A STUDY OF QUANTUM ELECTRON DYNAMICS IN PERIODIC SUPERLATTICES UNDER ELECTRIC FIELDS

DISSERTATION

Presented to the Graduate Council of the University of North Texas in Partial Fulfilment of the Requirements

For the Degree of

DOCTOR OF PHILOSOPHY

By

Daiqing Yuan, B.S. M.S.
Denton, Texas
May, 1996
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This thesis examines the quantum dynamics of electrons in periodic semiconductor superlattices in the presence of electric fields, especially uniform static fields.

Chapter 1 is an introduction to this vast and active field of research, with an analysis and suggested solutions to the fundamental theoretical difficulties. Chapter 2 is a detailed historical review of relevant theories, and Chapter 3 is a historical review of experiments. Chapter 4 is devoted to the time-independent quantum mechanical study of the electric-field-induced changes in the transmission properties of ballistic electrons, using the transfer matrix method. In Chapter 5, a new time-dependent quantum mechanical model free from the fundamental theoretical difficulties is introduced, with its validity tested at various limiting cases. A simplified method for calculating field-free bands of various potential models is designed. In Chapter 6, the general features of “Shifting Periodicity”, a distinctive feature of this new model, is discussed, and a “Bloch-Floquet Theorem” is rigorously proven. Numerical evidences for the existence of Wannier-Stark-Ladders are presented, and the conditions for its experimental observability is also discussed. In Chapter 7, an analytical solution is found for Bloch Oscillations and Wannier-Stark-Ladders at low electric fields. In Chapter 8, a new quantum mechanical interpretation for Bloch Oscillations and Wannier-Stark-Ladders is derived from the analytical result. The extension of this work to the cases of time-dependent electric fields is also discussed.
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CHAPTER 1

INTRODUCTION

The phenomenon I am attempting to understand in this work is the behavior of electrons in a periodic potential lattice under a uniform static electric field. This problem has been proposed from the beginning of the quantum theory for solids [2]. Because of the difficulties in observing the theoretically predicted effects like Bloch Oscillations (BO) and Wannier-Stark-Ladders (WSL) in bulk crystalline materials, these phenomena have remained as unconfirmed theoretical speculations for half a century. Recently [157, 180] the availability of semiconductor nanostructures or superlattices has made the experiments possible and basically confirmed the existence of these phenomena. Superlattices are man-made multi-atomic-layer structures from two or more kinds of materials, generally semiconductors, e.g. semiconductor superlattices made of GaAs-Ga$_x$Al$_{1-x}$As, that have lattice constants much larger than that of the bulk crystalline materials. Superlattices do not have to be periodic. However periodic superlattices are similar to bulk crystalline materials, except that they have larger lattice constants. The use of superlattices has made the needed electric field for these phenomena smaller than in bulk materials, and theories that treat the electric field as perturbations from the field-free periodic lattice are therefore more comparable to experiments. However, it is this perturbative theoretical treatment that has stimulated controversies. Before the experimental confirmation, there was a half-century long theoretical debate on the existence of these phenomena. Now
that their existence is confirmed, the debate is still going on about their characteristics. Despite the apparent simplicity, the problem of describing the dynamics of WS electrons is very complex and subtle. There are many technical difficulties in the theoretical treatments. Now it seems that the experiments lead the way, and a coherent global theory is still needed.

1.1 Defining Terms

Let’s first define the terms that I use in this work: When electrons are in a periodic potential lattice, they are called Bloch electrons. When Bloch electrons are under the influence of a uniform static electric field (bias potential), they are called Wannier-Stark (WS) electrons or dc WS electrons. When the field is uniform but alternating, the electrons are called ac WS electrons. WS electrons were predicted to have a periodic motion in momentum space and real space, called Bloch Oscillations (BO). When BO are realized in semiconductor superlattices instead of bulk crystalline solids, they are also called Esaki-Tsu Oscillations. WS electrons were predicted to be localized in real space, called WS localization (later theory proved that the localization is not square integrable, because there are no stable eigenstates for WS electrons [64, 97]). WS electrons have a ladder-like energy level structure, called Wannier-Stark-Ladders (WSL). When the electron tunnels to the higher energy bands, referred to as Zener Tunneling or Zener Breakdown, the above ladder-oscillation phenomenon may break down. In superlattices as defined in the last paragraph, the lattice constant is much larger than that of the bulk crystalline materials; therefore the Brillouin Zones (BZ) in momentum space, i.e. the unit of the periodical structure in the reciprocal lattice, are much smaller in size than the BZ’s in the reciprocal lattices of the bulk crystalline materials. The BZ’s of the superlattices are therefore called mini-BZ’s or minizones, and the energy bands are called minibands. In the whole dissertation,
I consistently use four acronyms: WS as for Wannier-Stark, WSL as for Wannier-Stark-Ladders, BO as for Bloch Oscillations, and BZ as for Brillouin Zones.

1.2 Theoretical difficulties

(1) Traditional solid state physics is built upon the spatially translational periodic symmetry of the crystalline structure of solids. Under a uniform static electric field, which adds a potential \( \varphi = -E x \), proportional to the real space position \( x \), where \( E \) is the electric field, this periodic symmetry is broken, and therefore all theories based on the field-free solutions are only valid for weak field situations. However it is hard to define what is a strong or weak field for infinite lattices, in which there will always be a point where the magnitude of the potential is larger than a set standard. If we redefine the electric field to be within the set standard then we have to change the origin, whose position is supposed to be non-physical. A non-perturbative approach is therefore needed to avoid this problem. Fundamental changes should happen due to the symmetry change. Since the new symmetry is less known, it is necessary to clearly identify, state and utilize the remaining symmetry for studying the WS electrons.

(2) Traditional solid state physics treats infinite lattices with periodic boundary conditions. However for infinite lattices the perturbation with a uniform electric field is singular, as stated above. If one treats a finite lattice, boundary conditions are needed if the treatment is done in the real space representation. Boundary conditions are supposed to be non-essential for (microscopically) large physical systems, therefore the results should not be sensitive to them. If the result is sensitive to the boundary conditions, then the problem is not the one we wanted to solve. It has been proven that periodic boundary conditions are not applicable for WS electrons [51]. Other types of boundary conditions, like the infinite well, change the problem, and the
solutions are sensitive to them. These solutions are not what we are looking for. Using the momentum representation seems to make us able to avoid setting a boundary condition in the real space, because only a requirement of the wavefunction vanishing at infinite momenta is needed.

(3) The traditional approach of solving a time-dependent quantum problem is to solve the time-independent Schrödinger's equation first, and use the superposition of the eigenstates with a phase factor related to the eigenenergy to form the time-dependent solution. However it has been proven that WS electrons have no discrete eigenenergies [64]. Their energy spectra are continuous. Therefore any time-dependent solutions based upon the superpositions of time-independent solutions are built upon not-well-defined states (non-square-integrable [97]). An approach of directly solving the time-dependent Schrödinger equation is therefore needed.

(4) Traditional solid state physics in the momentum representation considers that all information is stored in one BZ. By an umklapp process at the BZ's edge, that moves the particle to the other side of the BZ, all BZ's are folded into the central BZ \((-\pi/d \leq p < \pi/d\) for the one dimensional case, \(p\) is the momentum, \(d\) is the lattice constant), and therefore all BZ's are treated as one. However under the presence of a uniform electric field, the Ehrenfest's Theorem demands the electron to accelerate to higher momenta. In order to satisfy the correspondence principle when the lattice potential is considered weak and the electron is basically a free accelerating particle, the electron's wavefunction must be allowed to have values at momenta in all BZ's different from the initial one. Therefore a multi-BZ model or extended-momentum-space model is needed to include the acceleration regime into the theory. There are many complete sets of functions that can be used as basis functions: (a) Bloch functions (Wannier functions); (b) Houston functions (a modification of the Bloch function with the acceleration effect considered); (c) multi-BZ basis functions as in
this work. Expansions in all basis are valid if an infinite number of terms are kept. But only good physical bases converge in a few terms. Bloch functions only apply to the field-free case, Houston functions only to the weak-field case, but the multi-BZ basis functions apply to any field strength, because it is not functionally determined by the electric field. Like the Houston states, the multi-BZ states are eigenfunctions of the time-dependent Schrödinger's equation with continuous spectra, but the former is an approximation of the latter.

(5) The predicted basic features of BO and WSL, like the Bloch frequency \( \omega_B = eE d/\hbar \), where \( e \) is the electron charge, are independent of the functional forms of the potential functions. No matter what we chose as the potential models: square-wells, \( \delta \)-functions, or sinusoidal functions, as long as they are periodic, the solutions are expected to have the same general features. Therefore the functional form that must be chosen in order to proceed with solving the problem must reflect periodicity as the essential feature, and can be modified to have minor features. A general property of all periodic functions is that they can be expanded into Fourier series, the first order approximation of which is a sinusoidal model. More terms can be included in the series to make the approximation as close to other functional forms as we desire. For that reason it is reasonable to assume a sinusoidal model as potential, and leave open the possibilities of adding terms to model other types of potential, in order to get at the essentials of the problem.

(6) The above discussion is within the context of representing the uniform electric field by a scalar potential. However this is only one gauge, \( \varphi = -E x \) and \( A = 0 \), to represent a uniform static electric field with potentials (scalar \( \varphi \) and vector \( A \)) in the Schrödinger's equation. If we choose another gauge, called the vector potential gauge, \( \varphi = 0 \) and \( A = -E t \), where \( t \) is time, then we have the following benefits: (A) restoring the spatial translational periodicity in the Hamiltonian, therefore a certain
band structure is expected; (B) removing the perturbation singularity of the electric field at any finite time $t$. However it also brings in the following problems: (a) the Hamiltonian becomes time-dependent; (b) a singularity at time $t \to \infty$ is expected; (c) the Hamiltonian has no obvious periodicity in time to warrant a time-periodic solution like BO; (d) it is not in the "natural gauge" in which the Hamiltonian is identified as the total energy of the system: electron plus lattice plus field, therefore even if certain band structures exist due to the spatial periodicity, it is not the energy band of the whole system. I will present an argument that since a time-dependent approach is needed anyway, (a) is not a problem. Since I am only interested in the solution at a finite time, therefore (b) is also not a problem. I show that the Hamiltonian has a certain type of time-periodicity, termed shifting periodicity, in Chapter 6, therefore (c) is also not a problem. I also show that when the vector potential gauge is chosen, the Hamiltonian can be identified with the energy of the electron with the lattice, excluding the electric field, which is considered an external field, therefore the band I get is an energy band, so (d) is also not a problem. From the argument above I can choose the vector potential gauge as more advantageous than the scalar potential gauge.

(7) There have been many controversies on whether WSL and BO are single band or multiband phenomena. Some say that a single band model is enough to produce WSL and BO, and they also exist when multibands are considered [78]. Some say that the multiband interactions will destroy them [45]. Some say that interband interactions are strong so no single band approximation should be made [141]. I contend that they are each talking about different things, for I can show in my analytical solution of the approximate problem that WSL and BO can be single or multiband phenomena, depending on the initial conditions, therefore the controversies can be resolved (See Chapter 7). The only way to resolve the controversies is to solve
a full-Hamiltonian model, i.e. without a priori omission of any bands.

(8) The current experimentally observable situation is for excitons (electron-hole pairs), that are excited by short pulses of lasers, for which the microscopic effects of the Coulomb interaction between the electron and the hole, and scatterings by phonon etc, cannot be omitted. However since the complexity of microscopic models, the solution has to be obtained by single-band or a-few-bands approximations [140]. This omission of higher bands does not satisfy the requirement of the last argument for a full-Hamiltonian model. Traditionally microscopic models are solved by approximations as modifications to a solved independent-electron model or single-electron model. Currently the independent-electron model for WS electrons is still controversial due to the technical difficulties stated here, therefore it is hard to estimate which approximation in the microscopic models is valid and which is not. For this reason, the central issue in the current theoretical debate is to find a solvable Full-Hamiltonian Independent-Electron Model [102], before more microscopic effects are considered. In some of the literature [102], terms like “exact model” are used to represent the Full-Hamiltonian Independent-Electron Model. However, since all models are approximate, and single-electron models are very simplistic approximations, the word “exact” should only be interpreted in the context of comparing a full-Hamiltonian model to the single-band or a-few-band models. For the sake of appropriateness, I will use the full name instead of this short name.

(9) The initial conditions are found to be very important to the properties of certain WSL and BO [102]. However since no discrete eigenstates exist for the WS electrons, WS states (wavefunctions of the non-square-integrable localized WS electrons) are not well-defined, therefore the setting of the initial wavefunction has been quite arbitrary. Some authors use single Gaussian wave packets; some multiple neighboring Gaussians; some use multiple separated Gaussians; some use the field-
free Bloch states (eigenstates of electrons of the field-free Hamiltonian that satisfies the Bloch Theorem). The last one is the best defined physically, because before the electric field is turned on, the electrons are known to be in Bloch states. A physical approach is to include the turning-on of the uniform static electric field as a time-dependent problem, which can be solved as an extension of the work of this dissertation (See Chapter 8). For the current experiments in which localized excitons are excited into built-in electric fields (the field exists before the excitons), taking Gaussians to be the initial function have its validity. But for theoretical purposes, the Bloch states before the turning-on of the field is the only well-defined initial eigenstate, and it’s also related to the process of symmetry breaking.

(10) The experiments find BO to be short-lived oscillations, with the dephasing rate increasing with the electric field [180]. If scattering by phonons is the only reason for the scattering time, then it should only depend on the temperature, not the field. That dependence on the field suggests an intrinsic finite lifetime determined by the dynamics. The existing theories are yet to predict such a lifetime.

1.3 Scope of This Work

Chapter 2 and 3 give a historical review of the literature for both the theory and the experiments, respectively, and Chapter 4 discusses the time-independent quantum mechanics domain. The rest of the dissertation is oriented to overcome the last ten theoretical difficulties. Our current result is that I have overcome the first eight out of the ten difficulties; and for the last two, methods to tackle them have been designed in my work. The summary of my contributions is in §8.4; the method to deal with the initial value problem is presented in §8.3.3; and the direction to deal with the lifetime problem is presented in §8.1. The conclusion of this dissertation is that through my work, most of the theoretical difficulties have been removed, and
now a physically solid foundation can be laid for building a coherent global theory in the full-Hamiltonian independent-electron model for the study of quantum dynamics of WS electrons.
CHAPTER 2

HISTORICAL REVIEW OF THE THEORIES

2.1 Background

What started this area of research was a paper by Felix Bloch [2] (1929), who investigated the motion of electrons in crystalline solids modeled by a periodic potential lattice. Constructing the wavefunctions from Bloch functions which satisfy Bloch’s Theorem for electrons in periodic lattices, Bloch studied the motion of wave-packets localized in $k$-space under the influence of a uniform static electric field. Bloch’s Theorem is the application of Floquet’s Theorem [1] from the time-domain to configuration space.

