ21[x_] = (A g1[x] + B u1[x]) e^(-i k x) /. Exp2
Ψ22[x_] = (C g2[x] + D u2[x]) e^(-i k x) /. Exp2
```

Apply boundary conditions for two examples.

```
p11 = Ψ11[0] - Ψ12[0]
p12 = Ψ11'[0] - Ψ12'[0]
p13 = Ψ11[a] - Ψ12[-b]
p14 = Ψ11'[a] - Ψ12'[-b]
p21 = Ψ21[0] - Ψ22[0]
p22 = Ψ21'[0] - Ψ22'[0]
p23 = Ψ21[a] - Ψ22[-b]
p24 = Ψ21'[a] - Ψ22'[-b]
```

Form the coefficient matrices of four equations.

```
t1 = {{Coefficient[p11, A], Coefficient[p11, B], Coefficient[p11, C], Coefficient[p11, D]},
   {Coefficient[p12, A], Coefficient[p12, B], Coefficient[p12, C], Coefficient[p12, D]},
   {Coefficient[p13, A], Coefficient[p13, B], Coefficient[p13, C], Coefficient[p13, D]},
   {Coefficient[p14, A], Coefficient[p14, B], Coefficient[p14, C], Coefficient[p14, D]}}
t2 = {{Coefficient[p21, A], Coefficient[p21, B], Coefficient[p21, C], Coefficient[p21, D]},
   {Coefficient[p22, A], Coefficient[p22, B], Coefficient[p22, C], Coefficient[p22, D]},
   {Coefficient[p23, A], Coefficient[p23, B], Coefficient[p23, C], Coefficient[p23, D]},
   {Coefficient[p24, A], Coefficient[p24, B], Coefficient[p24, C], Coefficient[p24, D]}}
```

Obtain the dispersion relations for two cases.

```
dr = FullSimplify[ExpToTrig[Det[t1]]]
dr = FullSimplify[ExpToTrig[Det[t2]]]
```

$$A1^2\, C1\, D1\, e^{-i\,(a-b)\,k}\,\left(-2\,\alpha\,\beta\,\left(-\text{Cos}[a\,k]\,\text{Cos}[b\,k]+\text{Cos}[a\,\alpha]\,\text{Cos}[b\,\beta]+\text{Sin}[a\,k]\,\text{Sin}[b\,k]\right)+\left(\alpha^2+\beta^2\right)\,\text{Sin}[a\,\alpha]\,\text{Sin}[b\,\beta]\right)$$

$$A1^2\, C1\, D1\, e^{-i\,(a-b)\,k}\,\left(2\,\alpha\,\beta\,\left(\text{Cos}[(a+b)\,k]-\text{Cos}[a\,\alpha]\,\text{Cosh}[b\,\beta]\right)+(\alpha-\beta)\,(\alpha+\beta)\,\text{Sin}[a\,\alpha]\,\text{Sinh}[b\,\beta]\right)$$