2.1.1 Periodic Lattices

Not long after the birth of quantum mechanics, scientists started to study the quantum properties of electrons in periodic potentials, such as in crystalline solids. Bloch applied Floquet’s Theorem [1] to solids, and proved his theorem, that is: if the Hamiltonian is periodic in real space, then the wavefunction in real space can be written as a plane wave times a function that is periodic in real space. The proof of this theorem can be found in every standard solid state physics textbook, e.g. [203]. Brillouin [3] (1930) showed that for electrons in periodic lattices, the continuous energy-momentum relationship for the free electron breaks into energy bands at the border of Brillouin Zones (BZ) in $k$-space, and each BZ is physically
equivalent to others. Kronig and Penney [4] introduced the δ-function type potential barriers, which was later called the Kronig-Penney Model, and was used to study the transmission and reflection of quantum waves on multiple potential barriers. Wannier [9] (1937) found that the "atomic" part of the Bloch wavefunction is a complete set of functions localized in several neighboring sites, which was later called Wannier functions. Wannier functions are suitable as an expansion basis for the tight-binding models [11]. Slater [14] (1952) studied the Mathieu-type (sinusoidal) potential which is solvable in the absence of electric fields. Now the field-free scheme is established, in which the energy band structure is accepted as the normal result from the spatially periodic potential, and the wave functions have well-defined localized expression like the Wannier functions. This field-free scheme is a limit that the field-dependent theories must adiabatically approach as the strength of the electric field goes to zero. I will test my model at this limit.

2.1.2 Acceleration Regime

Darwin [8] (1936) studied the quantum acceleration of free electrons under static uniform electric fields. Houston [10] (1940) studied the acceleration of electrons in periodic lattices, and constructed a form of time-dependent wave-packets as an approximate solution for weak fields, far from the BZ edges. These wave packets are called Houston functions or Houston modification to Bloch functions, which in the case of free electrons reduce to Darwin's solution. The Houston functions or Houston states form a complete set, and therefore can be used as an expansion basis. However they are only useful when the field is weak and the band gap is large. The acceleration regime is also a limit that the field-dependent theories must adiabatically approach as the strength of the periodic potential approaches zero. I will test my model at this limit, too.
2.1.3 Bloch Oscillations

Bloch pointed out that an electron at the lower band edge of a BZ will increase its momentum as the result of acceleration under an electric field, moving toward the upper band edge (edge of BZ). If it loses its energy by scattering, it will always stay near the lower band edge, and on the average have a constant drift velocity. If the time between scattering is long enough, the electron may reach a region in $k$-space where its velocity starts to slow down, the turning point is called the inflection point. This reduction of velocity causes negative differential conductance that was later exploited by Esaki and Tsu [149].

However since Bloch's argument is only valid for electrons far from the BZ edge, what will happen at the inflection point is not clear. It was Jones and Zener [6] and Zener [7] (1934) who pointed out that at the band edge, the electron may have some probability to jump into the higher band. Houston [10] (1940) pointed out that if the electron does not undergo Zener Tunneling, then it will be Bragg reflected from the BZ edge (where $p = \pi/d$), and jump to the other end of the BZ (where $p = -\pi/d$), therefore reverse it's real space velocity, and start the same motion again. In this way the electron is oscillating in both the momentum and the real space. This oscillation was later called the Bloch Oscillations (BO). The Bragg reflection at the BZ edge is an Umklapp process, the physical meaning of which seems to be the equivalence of all BZ's at the field-free situation. This equivalence is broken when a uniform electric field is present, because a high momentum BZ now means more average momentum due to acceleration.

It was also Houston who pointed out that since the field potential is infinite in extent, and the origin of space coordinates has no physical meaning, a valid wavefunction for WS electrons should be independent of the boundary conditions. However if no such boundary conditions are used, the Bloch wavefunction series diverges. The
Houston function removes the divergence, but is also only valid for weak fields and large band gaps.

2.1.4 Zener Breakdown

Since BO electrons are localized, that makes the solid material not current-carrying, in other words, an insulator. Zener [7] (1934) estimated that as the electric field increases, the tunneling probability to the higher band will increase drastically, causing the material to be current carrying, thus a "breaking down" of the insulator happened and made it a conductor. Houston [10] (1940) also estimated the probability that the electron's transition to the next BZ with higher momentum, and showed that it increases drastically as the electric field increases, thus supporting the Zener Breakdown or Zener Tunneling to higher bands. The work herein shows the tunneling to higher momentum BZ's are more probable than tunneling to higher bands. I suggest that while the BZ to BZ tunneling is called Houston Tunneling, and the band to band tunneling the Zener tunneling, the entire process is a combination of the two, and should be called Zener-Houston Tunneling.
2.1.5  Energy Domain

The past theories of the above process at this moment in history are all semi-classical. Since time-domain quantum solutions can only be obtained from the time-dependent Schrödinger's equation, which is viewed as harder to solve than the time-independent one, people started to look into the energy domain manifestations starting with the time-independent Schrödinger's equation. James [12] (1949) studied qualitatively the biased periodic potential with the effective mass concept, and pointed out it's a partial Bragg reflection that causes BO in the time-domain. He calculated the Bloch period. But more importantly he realized that in the energy-domain, the discrete energy bands in adjacent wells are separated by the bias potential into a series of equidistant levels. Feuer [15] (1952) continued the time-independent quantum mechanical solution by a quantitative perturbative approach. With the help of computer calculations, the present work shows that the time-dependent problem is actually easier to solve than the time-independent one, because this model reduces the calculation to the diagonalization of a matrix of large dimensions, which is easier on computers than by hand, and it gives eigenstates with the continuous spectrum that theory demands, while the time-independent case either can't have eigenstates, or (with some boundary conditions) gives eigenstates with discrete energy, which the WS electrons don't have.

2.1.6  Change of Band Structures due to Fields

It was Wannier who started a rigorous quantum mechanical study on the quantum dynamics of WS electrons. He proposed [17] (1955) an auxiliary equation for the time-independent Schrödinger's equation to incorporate the Zener effect or acceleration effect into the energy bands, by replacing $x$ with $x + i\hbar \partial / \partial p$, which is very similar to the treatment in Wigner functions, that an average is taken in the $(x - p)$
phase space. In this way he speculated that the Zener effect will disappear until the field is at a threshold. Later Wannier [18] (1956) found that when a periodicity is artificially applied, the derivative of the free particle's wave function to $k$ will become discontinuous. Therefore the speculation was wrong but the idea to incorporate the Zener effect into the energy bands is still valid. Adams [19] (1957) asked a question of a fundamental nature: What is the status of the energy band concept in the presence of an external field that destroys the crystalline periodicity? His answer was that it is changed, and the function defined by Wannier then doesn't represent "physical energy bands" of the same nature. The words are vague then and now, because the basic ideas on the identity of the bands of WS electrons are still not well-defined. In this work I try to identify the bands as the energy bands of the electron and the lattice, with the momentum freely taking any value according the the acceleration. The idea of Wannier to “separate” the position $x$ with its operator $i\hbar \partial / \partial p$ persisted in later “exact” proofs by Emin and Hart [80, 83, 84]

2.1.7 Franz-Keldysh Effect

Franz [29] and Keldysh [30] (1958) independently calculated optical absorption spectra of electrons in bulk crystalline solids under uniform electric fields. They found a red-shift tail of optical absorptions, that is absorptions at long wavelength (low frequency) corresponding to energy levels in the forbidden gap. This is called the Franz-Keldysh Effect, which is the appearance of the Wannier-Stark-Ladder for bulk crystalline materials. Since later WSL refers only to the effects in the superlattices, the name Franz-Keldysh Effect remains for the bulk crystalline materials.

2.1.8 Wannier-Stark Ladder

Putting together the ideas of Peierls [5] (1933), Wannier [9] (1937), Luttinger
[13] (1951), Onsager [16] (1952), Adams [19] (1957), and Kohn [20] (1959), Wannier through a series of publications [21, 23, 24, 25] (1959-62), systematically studied the time-independent quantum mechanics of electrons in periodic lattices under electric fields. Since Stark first studied the splitting of energy levels in atoms under electric fields, which is called the Stark Effect, Wannier suggested to name the localization of wavefunctions caused by electric fields the Stark Localization. Later these electrons were called Wannier-Stark (WS) electrons, and the localization became WS localization.

Wannier found that if the function $\psi(x)$ is a solution of the one-dimensional
time-independent Schrödinger's equation

\[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + \left[ \sum_n V(x - nd) - e\varepsilon x \right] \psi(x) = E \psi(x) \] 

(2.1)

then \( \psi(x + nd) \) is also a solution of the above equation with energy \( E + ned\varepsilon \), where the separation of levels is \( \Delta E = h\omega_B, \omega_B = e\varepsilon d/h \) being the frequency of BO. The wavefunctions on the neighboring separate levels are localized in neighboring lattice wells. These equidistant energy levels (not for wavefunctions at the same lattice site in real space, though) are called Wannier-Stark-Ladders (WSL).

### 2.1.9 The Big Picture

In the semiclassical picture:

1. For electrons in periodic lattices, a natural representation to study their dynamics is the momentum representation (\( k \)-space). All information is folded into one Brillouin Zone (BZ), in which the allowed energies occur in bands, separated by forbidden energy gaps. All BZ's are considered equivalent. As an example, the discrete bands might be approximated as

\[ E_j(k) = B_j + \frac{W_j}{2} \left[ 1 - \cos(kd - j\pi) \right] \] 

(2.2)

where \( k \) is the wave number, \( B_j \) the bottom of the \( j \)th band, \( d \) the lattice constant, and \( W_j \) the band width of the \( j \)th band. The ground state is the 0th band. The electron’s wavefunction should be a superposition of Bloch wavefunctions:

\[ \psi(x, t) = u(x, t) \exp(ikx) \] 

(2.3)

where \( u(x + d) = u(x) \) and \( k \) is called the pseudo-momentum. When \( k \) is identified with the reciprocal-lattice vectors, \( u(x, t) \) can be written as Wannier functions, in which case the model is called the Tight-Binding Model.
(2) For WS electrons, the presence of the uniform static electric field biases the lattice, and destroys the periodic symmetry. Fundamental changes should happen to the quantum dynamics. However, if the field is so weak that it is considered a perturbation, approximate theories can be made based on the field-free picture. Within this picture, Bloch predicted the Bloch Oscillations for an electron narrowly localized in $k$-space, to oscillate in one BZ, and one band. The challenge of Zener Breakdown (Tunneling from band to band) and Houston Tunnelling (from BZ to BZ) suggested that people modify Bloch's wavefunctions using the Houston functions

$$\psi(x, t) = u_{k+\lambda t}(x) \exp[i(k + \lambda t)x] \times \exp[-(i/\hbar) \int E_{k+\lambda t} d\tau]$$

(2.4)

where $\lambda = eE/\hbar$, and the Wannier-Stark Wavefunctions, which are not well-defined theoretically, but are intuitively approximated with the shapes of Wannier functions which get more and more localized as the field increases. The Bloch Oscillations have frequency

$$\omega_B = eE d/\hbar$$

(2.5)

where $e$ is the electron's charge, $E$ the electric field, and $d$ the lattice constant. BO's amplitude in real space is

$$L = W/eE$$

(2.6)

where $W$ is the band width.

In the time-independent quantum mechanical picture:

The eigenstates of the WS electrons (WS states or WS wavefunctions) are localized in neighboring wells and have energy differences of size

$$\Delta E = \hbar \omega_B = eE d.$$  

(2.7)

For weak fields, the neighboring WS states have overlaps and coherent oscillating effects may happen like BO. For strong fields, the lattice turns into independent
quantum wells. At certain values of the field strength, the electron states can still be partially extended while the heavy-hole states are already fully localized, in which case interband transitions can lead to observable effects [185].

2.2 Theoretical Disputes: the Independent-Electron Model

Several of the original questions about the WS electrons persist till this day: (1) What is the status of the single BZ band picture in the presence of an electric field that breaks the periodic symmetry? (2) Is the weak field situation a smooth perturbation? How can the Zener Breakdown (acceleration regime) be integrated into the band picture? (3) Are WSL and BO single band or multiband phenomena? How accurate is the single-band-tight-binding predictions? (4) Is WSL absolutely stable or metastable? (5) Does BO have a finite or infinite lifetime? (6) How much should the microscopic details of the superlattice and bulk bands be incorporated into the single-electron models with minibands? There is yet to be a theoretical framework that can be a unified platform to answer all these questions.

2.2.1 Preparation for Round One

Under the assumption that the single BZ band picture is a valid approximation under weak electric fields, Wannier [25] (1962) gave an asymptotically “rigorous” proof for weak fields, that the Bloch bands are closed and therefore a single band model is warranted. Wannier’s derivation used a power series in terms of the magnitude of the electric field, with the concession that the acceleration regime under a finite field cannot be incorporated into the picture, neither for the free-electrons. Wannier et al. pointed out [46] that the negative answer for the “adiabatical connection” is because the field changes symmetry and therefore the quantum changes are “sudden”, and therefore can not be regarded as perturbations because they are singular. But even
with such theoretical difficulties, Wannier and others still believed in the existence of WSL and BO as physically stable phenomena. I will call the people with such opinions the Wannier School or the Prospective School.

Several experiments were explained by the theories of WSL, but the results were not conclusive, because the effects are very small. Callaway [33, 200] (1963-64) and Tharmalingam [34] (1963) calculated the optical absorptions, and concluded that there should be observable oscillatory effects, but later experiments had no success in measuring them for decades.

Subsequently there developed a school of physicists who suspected that the theoretical difficulties had led to faulty physical conclusions, and doubted the existence of WSL and BO at all as stable physical phenomena. This group was spearheaded by J. Zak, and so I shall call people of this opinion the Zak School or the Critical School. They first studied Bloch electrons in the presence of both electric and magnetic fields [43, 45] (1964-68). Later the focus was turned onto the static electric field case (the WS electrons). Zak developed a $kq$ representation that is a combination of momentum and real-space representations, as Schrödinger's equation for WS electrons, which is an exact treatment of the Wannier replacement of $x$ with $x + i\hbar \partial / \partial p$ [17, 18] (1955-56).

It seems that the Prospective School based their work on physical intuition, and the Critical School relied mainly on mathematical rigor. The experiments have finally proved that WSL and BO exist, therefore the basic idea of the Prospective School was right. On the other hand, these phenomena are not absolutely stable but only metastable, therefore the basic idea of the Critical School was also right. The pattern of this historical dispute was that each time a constructive attempt was given by the intuitive people to "rigorously" prove the existence of WSL and BO, a wave of criticisms arose from the "rigorous" people to point out some difficulties that the
authors had neglected. Those who criticised were themselves also criticised and the debate sharpened the arguments of both schools. A gradual focusing onto the key points of this debate has resulted in this thesis in which I attempt to synthesize all theories by greatly simplifying the model.

2.2.2 Round One: about WSL

Actually it was Callaway of the Wannier School [200] (1964) who pointed out that perturbation theories do not work for infinite crystals in the presence of external electric fields. Following Frische [42](1966), Zak pointed out [47] (1968) that previous calculations of Wannier [25] (1962) and Callaway [33](1963) on the Franz-Keldysh effect and WSL are based on inconsistent assumptions. He showed that within the one-band model with finite lattice size, WSL exists only if there is no overlap between electronic functions on different sites. The interband terms therefore are not to be neglected, and Bloch functions do not form a valid basis. By comparing with two limiting cases: the free electron (weak barrier) and the tight-binding (strong field) he concludes that no ladders related to the band structure ever exist, because where it is evident is in the continuous states where energy is allowed at every value, therefore no distinct ladders exist.

Wannier replied [48] (1969) that metastable WSL should exist. Zak replied to the reply [49] in the same issue of Physical Review, defending the “errors” he was accused of, and pointed out that there is still no “rigorous proof” that WSL exists. He depended on his \( kq \) representation in which no band index can be assigned to WS electrons.

The major result of round one is that Wannier admitted that WSL may not be a stable phenomenon, but he insisted on the existence of it as a metastable phenomenon.
2.2.3 Ripples of Round One

Rabinovitch of the Zak School pointed out [51] (1970) the fundamental problem of symmetry breaking, that the periodic (Born-von Karman) boundary condition used by Wannier et al. in their proofs of WSL is not consistent in the presence of electric fields that break the translational symmetry. He and Zak [52] (1971) also found that different boundary conditions changes the eigenfunctions of electrons in a Mathieu-type potential drastically, though the eigenvalues are not so sensitive to the boundary condition. No WSL was found in their numerical works. Zak gave a review of his school’s opinions in reference [53]. Rabinovitch and Zak [56] pointed out that Houston functions only satisfy the time-dependent Schrödinger’s equation for times shorter than the Bloch period.

Saitoh of the Prospective School [54] (1972) used a microscopic single-band model including phonons, with certain approximations (Tamm-Dancoff), and calculated the field-dependent conductivity. He suggested the existence of a process in which an electron at the $m$th ladder jumps to the $(m - n)$th ladder with the emission of an optical phonon. He asserts that WSL are resonance levels. They decay due to effects, if any, but they still have a physical significance if the lifetime is long enough. Shockley [55] (1972) used the methodology of Shockley surface states and qualitatively argued that WSL will only be minutely disturbed by tunneling effects. Fukuyama et al. [58] (1973) studied a two band model of this effect and decided that WSL survives.

Rabinovitch and Zak [56] (1972) again pointed out that due to the same theoretical difficulties in neglecting the interband terms, the Bloch electrons are not necessarily oscillating in time under an electric field.

Rauch and Wannier [59] (1974) and Avron of the Zak School [63] (1976) all agreed that WSL are metastable resonance states, not discrete stable eigenstates.
Avron pointed out that even though the electric field is a singular perturbation (divergence at infinite distance for infinite lattice models), so that it is not obvious what finite field can be regarded as small, there are two dimensionless parameters independent of the size of the lattice that can be used to define a small field. Avron et al. [64] (1977) also gave a proof that the bands of WS electrons are continuous, and the instability of the continuous spectrum, under the $N$-band approximation. It is interesting that Rabinovitch of the Zak School [65] (1977) who showed with a certain model calculation for a finite lattice that WSL exists "after all".

Some variations of WSL was also suggested. Moyer [57] (1973) reported that each band splits into not one ladder but many ladders. Banavar and Coon [67] (1978) calculated the width and spacing of WSL and suggest that they are not exactly equally spaced, but at high energy they approach the Wannier value. Kroemer [60] (1975) and Churchill [66] (1977) found that Bloch electrons in the field-free case do not propagate with constant shape and velocity. Rather they behave with certain eigenfrequencies determined by the lattice potential. Bassani et al. [61] (1975) treated the effect of the electric field to the interband transistions on the ground that if the initial state is Bloch-like, then the Hounston state is always Bloch-like. I shall give a comment here that the initial state in a built-in electric field is not a Bloch state. If the initial state is a Bloch state, then the electric field should have a turning-on time-dependent process, and is not a static field for a certain time.

During this period, even though no rigorous proof was available, theoretically it was established that WSL as a metastable phenomenon does exist.

2.2.4 Preparing for Round Two

From the Prospective School, Bentosela [68] (1979) proved that the probability of jumping to other bands are bounded by a term which is linear in time. Nenciu
and Nenciu showed [71, 72] (1980-81) that granted there is a qualitative difference between the field-free Bloch electrons and the WS electrons, so that one has a discrete energy band, and the other has a continuous spectrum, while the one band model for WS electrons still retains the discrete spectrum, yet for finite times some physical quantities like the interband transition probability behave "very gently" as functions of electric fields. So there should be a proof for the existence of WSL and BO.

From the Critical School, Churchill and Holmstrom [73] (1981) considered the limiting case of vanishing barriers with zero field, and found that by Ehrenfest’s Theorem there needs to be a non-periodic motion, which in no way can asymptotically approach the current picture of BO. They believe that there needs to be a substantial revision of theories to remove all these confusions. In a following paper [77], they constructed a solution of the time-dependent Schrödinger’s equation by taking linear combinations of the time-independent solutions at the energies corresponding to the WSL. Assuming the convergence of the series, they showed that the wavefunction can be written as a Bloch-like state with a time-dependent wave-vector in agreement with Wannier [23, 25], but the eigenenergy are allowed to have all continuous values as in agreement with Zak [45]. However the wavefunctions they got are not adiabatically connected to the zero field case as in agreement with Wannier and Van Dyke [46]. Their solutions do not satisfy the Born-von Karman boundary conditions. They argue that the wave functions is actually a standing wave, therefore no BO exists. The reason of the standing wave is due to the boundary conditions that they had used to get the eigenenergies.

Following Berezhkovskii and Ovchinnikov [62] (1976) and Banavar and Coon [67] (1978), whose usage of stair functions to approximate the linear potential are criticized by Zak [70], Bentosela et al. did numerical work with a periodic Kronig-Penney potential plus a stair potential (step-function), to consider the effects of interband
terms. They first [75] (1982) found approximate ladders of resonance with the real part close to Wannier model, and imaginary part very small. Then they [76] (1983) found the resonance' width oscillates strongly.

Luban [78] (1985) revived the constructive time-dependent quantum mechanical solution within a single-band-tight-binding model. He found an exact solution, and proved that all wavefunctions are necessarily periodic in time, because the WS electrons can be mapped to the quantum rotor system in the eikonal limit.

At this time, fifteen years after the proposed superlattice, there begins to appear more experimental evidence for the existence of WSL. However, the problem of the theories have been more obviously shown in the limiting case of weak barriers, when the semiclassical picture of BO violates the correspondence principle.

Round Two: for BO

From the Prospective School, Krieger and Iafrate [79, 81, 89] (1986-89) made a thorough analysis of former theories, and suggested using the vector potential gauge to represent the uniform electrical field in the time-dependent Schrödinger's equation in real space. They claim that it removes all theoretical assumptions that drew criticisms, and gave support for all semiclassical predictions. They analysed the three kind of bases people used to build solutions for WS electron: (1) the Wentzel-Kramers-Brillouin (WKB) generalization of Bloch functions by Zener [7], (2) the accelerated Bloch states (Houston function), and (3) the Crystal-Momentum Representation (CMR) by Kane [22] and Argyres [32]. They found that Houston functions are the short-time evolution of Bloch functions that represent the periodicity of potentials, but the solutions of the time-independent Schrödinger's equation with scalar potential gauge

\[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi + V(x)\psi - E\psi = E\psi(x)\]  

(2.8)
does not have translational invariance, therefore its solution, the only non-divergent
one is the Airy function, naturally do not look like the Houston functions, as Zak
and Rabinovitch [52, 56] had criticized. As they changed the gauge, they said their
instantaneous Hamiltonian

$$\hat{H}(x,t) = \frac{(\hat{P} - e\mathcal{E}t)^2}{2m} + V(x)$$ (2.9)

where $V(x + d) = V(x)$, is translationally invariant, therefore they have avoided the
sum of periodic functions to be a non-periodic function, as the traditional authors
were criticized for doing. They claim that the Zak School's criticisms are correct but
irrelevant. They also criticized the works of Churchill and Holmstrom [73, 74, 77] to
be invalid because their constructed solution, the linear combination of non-periodic
Airy functions to be a Bloch-like periodic function, do not reduce to the Bloch state
before the field is turned on, or reduce to the field-free Bloch state as $\mathcal{E} \to 0$. I
consider this criticism unwarranted because physically the wavefunctions under the
the built-in electric field should not be expected to smoothly connected to the field-
free wavefunction, because of the fundamental symmetry change. Turning on the
field should be a time-dependent problem, not an adiabatic change.

Zak wrote a comment [85] (1988) on the work of Krieger and Iafrate (K&I),
in which he claims that it's not so easy to remove the classical problems simply by
making a gauge transformation. Actually, he says, K&I only moved the problems
from the spatial domain to the time-domain, but didn't remove them. He pointed
out that although K&I know Houston functions are not a suitable expansion basis
because they are periodic in space while the Hamiltonian is not, the solution of K&I
is periodic in time at the lattice sites, while their Hamiltonian is not periodic in time.
I think that the implied shifting periodicity in the K&I's Hamiltonian (See Chapter
6) makes this criticism from Zak inapplicable.
K&I replied to Zak's comment in the same issue of Physical Review, in which they pointed out some errors in Zak's reasoning, but admitted the point by Zak, because they couldn't point out from where they get the time-periodicity. However they maintain that the validity of their work holds by a qualitative argument that since their instantaneous Hamiltonian is spatially translational invariant, therefore they can use the periodic boundary conditions, which results in the time periodicity at lattice sites. They therefore maintain their correctness in avoiding theoretical troubles, and continue their support of all the semiclassical pictures in WSL and BO. I think that their argument is invalid because the time-dependence of the Hamiltonian may result in changing the periodic boundary condition to be quasi-periodic by the multiplication of an unknown time-dependent phase factor.

The work of K&I is a significant contribution which pointed out that the constructive way to find the dynamics of WS electrons should be through the time-dependent vector potential gauge, in which certain aspects of the spatial periodicity (band structure) is kept untouched (more reasons are given in §1.2.) Their work is mathematically better, though not problem-free. But physically it was still not clear, because they could not demonstrate what kind of symmetry is left after the field is turned on. This work concludes that the spatial periodicity is turned into a translational similarity (not by scale change). When the electron moves into a neighboring well, the environment of the electron is similar to the former well, except that the energy is different. Motion to the right and left wells are not the same, because the spatial inversion symmetry is lost. But still some symmetry is present, that is the spatial translational periodicity minus the spatial reversal symmetry, which is manifested through the shifting periodicity in time in momentum space.

A direct response to K&I from Churchill and Holmstrom (C&H) came later [91, 92] (1990-91), in which they pointed out some inconsistencies in the K&I's papers.
When Ehrenfest's theorem is used on the proposed approximate solution of K&I to calculate the average acceleration, it is constant, without temporal variations whatsoever; however if one is to calculate the average velocity, and then take the time derivative for the acceleration, then it oscillates with the Bloch frequency. Therefore K&I were not justified in taking the one-term truncation of their expansion to get their solution, even though the expansion basis is a legitimate choice. In this way C&H has shown that K&I have failed to support the BO concept that was criticized. C&H further analysed through the free-space (weak barrier) limit, by their proposed method for studying semiclassical cases [82] (1987) that BO in the current semiclassical picture violates the correspondence principle. They pointed out that the Bloch frequency is totally independent of the lattice strength, i.e. the magnitude of the lattice potential, and is independent of the functional form of the potential, which seems counter-intuitive for any realistic motion of a wave-packet. They further constructed a Bloch-type wavefunction from the Airy function solution of the Schrödinger's equation in perfectly empty space, that has an apparent time-periodicity with Bloch frequency. But that is a paradox, since no physical oscillations happen in empty space.

The classical trajectory of a particle under a constant force in a sinusoidal periodic potential can be solved from an energy conservation equation

\[ \frac{1}{2} m \left( \frac{dx}{dt} \right)^2 + V_0 \cos k_0 x - F x = C, \]  

(2.10)

where \( C \) is the total energy which is a constant determined by the initial conditions. The trajectory \( x(t) \) is then determined by the inverse function of

\[ t(x) = t(x_0) + \int_{x_0}^{x} \frac{dx}{\sqrt{\frac{2}{m} (F x - V_0 \cos k_0 x + C)}}, \]

(2.11)

if that function is single-valued. Figure 2.3 show the qualitative argument from C&H on the requirement on quantum theories of WS electrons to correspond to this trajectory.
The Contribution Principle (CP) applied to the position and velocity of a WS electron as the lattice potential is turned on and off, described by the Hamiltonian \( H = \frac{p^2}{2m} + e\mathcal{E}x + \lambda V(x) \). It is evident that the 2nd group violates CP, and a theory of the 3rd type is demanded. (Reproduced from Ref.[91])

The contribution of C&H is very important, because they have shown from the critical side the need for a coherent pure quantum theory that satisfies the correspondence principle. Our result is exactly what they had hoped for in their paper [91], i.e. a comprehensive revision of the current theory that avoids the known technical difficulties. The acceleration regime that is needed by the correspondence principle in the weak barrier limit is built into the multi-BZ basis.
2.2.5 Ripples of Round Two

Niu [87] (1989) developed the idea of dynamical symmetry by taking the time-dependent vector potential gauge, and the periodic boundary condition. Through a tight-binding model, and a method called electric translations [28] developed after magnetic translations [26, 27], he found three Abelian subgroups representing (1) temporal uniformity, (2) spatial periodicity, and (3) temporal periodicity. The solutions for the WS electrons should exhibit these symmetries. He believes that if the electric field is turned on adiabatically, Berry’s phases [108, 122] change the symmetry property of the wavefunction.

Nazareno et al. [88] (1989) solved the BO problem in the one band model and periodic boundary conditions, predicted an oscillation, a diffusion, and the effects on the optical absorption. Even though they have used these approximations, their result is the closest to mine which is without those \textit{a priori} approximations.

2.2.6 Round Three: for WSL and BO

Emin and Hart (E&H) [80, 83, 84] (1987-88) published three papers that “rigorously proved” the existence of WSL and BO, through the method of separating the bias electric field into a sum of a saw-tooth shape potential that is periodic, and a step-function type potential that is not periodic. By treating the first effect, in a periodic square-well potential, there is a field-dependent electronic band structure, which has a Bloch-like wavefunction basis. By including the step-like potential, they claim that all interband matrix elements vanish, therefore WSL survives when multiple bands are considered. By taking the field-dependent basis states they believe they have solved the problem in the treatment of K&I [79, 85], where the basis states were chosen to be the field-free Bloch states. They gave a time evolution for an electron initially prepared as a field-dependent Bloch state. Their conclusion is that WSL and
BO validates each other, both surviving the multiband effects.

Criticism to the works of E&H came from Zak [93] (1991), and Leo and MacKinnon [178] later in one issue of Physical Review, along with the replies from E&H [94, 96]. Zak found E&H misused the $kq$ representation by splitting $x = i\partial/\partial k + q$ into $q$ and $i\partial/\partial k$, just like what Wannier had done before [17, 18] that was already criticized by the Zak School. In the reply by E&H to Zak, they rederived the questioned formula without using the $kq$ representation or crystal-momentum representation, and questioned the way Zak checked their work with empty space (weak lattice strength) limit, because the free-electron states are singular limits of Bloch states in which the basic properties of Bloch states abruptly disappear.

Leo and MacKinnon found some mathematical errors in the works of E&H, and pointed out that the thus invalid conclusion had already been cited in some publications. They pointed out that the final result of E&H is not a multiband result as it is claimed to be, but is a single band approximation. They quoted their recent work [90] (1989) where in a numerical calculation for the field-dependent band, the interband matrix elements are non-zero. In the reply to the comment, E&H rederived the questioned formula without further explanations.

2.2.7 Ripples of Round Three

Nenciu [97] (1991) gave a mathematical review and tried to rigorously justify the Peierls-Onsager effective Hamiltonian. Nenciu pointed out that the electric field is a singular perturbation, and it makes all states extended with continuous spectrum, therefore no square-integrable localized state exists. The doubts of the Zak School are well founded. The key point has to do with the interband matrix elements. WSL cannot exist as eigenvalues, but only possibly as resonances, which means long-lived states. For the free-electron limit the one-band approximations definitely break
down. The weak-field limit is mathematically singular but physically smooth. The controversies mostly involve technical difficulties. For δ-function potentials, WSL eigenenergies are not ruled out, but for finite potentials only resonances are possible, provided that the field-free electron has discrete bands. Nenciu's review also has an extensive mathematical literature regarding the WS electrons, which this thesis has omitted. Bastard et al. [98] (1991) gave a review on both theories and experiments.

Using the independent-electron model, Bouchard and Luban [99] (1993) theoretically predicted terahertz dipole radiations in semiconductor superlattices. At that time, a new experimental method of four-wave-mixing had enabled the observation of BO-like phenomena in semiconductor superlattices, but the lifetime of which are vary limited, contrary to the traditional picture.

The Iafrate group [100, 101] (1994) continued the K&I tradition [79, 81, 89] (1986-89) of using the vector potential gauge, and developed the treatment from a one-band short-time perturbation theory to a long-time multiband theory, by using the Wigner-Weisskopf approximation to deal with multiband couplings. They found the electric-field-induced broadening of the excited-state probability amplitudes, thus resulting in spatial lattice delocalization, the onset of smearing of discrete WSL, and band-to-band transitions due to the presence of the electric field.

Yu [103] (1995) developed the method by Churchill and Holmstrom [82] (1987) to construct a wavefunction of WS electrons from time-independent solutions, and claimed to have found BO in real space. Our criticism of this work will come in Chapter 5 when discussing the field-free limit.

Within the independent-electron full-Hamiltonian model, Bouchard and Luban [102] (1995) gave the most recent review. They used a piecewise-constant effective-mass model, and a high precision numerical method, to calculate the lifetime of BO. They predicted BO to have a longer lifetime than shown by the experiments, and
suspected that rough-edge effects on the potential boundaries destroyed the signal. They also found that BO can depend on many parameters, like the initial conditions of the wavefunction, and that there are many “modes” of BO like the “center-of-mass mode” or the “breathing mode”.

2.2.8 The Big Picture

The uniform static electric field is a singular perturbation, therefore the spectrum is continuous. No stable localized states with WSL exist, but certain resonance states with similar ladder-like structure exist, their lifetime determined by the interband mixing. The traditional BO picture is in contradiction to the correspondence principle, although certain interference effects with the Bloch frequency do exist. The choices of model, representation, gauge, functional form of potential, and basis states become essential since they focus the theory to a certain perspective that others can’t reach. They also cause certain difficulties when necessary approximations are made. A valid theory must have asymptotic correspondence to the field-free (weak-field) limit, the free-electron (weak-potential) limit, and the acceleration (strong-field) regime. The lifetime of BO may depend on the portion of microscopic models incorporated into the mesoscopic independent-electron model.

2.3 Related Research

Although the central line of debate related to the properties of WS electrons, i.e. electrons in periodic lattices under a uniform static electric field perpendicular to the lattice plane, is the studied within the independent-electron model, there are other research interests related to this topic, such as more complex and more microscopic models, and some basic research topic as follows:
2.3.1 Basic Research

Landauer [104] (1970) and Anderson et al. [105] (1980) studied the relationship between the transmission coefficient and the conductivity, and found that they are proportional by the universal constant $2e^2/h$. This gives my study of the transmission spectrum more physical meaning.

Kobe et al. [106, 109] studied the gauge-invariant energy operator and power operator. They argued that the Hamiltonian is gauge-dependent and therefore not physical, but the Hamiltonian minus the scalar potential is gauge-independent, and its time derivative is the power operator that is equal to the energy input rate from external fields. For static uniform electric fields, the natural and physical gauge is the scalar potential gauge, in which the scalar potential is a potential energy, and the Hamiltonian is the energy operator identified as the total energy of the system. By gauge transforming the Hamiltonian into the vector potential gauge, the Hamiltonian is not supposed to be the energy operator. However the dynamics of the wavefunction governed by the Hamiltonians in different gauges is not changed. This assures that my change of gauge is warranted for the problem I am studying. I show in Appendix C that the Hamiltonian in the vector potential gauge is still an energy operator, identified not as the total energy, but only the energy of the electron and the lattice, excluding the field.

Berry et al. [111] found a nonspreading accelerating non-square-integrable Airy wave-packet which is related to the WS electrons’ weak potential limit. Nassar et al. [114] developed the idea for expandable and contractible packets, and explained that the non-integrable packet does not represent one single electron, but an ensemble of them.

Berry’s phase [108] (1984) has some connection to the symmetry groups in the WS electrons [87], for if the electric field is turned on adiabatically, the Berry’s phase
will change the symmetry properties of the wavefunctions.

Büttiker et al. [107] (1983) and Ignatov et al. [110] (1993) have compared the Josephson effect to the motion of WS electrons, because the WS electrons have probabilities to jump over the biased energy band gap just like the Josephson electrons tunneling through the barrier.

Due to the emerging of free-electron lasers [112], the possibility of prolonged investigation of WS electrons under harmonic electric fields is becoming important. The WSL now has found an application in quantum cascade laser [113].

2.3.2 Transmission Properties

Lei et al. [115] (1992) studied the temperature dependence of the electron drift velocity versus the electric field from a microscopic balance-equation theory, and found agreement with the predictions of Esaki-Tsu [149] from semiclassical ideas, and qualitative agreement with experiments. The transfer-matrix method (invented by Kramers) was applied to study various transmission properties in solids with plane waves by Griffith et al. [116] (1992), Blundel [117] (1993), Sprung et al. [118] (1993), and Walker et al. [119] (1994). Our work [120] (1995) on the electric-field-induced changes to the transmission spectrum is a study of the details of Zener-Houston Breakdown.

2.3.3 Complex Models: Nonperiodic Lattices

Soukoulis et al. [121] (1983) studied the electrons in one-dimensional disordered systems in the presence of an electric field. They found power-law localizations (non-exponential localization) for small fields. Delyon et al. [123] (1984) found a transition between the regime of extended states for large field to the regime of power-law localized states for small field. Luban et al. [124] (1986) found that all eigenstates are
localized in a general nonperiodic potential under electric fields, within the single-band-tight-binding model. Niizeki et al. [125] (1993) studied quasiperiodic lattices. Cai et al. [126] studied nonlinear lattices under time-varying, spatially uniform electric fields, and found a nonlinear counterpart of BO, and a dynamical localization.

2.3.4 Complex Models: Other Materials


2.3.5 Complex Models: Time-dependent Fields

Ignatov et al. [127] (1976) and Dunlap and Kenkre [128] (1986) studied the dynamical localization when the average velocity of electrons vanish. Holthaus et al. [129, 130] (1992-93) studied the effect of strong harmonic time-dependent electric field on the miniband structure. He found a band-collapse or dynamical localization, when the width of the miniband approaches zero if the ratio of the Bloch frequency and the laser frequency approaches a zero of the Bessel's function $J_0$. He also found the avoided-crossings in the quasienergy spectrum of the two-state system is related to the frequency spectrum of radiation scattered from a laser-driven double well. Alekseev et al. [131] (1994) discussed the possibility of dynamical instabilities and deterministic chaos for electrons in superlattices with alternating electric field. Zhao et al. [132] (1995) found that a single band splits into a series of fractional Stark-ladders in dc-ac fields, in which case the level separations of the WS states are not integer multiples of $\hbar \omega_R$, but fraction of integers.
2.3.6 Microscopic Models: Details of the Superlattices

Bleuse et al. [135] (1988) numerically calculated the WS states in the superlattices, and found them to be gradually localized with increasing electric fields.

Dignam and Sipe [136, 137] (1990) and coworkers [191] (1994) developed the dynamics of exciton for WS electrons, for Type-I GaAs/Ga$_x$Al$_{1-x}$As superlattices, where the coherent electron-hole pairs are only in the same layer, and Type-II GaAs/AlAs superlattices, where the electrons and holes are in different layers, but still with coherent motions. In their calculation for exciton WSL in Type-I superlattices, they found significant differences with the single-band model results, particularly at low field strengths. They misquoted the paper of Emin and Hart [80] as the rigorous proof of the existence of WSL, but their result is in agreement with the experiment by Agulló-Rueda et al. [163] (1989). They found evidence of excitonic BO, with the spatial amplitude strongly dependent on the initial conditions, and independent of Coulomb interactions, except that with Coulomb interactions, there is no “breathing mode” BO.

Yu [138] (1994) studied the WSL in modulation-doped finite length superlattices, and found that WSL exists only for strong field domain, and that the electronic states are not evenly spaced. Meier et al. [140] (1994) considered Coulomb interactions and calculated the signals of BO in terahertz emission and four-wave-mixing. They found that BO should exist even for high exciton energies near the band width. Rotvig et al. [141] (1995) studied a two miniband microscopic model, and found that for static fields, strong interband transitions occur, and a series of stable plateaus appear for low fields.

2.3.7 The Big Picture

A biased periodic lattice is a fundamentally important configuration for phys-
ical investigations, and is applicable in many areas of study. Complex models and microscopic models may tell us more about the specific systems, but not necessarily more accurately, because in general the more complex a model is, the harder it is to solve. Usually we develop a simplified model that's easier to solve, like an independent-electron model, then the solution is used as the backbone for analytical approximations to complex models, to check if the approximations are reliable. When the validity of the basic concepts are still in doubt, it is best to get the most out of simple independent-electron models, without any a priori analytical approximations, to get the basic physical features, so that further development of the microscopic and complex models can be made.

2.4 Summary

The theory for WS electrons is complicated by the following problems, which are also addressed in §1.2, here I only list the names as a summary for this chapter:

(1) The issue of symmetry and perturbation;
(2) The issue of boundary conditions and representations;
(3) The issue of continuous spectrum and time-dependency;
(4) The issue of acceleration and multi-BZ basis;
(5) The issue of lattice potential strength and functional form of potentials;
(6) The issue of gauge and energy band;
(7) The issue of one-band or multiband nature;
(8) The issue of microscopic effects;
(9) The issue of initial conditions;
(10) The issue of lifetime of BO.

A completely successful theory must deal with each of these problems.
CHAPTER 3

HISTORICAL REVIEW OF THE EXPERIMENTS

3.1 Bulk Crystalline Materials

The first attempts to confirm WSL in bulk crystalline material were done by Wannier and coworkers [142] (1960), by studying the tunneling currents through a narrow p-n junction of indium antimonide. The result was inconclusive at best, because of the smallness of the effects. So are several other attempts by Snavely [144] (1965), Vavilov [145] (1967), Hamakawa [146] (1968), and Maekawa [147] (1970). Various theoretical attempts were made to explain the unsuccesfulness of the experiments, by Franz [31] (1961), Argyres [32] (1962), Yacoby [36] (1965), Bychkov et al. [37] (1965), Snavely [38] (1966), Kurskii et al. [39] (1967), Döhler et al. [40], and Hacker [41] (1969).

The result of this round of investigation was two-fold: (1) It resulted in the full-scale theoretical investigation on the validity of the traditional concepts, spearheaded by Zak [45] (1968). (2) It made people know that electron scattering by the Coulomb interactions and lattice (thermal) interactions can not be overlooked. Although the major physical feature is predicted in the independent-electron model, making the scattering time longer than the Bloch period is the major experimental task. Getting lower temperature and cleaner samples so as to lengthen the scattering time were the first ideas. But it can be estimated that even the best limit is not good enough for bulk materials, in which the lattice constant is $d \approx 5\text{Å}$, and typical scattering
time is $\tau_S \approx 1 \times 10^{-13}s$. To make the Bloch period $\tau_B = h/e\mathcal{E}d$ less than $\tau_S$, the electric field $\mathcal{E}$ has to be $6 \times 10^7 V/m$. For such high fields, no semiclassical predictions are valid because they are only good for "slowly varying potentials". In bulk materials the band width is $W \simeq 1eV$, therefore the real space amplitude of BO will be $L = W/e\mathcal{E} \simeq 10^{-2} cm$.

A high note of the investigation in bulk materials came when Koss and Lambert [148] (1972) positively observed for the first time several Wannier levels as predicted by Callaway [33], in optical absorption in direct-transition semiconductor GaAs. Lederman et al. [150] (1976) observed positively the Franz-Keldysh effect. Recently Sha et al. [197] (1995) observed coherent plasma oscillations in bulk semiconductors. As promising as they sound, the experiments in bulk materials are still considered not definitive for this highly theoretically debated area.

### 3.2 Semiconductor Superlattices

In a theoretical paper, Esaki and Tsu [149] (1970) imagined building "superlattices" by laying on monolayer crystalline semiconductors with different impurity contents during the epitaxial growth procedure. In superlattices the lattice constant could be two magnitudes larger than the bulk crystal lattice constants, therefore the Bloch period is lowered by two magnitudes, and the electric field required is smaller by two magnitudes. In momentum space, among the bulk BZ's there are mini-BZ's of two magnitudes smaller, and above the bulk energy bands there will be minibands of band width two magnitudes smaller. The real space amplitude of BO will still be of the same amplitude $10^{-2} cm$, but is of a smaller number of lattice units, only about $10^2$ quantum wells. If BO exists in superlattices, then a negative differential conductance will appear. Their paper changed the direction of the investigations on WS electrons to the semiconductor superlattices. From now on when I talk about
bands or BZ's of the WS electrons, I mean minibands and mini-BZ's, and I mean superlattices when I say lattices.

3.2.1 Preparations


3.2.2 Concepts

Given a semiconductor superlattice, with the Fermi energy between one band (miniband) and another, then we have a valence band below and a conduction band above. By letting a laser beam with a frequency matching the band gap, an electron in the valence band can be excited to the conduction band, and a positively charged hole is left in the valence band. If the electron-hole pair has coherent motion, it’s called an exciton. For some materials where the effective-mass of the hole is heavy, the heavy-hole (hh) is basically localized, while the electron (el) is moving around the hh. In a static uniform electric field each band separates into several WSL and the el eigenfunctions of different ladders are localized around neighboring wells. By exciting the el-hh pair with a short laser pulse, the exciton wave function is only composed of several neighboring WS states. If the Coulomb interaction between the el-hh pair can be neglected, then the el-hh separation undergoes the BO, and the el wavefunction evolves around several WSL, creating quantum beats, which can be
detected by a second short laser pulse. For some light-holes (lh), the motion becomes more complicated.

![Figure 3.1. Optical absorptions between a WS electron state in the conduction band and the heavy-hole states in the valence band. (Reproduced from Ref. [185])](image)

3.2.3 Interband Optical Transition

Since the electron wavefunction is partially extended to several wells in the conduction band, and the hh wavefunction is fully localized in different wells, therefore occupying different levels of WSL in the valence band, absorbing or emitting a photon
would cause an interband optical transition between the electron and hole states, which would give rise to a well-defined absorption and emission spectra, with the following properties:

(1) The spectra lines are equidistant in energy with a separation of the Stark energy \( \Delta E = \hbar \omega_B = eEd \).

(2) The energy of the central line (representing the optical transition between the electron and the hole right below the central well of the electron) would be independent of the field, but its strength should be increasing with the field, since the electron is more localized in the central well at high fields.

(3) The upper lines would increase in energy relative to the central line. If we let \( n = 1, 2, 3, \ldots \) represent the neighbor index relative to the central line, then the increases are \( ned\). The lower lines decrease with the electric field similarly.

(4) The strength of the upper and lower branches will decrease with increasing field, and the strength of a higher neighbor index line is smaller than the lower neighbor index line at a given field.

### 3.2.4 Observing WSL

The methods to measure the interband optical transitions include Photocurrent (PC) spectra and Photoluminescence (PL) spectra by Mendez et al. [157] (1988), Electro-Reflectance (ER) by Voisin et al. [158] (1988), and Direct Absorption (DA) by Bleuse et al. [135] (1988). Mendez et al. [157] (1988) was the first group to observe WSL through interband optical transition using the PC and PL spectra. Their result proved beyond a doubt that certain ladder-like resonance states exist, because the above descriptions of interband optical transitions are clearly evident in the data.
3.2.5 Intrasubband Optical Transitions

The Intrasubband Optical Transitions, between two states in the same ladder, are involved with the resonant Raman scattering by Agulló-Rueda [161] (1988), when a triple resonant Raman scattering was observed.
Figure 3.3. Observation of intrasubband optical transitions for WS electrons by Raman scattering. On the left is the mechanism, on the right is the signal enhancement at the right field strength. (Reproduced from Ref. [185])

3.2.6 More Developments

Moore et al. [159] (1988) studied the effects of thin barriers to the band alignments. Bar-Joseph et al. [162] (1989) reported the observation of WSL at room temperature. Agulló-Rueda et al. [163] (1989) found that quantum coherence increases as the superlattice constant is decreasing, even to $d = 60\text{Å}$, when more numbers of interband optical transitions are observed. Agulló-Rueda et al. [165] (1990) found that the electric field induces a change of dimensionality of the exciton in superlattice from three to quasi-two dimensions. Schneider et al. [166] (1990) found electro-optical multistability, while discovering the coherent length of WSL is at least five superlattice periods, therefore WSL is a mesoscopic phenomenon. Dharsai et al. [168] (1990) studied the effect of interface roughness scattering, and found they are not of great
influence to electron mobility. Brozak et al. [170] (1990) studied the effect of thermal saturation of band transport in superlattices. Fox et al. [172] (1991) studied electron subband anticrossing in WSL. Sibille et al. [173] (1992) observed the coexistence of WSL and negative differential velocity (NDV) and negative differential current (NDC) in the superlattices at certain strong fields. Since the idea of NDV and NDC was proposed by Esaki and Tsu [149] (1970) based on the semiclassical picture of BO in the miniband, and WSL is a breaking up of the miniband into separate levels, their coexistence is an interesting mixture of the validity of both semiclassical and quantum pictures. Schneider et al. [174] (1992) found that when the barrier width goes to zero, WSL turns into Franz-Keldysh Effect in bulk materials. But even for one monolayer of barrier, WSL still exists for low fields. Mendez et al. [169] (1990) studied the temperature dependence of WSL and found that it's not very strongly dependent on the temperature, changing from 17 periods at 5K to 9 periods at room temperature 292K. A good review of this field was given by Mendez [185]

3.2.7 The Big Picture

When an exciton is created by a laser pulse in a superlattice with built-in bias electric fields, both the electrons and the holes have separate resonance states in the continuous spectrum which includes bands and band gaps in the field-free situation. The physical reality must include the Coulomb interaction and the scattering from phonons etc, but the physical features are exactly as predicted by the independent-electron model in the quantum theory of WSL, with only small modifications from temperature and rough interfaces etc. The existence of such states are now without a doubt, and a score should be given to the Wannier School in theoretical study. But the questions posed by the Critical School is still well founded [97], and it's now a question of how does WSL evolves in time, at the field-free limit, the free-space limit,
and the semiclassical limit.

3.3 Four-Wave-Mixing

Four-wave-mixing (FWM) is a powerful technique of nonlinear-optical spectroscopy, well documented in textbooks by e.g. Bloembergen [201] (1965). The question is whether experimental techniques can make the laser pulses so short that one can have time-resolved FWM. Becker et al. [164] (1989) performed four-wave-mixing (FWM) experiments with femtosecond resolution. This made it possible to study ultrafast (pico to femtosecond) processes, which is the range of Bloch periods in superlattices. When the resolution of the effects of a laser pulse is so high, the time-evolution of a signal can be measured to see how it decays etc.

3.3.1 Time-domain

Göbel et al. [176] (1990) reported quantum beats (oscillatory modulation) during the excitonic polarization decay, and found that the decay not only depends on the scattering process, but also how the initial state was excited to be. It's the Coulomb interaction that gives rise to the appearance of exciton bound states within the energy gap. The study of WSL now starts to turn to the time-domain. Leo et al. [177] (1990) observed coherent polarization interactions in dense media with the FWM method. A slightly different group Leo et al. [178] (1991) applied subpicosecond FWM in superlattices.

3.3.2 Degenerate-Four-Wave-Mixing

A saying is that the most practical thing is a good theory. Just like the theoretical paper by Esaki and Tsu [149] (1970) turned the experiments to superlattices, it's also a theoretical paper by Plessen and Thomas [179] (1992) that led to the
discovery of BO signals (I stress here that I say BO signals instead of BO per se because whether or not these signals represent a center-of-mass oscillation is still in question) by Degenerate-Four-Wave-Mixing (DFWM) method. Developed upon the ideas of Zakharov and Manykin [175] (1973) that for high enough fields the photon-echo-signal should have a characteristic modulation with the periodicity of BO, they calculated and found this signal should be observable at moderate fields. By varying the time-delays between the laser pulse signals, it is predicted that the echo-amplitude should peak at the time of \( n\tau_B \) where \( n \) is an integer, and \( \tau_B \) is the period of BO (Bloch period).

3.3.3 Observing BO signals

Feldmann et al. [180] (1992) was the first to discover BO signals with the DFWM method, not long after its proposal. They also discovered the dephasing rate of BO increases with higher electric field. They attribute this to interband tunnelling. Leo et al. [181] (1992) and others groups soon repeated and improved the observation that a periodic signal in WS electrons exist, that is equal to the Bloch period, that is tunable by the electric field by 400\%, and the dephasing time is about 4\( \tau_B \).

Other methods were later developed like observing Terahertz (microwave) emission spectroscopy (THz) by Roskos et al. [182] (1992) in a double-well potential, and Waschke et al. [187] (1993) in superlattices; and the Transmittive Electro-Optic Sampling (TEOS) by Dekorsy et al. [190, 199] (1994-95), all confirming the existence of BO signals, and the best value of dephasing time is observed to be 15\( \tau_B \).
Figure 3.4. Observation of BO signals by the TEOS method. On the top is the photoecho signal to short laser pulses at different time-delays. Bottom left is the Fourier spectrum. Bottom right shows the proportion of the maximum frequency to the electric field. (Reproduced from Ref. [190])

3.3.4 Other Developments

Schmitt-Rink et al. [183] (1992) studied the damping of the BO signals, and the dependence on the polarization of the laser signals. Koch et al. [184] (1992) were able to distinguish quantum beats and the beats due to the interfering polarizations
of independent quantum systems.

Piazza et al. [186] (1993) studied the transport properties of electrons in superlattices through optical techniques. Plessen et al. [188] (1993) studied the escape tunneling out of the shallow quantum wells, and found the tunnelling time is of the scale of picoseconds, therefore DFWM experiments are sensitive to this tunnelling. Lefebre et al. [189] (1993) tried to use the fractional dimension of excitons in electric fields to unite the excitonic absorption spectra in quantum wells, quantum wires and superlattices. Minot et al. [192] (1994) investigated the nonlinear conduction and electron heating effect in biased superlattices. Plessen et al. [193] (1994) studied the critical (minimal) field requirements for the onset of WSL and BO and concluded that they are strongly dependent on the band width of the miniband. The wider the band width is, the higher the field needs to be.

Leisching et al. [195] (1994) gave a thorough review of the experiments. Roskos et al. [196] (1995) reported WSL-BO induced by photo-excitation of continuum states far above the fundamental band-gap, instead of the traditional simultaneous optical excitation of several excitonic WS states at the band edge of the first band.

Grenzer et al. [198] (1995) and Dekorsy et al. [199] (1995) reported observations of BO signals at room temperature.

3.3.5 The Big Picture

It is natural that as the existence of WSL is confirmed, so will be the interference or beats from these WS states that will give a time-oscillatory signal. What is detected is a signal that has the period of BO, not necessarily a direct visible evidence of a center-of-mass oscillation. That picture of BO is still in theoretical doubt, but the existence of a oscillatory signal with Bloch frequency is undeniable now. A general feature of the detected BO signals is that they are all short-lived, details depending
on the configuration. The dephasing rate depends on the temperature due to phonon collisions, but not very sensitively. The dephasing rate also was found to depend on the electric field, which is only attributed to interband tunnelling, but could be explained by a time scale of intrinsic lifetime. The challenge by the experiments to theories is how to explain the finite lifetime and its dependence on the electric field. The single-band-model’s answer of infinite lifetime is certainly not adequate.

3.4 Summary

The semiclassical theories of WS electrons were built on the symmetry of spatial translational periodicity for systems without electric fields, and therefore was only supposed to work for “weak fields”. In bulk crystalline materials, no visible effects can be seen unless the field is extremely high, so that there was a delay of the experimental confirmation of the existence of WSL and BO. This delay had greatly enhanced the theoretical debate. The late “confirmation” for “theoretically not well-defined” WSL and BO also did not quench the debate, but intensified it by bringing new challenges like the lifetime issue. The theoretical debate intensified the experimental pursuit until the superlattice was made and great technological achievements followed as a result. The experimental achievements reaffirms the value of intuitive physical ideas like the “theoretically not well-defined” WSL and BO, but credits should also be given to the theoretically rigorous Critical School for the pursuit of a mathematically rigorous truth. Without them certain errors would not have been so readily found, and a better understanding of these phenomena would have taken much longer.
CHAPTER 4

TRANSMISSION SPECTRUM

The study of the transmission properties of the crystalline materials under electric fields was initiated by Bloch [2] (1929), Zener [7] (1934), and Wannier [25] (1962). The proposed Wannier-Stark Ladder (WSL) and Bloch Oscillations (BO) has been discussed and debated over the years (See the Historical Review in Chapter 2). Recently, both WSL and BO signals have been experimentally realized in GaAs/Al_xGa_1-xAs superlattices (See the Historical Review in Chapter 3). But the details of Zener Breakdown and other transmission properties was somewhat neglected in the theoretical research.

4.1 Motivation

In dealing with quantum well problems in the presence of an electric field, I notice that the following considerations can significantly affect the results:

(a) whether one considers an infinite lattice or a finite one;
(b) whether or not one uses plane wave approximations and staircase potentials to discretize the continuous electric field; and
(c) whether or not perturbation theory and a weak (or strong) field approximation is used.

The reason that (a) is important is because Bloch functions cannot in general be built out of a finite set of atomic wavefunctions in the presence of an electric field, and
the effect of boundary conditions becomes increasingly evident for smaller lattices.

The reason that (b) is important is because difference equations usually have more complicated spectra than the corresponding differential equations, and therefore discretization of a continuous process may easily introduce artificial spectra (even artificial chaos in a nonlinear case) into the system.

The reason that (c) is important is because perturbation series usually diverge in critical parameter regions where the system undergoes fundamental changes or transitions.

There has been a lot of works concerning the discrete energy spectrum of electrons in a quantum well or in a superlattice consisting of many quantum wells in an electric field, usually in the limit of an infinite lattice. Less attention has been paid to the transmission of electrons with energies considerably higher than the bandwidth of the first gap. I found that contrary to my intuition, electric field in general plays quite a negative role for electronic transport, rather than enhancing electron transport, it suppresses the coherence of the electronic waves in consecutive wells. One of the reasons for studying transmission spectra, besides the inherent interests, is that the transport properties are directly related to the transmission coefficient of quantum mechanical waves. As shown by Landauer and others[104, 105], the electric conductance is related to the transmission coefficient by the elementary factor of $2e^2/h$.

In this chapter, I study a finite quasi-one-dimensional superlattice in the presence of a constant electric field, and see how the transmission spectrum is affected by the field. Figure 4.1. shows the schematic picture of the superlattice and the tilted potentials inside it.
I consider a superlattice that consists of alternating layers of two media, and study the transport property of electrons travelling in it. At low temperatures, electrons have long free mean path, and interactions with phonons are negligible. Quantum mechanical wave coherence and interferences become important when the wavelengths of electrons are comparable with the superlattice constant (interval between two neighboring unit cells). Electrons experience a potential barrier and are consequently scattered at each interface between two layers. In other words, I consider a model of periodic rectangular wells. When an external electric field is applied to the superlattice, the potential wells become tilted, and the parity symmetry in wavevector $k$ is broken, i.e., a wave travelling to the left experiences a different potential from that travelling to the right, and each site has a potential energy different from its neighbors. This model can be solved exactly, without treating the electric field as a weak field or discretizing the potential, and the formal solution will be given later. I show that the gap regions are shifting toward lower energy band and become wider and wider under an increasing field. In particular, I find that the transmission spectrum undergoes a transition, i.e., from transmission to gap, and back to a transmission state, with stronger fields. I illustrate how a gap state can be gradually brought into an extended state under the influence of the field and vice versa.

Figure 4.1. The superlattice consists of two types of layers (upper part); when an electric field is applied, the periodic potentials become biased (lower part).
4.2 Method

Based upon the work of Walker et al. [119] (1994), who used the Transfer Matrix Method on barrier chains without an electric field, I extend the method to study Wannier-Stark electrons (electrons in a periodic lattice in the presence of a uniform static electric field).

I start with the time-independent one-dimensional Schrödinger's equation of a single electron in an external electric field $\mathcal{E}$, with eigenenergy $E > 0$, whose wavefunction entering a lattice sample of $N$ periodic potential barriers.

$$\frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + \sum_{n=1}^{N} V(x - x_n) - e\mathcal{E}x \psi(x) = E \psi(x) \quad (4.1)$$

where $V(x - x_n)$ is the potential well at site $n$, $V(x - x_n) = 0$ except when $x_n < x < x_n + b$, where it equals $V_0$; $x_n = na$, where $a$ is the lattice constant, and $b$ is the well width. Before I look for the solutions, I notice that in the presence of the electric field, plane waves are not eigenfunctions of Eq.(4.1), nor is wavenumber $k$ a good quantum number. Nevertheless, if the electric field is relatively weak, one can still use plane waves and treat $k$ as a semiclassical quantity, which changes by a discrete amount from site to site; band shifts are expected owing to the lifted energy levels of the left-hand side of the lattice relative to the right-hand side. However, when the field is larger, a full quantum-mechanical approach is needed to reveal the electronic transport behavior.

Now let's start to solve Eq.(4.1). If we define a characteristic length

$$l(\mathcal{E}) = (\hbar^2/2me\mathcal{E})^{1/3}, \quad (4.2)$$

and a dimensionless parameter

$$\lambda(\mathcal{E}, U) = (2m/\hbar^2 e^2 \mathcal{E}^2)^{1/3} U, \quad (4.3)$$
where \( U = E \), or \( (E - V_0) \), for the first and the second media, respectively, then, it can be shown that inside each layer, Eq.(4.1) can be transformed into a Bessel’s Equation of order \((1/3)\) (see Reference [202] on the transformation), and the solutions for propagating waves can be expressed as a combination of Hankel functions of the first and second kinds (or equivalently as Airy functions). The forward and backward propagating waves between \( x_{n-1} \) and \( x_n \) consequently are combined to give the following solution:

\[
\psi^{(i)}(z) = A_n^{(i)} z^{1/3} H_{1/3}^{(1)}(z) + B_n^{(i)} z^{1/3} H_{1/3}^{(2)}(z)
\]  

(4.4)

where \( i = 1,2 \) indicating the first and second medium respectively, and

\[
z(x,\varepsilon, U) = \frac{2}{3}(\lambda(\varepsilon, U) + x/x(\varepsilon))^{3/2}
\]

(4.5)

is the new dimensionless coordinate; \((A_n^{(i)}, B_n^{(i)})\) are amplitude constants, which will be determined solely by boundary conditions; and \( H_{1/3}^{(1,2)}(z) \) are the Hankel functions of the first and second kind, respectively.

Considering the continuity of \( \psi(x_n) \) and \( d\psi/dx \) at the interfaces of different layers, a transfer matrix between consecutive unit cells can be found. For the simplicity in presentation, I only give specific result for the \( \delta \)-function case (Kronig-Penney Model for potentials): the rectangular potentials are replaced by \( \delta \)-functions so that in each unit cell the particle is only scattered once. The unit-cell transfer matrix is shown as follows,

\[
\begin{pmatrix}
A_{n+1} \\
B_{n+1}
\end{pmatrix} = \begin{pmatrix}
1 + w_n h_n^{(1)}/h_n^{(0)} & w_n h_n^{(2)}/h_n^{(0)} \\
-w_n h_n^{(3)}/h_n^{(0)} & 1 - w_n h_n^{(1)}/h_n^{(0)}
\end{pmatrix} \begin{pmatrix}
A_n \\
B_n
\end{pmatrix}
\]

(4.6)

where

\[
w_n = 2ml/h_n^2(3/2 z_n)^{-1/3} g_0 a,
\]

(4.7)

with \( g_0 \) being the average potential height in a unit cell for the original lattice without the field; and all the \( h_n \)’s are products of Hankel functions of argument
\( z_n = z(n\alpha, E, E) \), shown as follows:

\[
\begin{align*}
    h_n^{(0)} &= H_{1/3}^{(2)}(z_n) H_{-1/3}^{(1)}(z_n) - H_{1/3}^{(1)}(z_n) H_{-1/3}^{(2)}(z_n), \\
    h_n^{(1)} &= H_{1/3}^{(1)}(z_n) H_{1/3}^{(2)}(z_n), \\
    h_n^{(2)} &= H_{1/3}^{(2)}(z_n)^2, \\
    h_n^{(3)} &= H_{1/3}^{(1)}(z_n)^2.
\end{align*}
\]

The analytical solutions of Eq. (4.1) are therefore completely determined:

\[
\begin{pmatrix} A_N \\ B_N \end{pmatrix} = T_N \begin{pmatrix} A_0 \\ B_0 \end{pmatrix} = \prod_{n=N}^1 M_n \begin{pmatrix} A_0 \\ B_0 \end{pmatrix} \tag{4.8}
\]

where \( A_0, B_0 \) are the initial amplitudes of the wavefunction, \( T_N \) is the final transfer matrix, and \( M_n \) is the \( n \)th transfer matrix in Eq. (4.3). The transmission coefficient \( \mathcal{T} \) is related to the final transfer matrix by

\[
\mathcal{T} = |\det(T_N)/(T_N)_{22}|^2 \tag{4.9}
\]

4.3 Result

To simplify my numerical results, I first define two normalized dimensionless quantities for eigenenergy and electric field strength. I define the dimensionless energy as \( \tilde{E} = E/g_0 \), where again, \( g_0 \) is the average barrier height in a unit cell; so if \( \tilde{E} = 1 \), it means that the eigenenergy is at the average height of the barrier. I also define a dimensionless electric field as \( \tilde{E} = e\alpha/a/g_0 \), where \( e \) is the electron’s charge, and \( a \) is the lattice constant, so that \( \tilde{E} \) can be seen as the relative potential drop within a cell caused by the electric field. I then can study how the transmission spectrum, as shown in Figure 4.2, is changed by the electric field.
As I increase the field strength, I find the second gap (gap II) becomes wider, and shifts to the left (lower value), as can been seen from Figure 4.2 (b) and (c). The shift of the gap is not a surprise, because a similar result is expected from the semiclassical theory for conductivity. However, when I further increase the field strength, the original band structure collapses and gap II disappears; the first transmission band is combined with gap II to form a new low-transmission band (Figure 4.2 (e) and (f)). In the final situation, almost the whole spectrum becomes a transmission band, but
with significantly different probability for electrons with different energy. This new band structure cannot be obtained by any weak field approximation, and it is not predicted by any semiclassical calculations. Actually, what is described here seems to be the details of the Zener Breakdown, when the electric field is strong enough to make the nonconducting crystal become conducting, although of low conductivity.

From the changed spectrum, one can obtain the following conclusions: (1) the first gap, which has been studied extensively in the literature undergoes moderate shifts in the presence of an electric field, whereas the second gap is greatly expanded for moderate field strength; (2) an electron with an eigenenergy initially at a transmission (conduction) state may become a gap electron in the field and vice versa; (3) as the field strength is increased, the whole spectrum undergoes a drastic reconstruction, i.e. the first transmission band collapses, and then rises again, and merges with gap II to become a lower transmission band. These changes in transmission spectrum affect the electronic conductivity, and results, in some cases, in an oscillation between negative and positive differential resistances. I now study the transition processes at the transmission band edges.

Figure 4.3 shows how the electric field affects the transmission coefficient of the electron at the left and right gap edges; (a) for $E = 15$, a gap point when there is no electric field, is transformed into a transmission point by the electric field when $E \geq 0.06$; (b) for $E = 12$, a transmission point when there is no field, is transformed into a gap state when $0.02 < E < 0.05$, and then return to a transmission point for larger field strengths. In both cases after escaping from the gap, the transmission coefficient increases smoothly over an interval of about 0.1, and then oscillates as the field is increased. I can see that on the average, the nonconducting insulator had become a conductor with some erratic behavior, which is the result of the Zener Breakdown [7].
4.4 Conclusion

I have shown in the framework of time-independent quantum mechanical treatment that the transmission spectrum of a superlattice undergoes fundamental changes in the electric field. Such changes will show up in electric conductivity of the superlattice. In particular, one can calculate the conductivity by considering all the channels for a specific energy configuration of electrons. I notice that the localization behavior in a disordered or quasiperiodic infinite system in the presence of an electric field has been studied extensively within the tight-binding model [121, 123, 125], and it has been found that localization is either weakened or sometimes totally eliminated by the field. It would be interesting for one to use the present model to study how disorder in a finite system would affect the transmission property and hence the conductivity of the electrons in the electric field.
It is clear from the introduction and historical reviews that I need to develop a full-Hamiltonian independent-electron model that either solves or avoids those clearly stated problems in §1.2. Within the framework of the independent-electron models, one has to make a choice between a constant-mass model or a piecewise-constant effective-mass model. I argue here that since I am looking for BO, a mesoscopic quantum oscillation involving several neighboring wells, the detailed local phenomena determined by the local properties are averaged out. We are focusing on the minibands determined by the global potential, not the bulk bands determined by each materials' crystalline lattice. After some coarse graining, one uses a global constant mass, either as an effective mass determined by the global potential, or the bare electron mass, and let the phenomenological value of potential $V$ carry most or all of the information from the real superlattice. In this chapter, I build a simple time-dependent quantum mechanical exact model with constant-mass, taken as the bare electron mass.

5.1 Framework

To simplify the problem, I restrict the solution here to (i) a time-independent electric field, and (ii) a sinusoidal (Mathieu-type) lattice potential model. But the method can be expanded to accommodate time-dependent fields, square-well or \( \delta \)-function lattice potentials.
Since Bloch [2] initiated the problem by proposing BO in momentum space (who used the scalar-potential gauge to represent the electric field), it seems that the momentum representation is the natural representation. And the advantage of choosing a vector potential gauge is evident in the work of Krieger and Iafrate [79] (who used the real-space representation). I make two \textit{a priori} choices: (1) momentum representation (\(k\)-space); and (2) vector potential gauge

\[
A = -\varepsilon t,
\]

\[
\varphi = 0
\]

so that

\[
\varepsilon = -\nabla \varphi - \frac{\partial A}{\partial t}
\]

is a constant.

The last two choices wouldn't help anything unless we expand the periodic potential in a Fourier series, as Churchill and Holmstrom once did [77] (who used the real space representation and scalar potential gauge), and use the momentum-space translation operator, which becomes obvious after I've chosen the Mathieu-type potential as a first-order representation of any periodic lattices. To make the energy non-negative, I choose

\[
V(x) = V_0[1 + \cos(k_0 x)],
\]

therefore in the momentum space, the potential energy operator is

\[
V(\hat{x}) = V_0 + \left(\frac{V_0}{2}\right)[\exp(p_0 \frac{\partial}{\partial p}) + \exp(-p_0 \frac{\partial}{\partial p})],
\]

where \(k_0 = 2\pi/\ell\) is the width of the Brillouin Zone (BZ), and \(p_0 = \hbar k_0\). Using the displacement operator

\[
\exp(p_0 \frac{\partial}{\partial p}) \phi(p) = \phi(p + p_0),
\]
the time-dependent Schrödinger's equation in the momentum representation is

\[ i\hbar \frac{\partial}{\partial t} \phi(p, t) = \left( \frac{(p - e\mathcal{E}t)^2}{2m} + V_0 \right) \phi(p, t) + \frac{V_0}{2} [\phi(p + p_0, t) + \phi(p - p_0, t)]. \]  (5.7)

Thus the wavefunction in one BZ is coupled to wavefunctions in the nearest BZ's. There are three time scales in this equation which are defined by:

\[ \tau_A = \frac{\hbar}{(p_0^2/2m)} = \frac{m\mathcal{E}}{\hbar} \]  \hspace{1cm} (5.8)

\[ \tau_B = \frac{p_0/e\mathcal{E}}{\hbar/e\mathcal{E}d} \]  \hspace{1cm} (5.9)

\[ \tau_C = \frac{\hbar}{V_0}. \]  \hspace{1cm} (5.10)

The first is related to the time for a free particle, having momentum \( p_0 \), to travel a lattice spacing \( d \): that time is \( \pi\tau_A \). The second is the Bloch period. The third is related to the barrier height. There is a fourth relevant time scale that does not appear in Eq.(5.7), that is the wavefunction's dephasing time \( \tau_S \) which is due to scattering.

To analyse Eq.(5.7), divide the momentum axis into segments of length \( p_0 \),

\[ p = p_0(n + \bar{p}), \]  \hspace{1cm} (5.11)

where \(-1/2 \leq \bar{p} < 1/2\) is the reduced momentum in one BZ, and \( n = \text{integer} \). Changing the notation slightly \( \phi(p, t) \rightarrow \phi_{\bar{p},n}(t) \), then Eq.(5.7) becomes

\[ i \frac{d}{dt} \phi_{\bar{p},n}(t) = \left( \frac{1}{\tau_A} (\bar{p} + n - \frac{t}{\tau_B})^2 + \frac{1}{\tau_C} \right) \phi_{\bar{p},n}(t) + \frac{1}{2\tau_C} [\phi_{\bar{p},n+1}(t) + \phi_{\bar{p},n-1}(t)]. \]  (5.12)

We can always nondimensionalize the last equation using any of the four time scales as the situation requires. Then the problem is reduced to a set of coupled first-order differential equations in a tridiagonal matrix form

\[ i \frac{d}{dt} f_{\bar{p}}(t) = H_{\bar{p}}(t) f_{\bar{p}}(t) \]  \hspace{1cm} (5.13)
where $f^\rho(t)$ is the wavefunction for reduced momentum $\vec{p}$ in a column vector form
\[
f^\rho(t) = \begin{pmatrix} \vdots \\ \phi^\rho_{\mu,-1}(t) \\ \phi^\rho_{\mu,0}(t) \\ \phi^\rho_{\mu,1}(t) \\ \vdots \end{pmatrix} \tag{5.14}
\]
and the "Hamiltonian matrix" is
\[
H^\rho(t) = T(q) + V, \tag{5.15}
\]
where
\[
q = \vec{p} - t/\tau_B. \tag{5.16}
\]
The "kinetic matrix" is
\[
T(q) = \frac{1}{\tau_A} \begin{pmatrix} \vdots \\ \cdots (q-1)^2 \\ \cdots (q+0)^2 \quad 0 \\ \cdots (q+1)^2 \\ 0 \end{pmatrix}, \tag{5.17}
\]
and the "potential matrix" is
\[
V = \frac{1}{\tau_C} \begin{pmatrix} \vdots \\ \cdots 1/2 \\ \cdots 1 \quad 1/2 \\ \cdots 1/2 \\ 0 \end{pmatrix}, \tag{5.18}
\]
In general since $H^\rho(t)$ is time-dependent and non-diagonal, closed-form analytical solutions are hard to obtain. But the whole problem is already simplified to a set of coupled first-order differential equations without making any approximations at all. Given the initial condition of the electron wave packet in real or momentum space, then its time-evolution is determined, and can be obtained numerically by integrating this set of equations. In its matrix-vector form, this equation becomes the starting point of my later analysis.
5.2 Limiting Cases

How a model behaves in the limits of known situations is the testing ground of a new model. For WS electrons, a good model must behave reasonably at the field-free, free-space, and semiclassical limits.

5.2.1 The Field-free Limit

Our model reproduces the mainline thoughts of traditional solid-state physics on this topic in the field-free limit (see Appendix A), when the wave function is composed of superpositions of Bloch functions, summed over the first BZ, which can be expanded by eigenfunctions of different energy bands.

At zero field the electron oscillates with eigenfrequencies determined by the lattice. When a uniform static electric field is present, no matter how weak it is, no such solution exists. Some have tried \[82, 103\] to solve the problem in real-space, by putting a specific boundary condition like infinite-well at the end of a finite lattice model, solving for the eigenstates and eigenenergies, then composing by superposition to get a wavefunction to represent the time-evolution of WS electrons. These solutions are inadequate, because by bringing specific boundary conditions one gets discrete eigenenergies, which WS electrons don't have. Their energy spectra has been rigorously proven to be continuous \[64\] (commented in \[97\]), and the so-called BO \[103\] resulting from such algorithms are therefore not physical.

5.2.2 The Free-space Limit

When \( V_0 \to 0, \tau_c \to \infty \), therefore all the off-diagonal terms go to zero. No bands are formed, and the electrons motion should return to free-electron motion. Since the Hamiltonian becomes diagonal

\[
\frac{id}{dt} \phi_{\mathbf{p},n}(t) = \frac{1}{\tau_A} (\mathbf{p} + n - \frac{t}{\tau_B})^2 \phi_{\mathbf{p},n}(t),
\]

(5.19)
it has closed form solution (remember \( p = p_0(\bar{p} + n) \), and \( \phi(p, t) = \phi_{p,n}(t) \))

\[
\phi(p, t) = \exp \left\{ i\left( \tau_A \frac{p}{p_0} - \frac{t}{\tau_B} \right)^3 - \left( \frac{p}{p_0} \right)^3 \right\} \phi(p, 0). \tag{5.20}
\]

The Fourier transform of which

\[
\psi(x, t) = \frac{1}{\sqrt{2\pi\hbar}} \int \phi(p, t) \exp(ipx/\hbar) dp \tag{5.21}
\]
describes the real-space motion. Assume the initial condition to be a resting Gaussian packet

\[
\psi(x, 0) = \sqrt{\frac{1}{\sqrt{\pi}\sigma}} \exp(-x^2/2\sigma^2), \tag{5.22}
\]

\[
\phi(p, 0) = \sqrt{\frac{\sigma}{\hbar\sqrt{\pi}}} \exp(-\sigma^2p^2/2\hbar^2), \tag{5.23}
\]

then we can find the wave function

\[
\psi(x, t) \propto \exp\left[\frac{-x(t)^2}{2\sigma(t)^2}\right], \tag{5.24}
\]

where \( x(t) = x + eEt^2/2m \), and \( \sigma(t) = \sqrt{\sigma^2 + \hbar^2t^2/m^2\sigma^2} \), which is an expanding free-particle Gaussian wave packet with it’s center moving with an acceleration of \( a = eE/m \). Thus this model satisfies the acceleration theorem at the free-space (weak barrier) limit.

### 5.2.3 The Semiclassical Limit

From Eq.(5.8)-(5.10), as the Planck’s constant \( \hbar \to 0 \), we can see that \( \tau_A \to \infty \), \( \tau_B \to 0 \), and \( \tau_C \to 0 \). Then the Hamiltonian matrix will be \( \bar{p} \)-independent, for any nonzero time, and also independent of the BZ index \( n \), since

\[
\frac{1}{\tau_A}(\bar{p} + n - \frac{t}{\tau_B})^2 \to \frac{t^2}{\tau_A\tau_B^2} \tag{5.25}
\]

and

\[
\tau_A\tau_B^2 = \frac{2m}{e^2E^2\hbar} \tag{5.26}
\]
is of the same order with $\tau_C = \hbar/V_0$. Since now the "kinetic matrix" of Eq.(5.17) has become a $c$-number times the identity matrix

$$T = \frac{e^2 \mathcal{E}^2 t^2}{2m\hbar} I,$$

(5.27)

it can be transformed away by a universal phase factor which has no physical effect. Let

$$f(t) = \exp[-i\frac{e^2 \mathcal{E}^2 t^3}{6m\hbar}]g(t),$$

(5.28)

then $g(t)$ is determined by the equation

$$i\frac{d}{dt}g(t) = Vg(t)$$

(5.29)

that is independent of the electric field. Thus all electric-field-induced physical effects are pure quantum effects, and have no classical correspondence. The criticism of Churchill and Holmstrom [82] that BO does not satisfy the correspondence principle was right, that the true BO should simply disappear at the semiclassical limit, and have no classical correspondence.

5.3 Method for obtaining Field-free Bands of Different Potential Models

Traditionally, people calculate the energy bands by resorting to a Kronig-Penney model ($\delta$-function potentials) (e.g. [195]), therefore the results are analytically approximated and the errors are hard to assess. A product of the new model is that it provided an easy method to calculate the field-free bands simply by numerically diagonalizing the truncated Hamiltonian matrix $\mathcal{H}_p$ for a selection of $\widetilde{p}'s$ in the first BZ.
When the electric field is zero, \( r_B \to \infty \), therefore \( H_p \) is independent of time

\[
H_p = \frac{1}{\tau_C} \begin{pmatrix}
\ddots & \ddots & \ddots \\
\frac{1}{2\tau_C} & \frac{1}{\tau_A}(\bar{\beta} - 1)^2 & \frac{1}{2\tau_C} \\
0 & \frac{1}{\tau_A}(\bar{\beta} + 0)^2 & \frac{1}{2\tau_C} \\
\end{pmatrix} I + \begin{pmatrix}
\ddots \\
\frac{1}{2\tau_C} \\
0 \\
\end{pmatrix}
\]

The diagonal elements increase quadratically with the matrix element's index, and the off-diagonal terms are constant. When that index is large enough, say \( n \gg \sqrt{\tau_A/\tau_C} \), then that diagonal element is about equal to an eigenvalue of \( H_p \), and a unit vector with element zero everywhere but one at that index is an eigenvector. We can truncate the matrix to be dimension \( 2N+1 \), where the index \( n \) in the diagonal elements satisfies \(-N < n < N\), and \( N \) satisfies \( N \gg \sqrt{\tau_A/\tau_C} \).

By diagonalizing numerically \( H_p \) and scan \( \bar{p} \) over the first BZ \((-1/2 < \bar{p} < 1/2)\), I get the dispersion relation. We can change the \( N \) in the truncation dimension \( 2N+1 \) to observe the quadratic pattern in the eigenvalues in order to determine the accuracy of calculation. More rigorous estimate of the converging rate is yet to be done, but numerically it converges very fast. The results are only numerically approximated, and can be calculated to any required accuracy by increasing the matrix size. The lowest few bands can be gotten by very low truncation dimensions like \( 20\sqrt{\tau_A/\tau_C} \).

This method can be used on all kinds of potential models. A Sinusoidal Model (SM) (Mathieu-type potential) is the first Fourier component of a periodic potential. If \( V(x) = V(x + d) \), then

\[
V(x) = \sum_{n=0}^{\infty} a_n \cos(nk_0 x) + \sum_{n=1}^{\infty} b_n \sin(nk_0 x) \tag{5.31}
\]

where \( k_0 = 2\pi/d \), and

\[
a_n = \frac{2}{d} \int_{-d/2}^{d/2} V(x) \cos(nk_0 x) dx, \quad n = 0, 1, 2, \ldots \tag{5.32}
\]

\[
b_n = \frac{2}{d} \int_{-d/2}^{d/2} V(x) \sin(nk_0 x) dx, \quad n = 1, 2, \ldots \tag{5.33}
\]
If $V(x)$ is symmetric about the origin, i.e. $V(x) = V(-x)$, then $b_n = 0$.

5.3.1 Square-Well Model

For the well-known Square-Well Model:

$$V(x) = \begin{cases} V_0, & (nd - \frac{b}{2} \leq x < nd + \frac{b}{2}) \\ 0, & (nd + \frac{b}{2} \leq x < (n + 1)d - \frac{b}{2}) \end{cases}$$

(5.34) \hspace{1cm} (5.35)

where $b$ is the barrier width, $d$ is the lattice constant, $w = d - b$ is the well-width, and $n = \text{integer}$, (The potential is chosen to be symmetric about the origin so that the odd terms in its Fourier series disappear), then

$$V(x) = \frac{V_0 b}{d} + \sum_{n=1}^{\infty} \frac{2V_0}{\pi n} \sin \left( \frac{n \pi b}{d} \right) \cos (nk_0 x).$$

(5.36)

By applying the displacement operator, and defining the same time scales as before, we get the same equation set as Eq.(5.13). The Hamiltonian matrix is still the sum of the same "kinetic matrix" as in Eq.(5.15), and a new "potential matrix" which has more off-diagonal terms that decreases as they get further from the diagonal. $H_p(t) = T(q) + V$, where $q = \ddot{p} - t/\tau_B$, and the new "potential matrix" is

$$V = \frac{1}{\tau_c} \begin{pmatrix} \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & a_0 & a_1 & a_2 & a_3 & a_4 \\ \cdots & a_1 & a_0 & a_1 & a_2 & a_3 \\ \cdots & a_2 & a_1 & a_0 & a_1 & a_2 \\ \cdots & a_3 & a_2 & a_1 & a_0 & a_1 \\ \cdots & a_4 & a_3 & a_2 & a_1 & a_0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix},$$

(5.37)

where $a_0 = b/d$, and

$$a_n = \frac{2 \sin (n \pi b/d)}{\pi n}$$

(5.38)

for $n = 1, 2, 3, \ldots$. As $n \to \infty$, $a_n \to 0$. 
5.3.2 Kronig-Penney Model

For the Kronig-Penney Model (KPM) ($\delta$-function potentials, Dirac Combs), if I choose the potential to be symmetric about the origin

\[ V(x) = \sum_n [(V_0d) \delta(x - nd)], \quad n = \text{integer}, \quad (5.39) \]

where I've inserted $d$ to make $V_0$ an energy, because the dimension of $\delta(x)$ is the inverse of length, then its Fourier expansion is

\[ V(x) = V_0 + \sum_{n=1}^{\infty} 2V_0 \cos(nk_0x); \quad (5.40) \]

therefore in its “potential matrix” $V$, $a_0 = 1$, and $a_n = 2$, for $n = 1, 2, 3, \ldots$. Since all off-diagonal terms are the same no matter how far from the diagonal, it is hard to estimate legitimate truncation dimensions. However numerically the eigenvalues of the Kronig-Penney model still appear to converge to a quadratic pattern as $N$ increase, just slower than the square-well or sinusoidal model.

In general the algorithm, or rather method, to calculate the energy band of a one-dimensional periodic potential is: (1) write down the Fourier series of the potential; (2) write down a “potential matrix” according to the Fourier coefficients; (3) adding the “kinetic matrix” for certain reduced momentum $\tilde{p}$ to have the “Hamiltonian matrix”; (4) numerically diagonalize the above Hamiltonian matrix in any reliable software packages, such as using the command “Eigenvalues[ ]” in Mathematica. (5) Do the above for a sufficient number of reduced momenta to determine the dispersion relation.
CHAPTER 6

EXISTENCE OF LADDERS

Now that I have built a full-Hamiltonian independent-electron model which fits the physical requirements at interesting limiting cases, the challenge now is whether it produces a ladder-like structure like WSL which has been convincingly observed by experiments.

6.1 General Features

Notice the following characteristics of the Hamiltonian matrix $\mathbf{H}_p(t)$

$$\mathbf{H}(q) = \frac{1}{\tau_C} \mathbf{I} + \begin{pmatrix}
\cdots & \frac{1}{2\tau_C} & \frac{1}{\tau_A}(q-1)^2 & \frac{1}{2\tau_C} & \frac{1}{\tau_A}(q+0)^2 & \frac{1}{2\tau_C} & \frac{1}{\tau_A}(q+1)^2 & \frac{1}{2\tau_C} & \cdots \\
0 & \frac{1}{2\tau_C} & \frac{1}{\tau_A}(q-1)^2 & \frac{1}{2\tau_C} & \frac{1}{\tau_A}(q+0)^2 & \frac{1}{2\tau_C} & \frac{1}{\tau_A}(q+1)^2 & \frac{1}{2\tau_C} & \cdots \\
\end{pmatrix}, \quad (6.1)$$

where $q = \tilde{p} - t/\tau_B$:

1. It is real and symmetric, therefore Hermitian, and so there is no dissipation of the wavefunction $f_p(t)$.

2. Every wavefunction in one BZ is coupled to the wavefunctions in two neighboring BZ’s with the same $\tilde{p}$ (wavefunctions in the nearest and next-nearest minibands). If $V_0 \to 0$, so $\tau_C \to \infty$, then the interzone coupling disappears, but that results in an accelerating free electron without BO. Therefore the dynamics of BO described here is an inherently multi-BZ phenomenon. There is a difference between
the concepts of multiband and multizone. If the particle is sharply localized in momentum space and nearly free, then moving to a different BZ does mean changing to the next energy band, because the nearly-free particles have a parabolic dispersion relation, and just breaks a little at the BZ edge. However if the particle's wavefunction is extended in momentum space and is tight-bound, then moving a portion (even the major part) of the wavefunction to a different BZ does not mean the particle changes energy bands. This shows the ineptness of the concept of 1-BZ energy bands in the presence of an external field which breaks the periodic symmetry. A multizone model that gives the probability of the particle at different momenta and different bands is more complete in describing the particle's quantum motion.

(3) Because $H_p(t)$ is an infinite matrix, it comes back to itself after a time elapse of one Bloch period $\tau_B$, by shifting down one row and one column to the right. In other words, $H_p(t)$ has a “Shifting Periodicity”. i.e.

$$H_p(t + \tau_B) = S H_p(t) S^{-1},$$

where $S$ is the Shifting Operator, which is the infinite identity matrix shifted one column to the right

$$S = \begin{pmatrix}
... & ... & ... & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 \\
\end{pmatrix}. \quad (6.3)$$

The shifting adds 1 to all indices of each element in the matrix $H_p(t)$, and we have $S^{-1} = S^T$, where $T$ stand for transpose.

6.2 Shifting Periodicity

Shifting Periodicity is a special kind of periodicity related to the special kind of symmetry that remains after the spatial periodicity is broken by the presence of the
uniform static electric field. To an electron in a quantum well, its surroundings is still similar to the electron in the neighboring wells, even though their energies are not the same. This is a symmetry of less order than the spatial translational periodicity. It may be called translational similarity.

Shifting periodicity was implicitly contained in the works of early authors like Houston [10]. If the initial wavefunction is a Bloch function \( \psi_n(k_0, x) \), the wavefunction at time \( t \) is

\[
\psi(x, t) = \exp(-iHt/\hbar) \psi_n(k_0, x),
\]

where \( H = H_0 + eE x \), where \( H_0 \) is the crystal Hamiltonian. By applying a crystal translation \( d \), we get

\[
\psi(x + d, t) = \exp[ik(t)d] \psi(x, t),
\]

where

\[
k(t) = k_0 - \frac{eEt}{\hbar}.
\]

So the wavefunction will always be a Bloch function. What is interesting is that if \( t \to t + \tau_B \), where \( \tau_B = \hbar/eEd \), then a change of \( k_0 \to k_0 + 2\pi/d \) will keep the dynamical momentum \( k(t) \) unchanged. An apparent time-momentum symmetry!

A word that should be addressed is that the initial state being a Bloch function and the electric field being a constant are not compatible. Physically a Bloch state can only be prepared if there is no electric field present. A process of turning-on the field would make the field not a constant for all times. That’s why Houston’s function is only an approximation for weak field and strong barriers. In this case I haven’t assumed any functional requirement for initial wavefunctions, and therefore my claims are more general. So even though this “shifting periodicity” symmetry in momentum and time was implied in the results of earlier authors, it had not been identified, stated, emphasized or utilized to study the dynamics of WS electrons as I
have done, according to the knowledge we currently have through investigating the literature. For the remaining symmetry of a periodic lattice at the presence of a uniform electric field, here is a general result:

6.2.1 Bloch-Floquet Theorem

For a Hamiltonian that has time-periodicity

\[ H(t + T) = H(t), \quad (6.7) \]

there is Floquet's Theorem [1], which states that the wavefunctions can be written as

\[ \psi(t) = u_E(t) \exp(iEt), \quad (6.8) \]

where \( E \) is called the pseudo-energy, and the function \( u_E(t) \) satisfies

\[ u_E(t + T) = u_E(t). \quad (6.9) \]

For a Hamiltonian that has spatial periodicity

\[ H(x + d) = H(x), \quad (6.10) \]

there is Bloch's Theorem [203], which states that the wavefunctions can be written as

\[ \psi(x) = u_K(x) \exp(iKx), \quad (6.11) \]

where \( K \) is called the pseudo-momentum, and the function \( u_K(t) \) satisfies

\[ u_K(x + d) = u_K(x). \quad (6.12) \]

For a Hamiltonian that has "Shifting Periodicity", that is, a combination of time and "(momentum) space" (position in the matrix) periodicity

\[ H(t + T) = SH(t)S^{-1}, \quad (6.13) \]
I can prove the following result which I named the “Bloch-Floquet Theorem”: that (a) the eigenvalues $E(t)$ of $H(t)$ are periodic

$$E(t + T) = E(t);$$

(6.14)

and (b) the eigenvectors are shifting-periodic, and can be written as

$$f(t) = u_\omega(t) \exp(i\omega t)$$

(6.15)

where $\omega$ is called the pseudo-energy, and the function $u_\omega(t)$ satisfies

$$u_\omega(t + T) = Su_\omega(t),$$

(6.16)

where $S$ is the shifting operator. The proof is given in Appendix B.

Bloch’s theorem is mathematically the same as Floquet’s theorem. Bloch simply extended it to three dimensions and utilized ordinary space rather than time. To the same extent the above Bloch-Floquet Theorem can be called a theorem, because even though there is nothing new in essence, there is something new in application.

6.2.2 Expectations

There are two aspects of Shifting Periodicity, one is the shifting, one is the periodicity. I expect the periodicity will cause the Wannier-Stark level-splitting and therefore the BO. In the case of 1-d time-periodic Hamiltonian e.g.

$$H(t) = \omega_0 + \cos(\omega_1 t),$$

(6.17)

the solution to the equation

$$i \frac{d}{dt} f(t) = H(t) f(t)$$

(6.18)

is

$$f(t) = e^{(-i\omega_\omega t)} e^{(-i\omega\sin(\omega_1 t))} f(0).$$

(6.19)
Since

\[ e^{(iz \sin \theta)} = \sum_{n=0}^{\infty} J_n(z) e^{in\theta}, \]  

(6.20)

where \( J_n(z) \) is a Bessel's function of the first kind, therefore the Fourier spectrum of \( f(t) \) is

\[ F(\omega) = \sum_{n=0}^{\infty} J_n(-a) \delta(\omega - (\omega_0 + n\omega_i)) f(0). \]  

(6.21)

So there is a ladder of oscillating frequencies \( \omega_i \) above the original inherent frequency \( \omega_0 \). I expect that the same kind of ladder exists for the vector-matrix case due to the existence of a periodicity.

6.3 Numerical Evidence

To numerically calculate the time evolution of the wavefunction in \( k \)-space, we need to truncate the infinite matrix. The justification comes from the setting of initial conditions. I take the initial wave packet in \( x \)-space to be a few neighboring Gaussian packets at rest centered in wells near the center of the lattice, each with a width of one lattice constant; then it's also localized in \( k \)-space, centered around zero momentum in the first BZ. The neighboring elements in the vector \( f_p(t) \) are wave-functions in \( k \)-space that are separated by \( \text{integer} \times p_0 \), and therefore initially only the few elements of \( f_p(t) \) in the low momentum BZ's are nonzero. I expect the majority of the electron's wave packet to continue being localized in the low momentum BZ's and oscillate, rather than accelerating to higher momenta, unless the barrier strength is very weak and the electric field is very strong. This is an assumption supported by both semi-classical theory and my numerical calculations. Even if part of the packet accelerates, in time \( t = n\tau_B \) it's no further than \( p = mv = m(at) = m(eE/m)n(h/eEd) = nh/d = np_0 \) away from the initial position in momentum space. So I truncate the matrix to \( 2n + 1 \) dimensions, where \( n \) is greater than the total number of Bloch periods I want to calculate. I make a discrete Fourier transform on the time evolution data.
of wavefunction in $k$-space in the central BZ to get the dispersion relationship. For parameters like $d = 100\,\text{Å}$, $V_0 = 20\,\text{meV}$ and $E = 10^8\,\text{V/m}$, we can set $\tau_A = \tau_C = 1$ and $\tau_B = 10$, in the unit of $4 \times 10^{-14}\,\text{sec}$. I also set the total number of lattice periods to be $N = 50$. I find that we do get uniform splitting of one energy level, i.e. the WSL.

Figure 6.1. Dispersion relation of a WS electron, calculated from the time series of a wavefunction in momentum space, under the condition of $\tau_A = \tau_C = 1$, and $\tau_B = 10$, for a total time of $10\tau_B$'s, with $k$ between 0 and $2\pi/d$, where $d$ is the lattice constant, taken to be 1 here. The frequency is in arbitrary units. The initial condition was 11 Gaussians in neighboring wells. For the purpose of visual clarity I plotted $\sqrt{|\phi(k,\omega)|}$ rather than $|\phi(k,\omega)|^2$ on the third axis.
It is not clear why the splitting is only seen on the third band, but what's important is that it exists. All of the high frequency information cannot be retrieved because of the discrete time interval used in the time-evolution calculation. They are confined together in a high pseudo-level. The magnitude of the splitting in the third band appears to be $\omega_B$, which should be one tenth of the band gap. Thus BO seems to exist as a quantum beat between waves that differ in frequency by $n\omega_B$, where $n = 1, 2, \ldots$. The Bloch frequency is the envelope frequency, with the carrying frequencies due to a combination of motions with lattice eigenfrequencies and the increasing high frequencies due to the kinetic term in Eq.(5.12), which causes acceleration. Thus I have numerical indications that shifting periodicity causes a ladder-like structure like WSL in dispersion relations, and results in a certain oscillations with the period of BO, as the result of a multi-BZ coupling.

Since the bands are curved, when the field is weak and the separation is small, the split-levels that rise above the band will fill the whole energy domain to make it continuous. Even though they can be seen in the dispersion relations clearly, they are not discrete energy levels, only resonance levels. The mixture of the split-levels and the original bands make the so-called electric-field-induced changes to energy bands by early authors like Wannier [17]. The transitions between these resonance states causes the red-shift tail of optical absorptions (energy smaller than band gap), that is Franz-Keldysh effect.

6.4 Conditions of Observability

For the effect described above to be observable before the collision processes erase it, it is reasonable to set the three time-scales $\tau_A$, $\tau_B$ and $\tau_C$ to be smaller than the scattering dephasing time $\tau_S$. The first one means that the electron can drift long enough without being scattered; the second means that the electron can oscillate long
enough with being scattered; the third means that the electron can stay in the well long enough without being scattered. These three conditions

\[
\tau_A = \frac{md^2}{\pi\hbar} < \tau_S, \quad (6.22)
\]
\[
\tau_B = \frac{\hbar}{eE_d} < \tau_S, \quad (6.23)
\]
\[
\tau_C = \frac{\hbar}{V_0} < \tau_S, \quad (6.24)
\]

leads to

\[
d_{\text{min}} < d < d_{\text{max}}, \quad (6.25)
\]
\[
V_0 > V_{0\text{min}}, \quad (6.26)
\]

where

\[
d_{\text{min}} = \frac{\hbar}{eE\tau_S}, \quad (6.27)
\]
\[
d_{\text{max}} = \sqrt{\frac{\pi\hbar\tau_S}{m}}, \quad (6.28)
\]
\[
V_{0\text{min}} = \frac{\hbar}{\tau_S}, \quad (6.29)
\]

For \(d_{\text{min}} < d_{\text{max}}\) to be true, one gets the general requirement for electric field and scattering time

\[
E^2\tau_S^3 > \frac{m\hbar}{\pi e^2} = 7.38 \times 10^{-27} (V/m)^2 s^3, \quad (6.30)
\]

where \(m\) is taken to be the electron's naked mass \(m_e = 9.1 \times 10^{-31} kg\). This means that for a given scattering time determined by the material and temperature, a minimum electric field is required. For typical value \(\tau_S = 10^{-13} s\), the minimum field is \(E = 2.7 \times 10^6 V/m\) which is very high at that small scale. A slight increase in the scattering time will greatly decrease the required electric field strength. At these values we have

\[
d = 150\text{Å}, \quad (6.31)
\]
\[
V_{0\text{min}} = 6.6 \text{meV}, \quad (6.32)
\]
which are all in experimentally achievable ranges these days. That means the WSL observed by experimentalists today are probably the effect described above.
CHAPTER 7

EXISTENCE OF OSCILLATIONS

Energy levels of constant spacing produce quantum beats of wavefunctions that exhibit oscillatory motions with the frequency proportional to the level difference. It is a general belief that WSL and BO validate each other.

7.1 An Analytical Solution

Since all time-dependence of the Hamiltonian matrix \( H_p(t) \) is through the parameter \( q = \bar{p} - t/\tau_B \), I can expect the time-dependence in the eigenvalues and eigenvectors of \( H(q) \) to be through the same intermediate parameter \( q \). Now for simplicity, I drop the label of \( \bar{p} \) in notation, and diagonalize the real and symmetric Hamiltonian matrix

\[
H(t)\psi_j(t) = E_j(t)\psi_j(t),
\]

where the eigenvectors can be taken to be real. (In numerical calculation we always get a real answer, except a possible difference of \( \pm 1 \). I have to "smooth" it by calculating them at very close time moments and require their inner product to be almost one (normalized), otherwise change the sign of one of them. This way we get the eigenvectors to have the same phase factor.) Since \( H(t) \) is shifting periodic, then \( E_j(t) \) is periodic with period \( \tau_B \), and \( \psi_j(t) \) is shifting periodic. (See Bloch-Floquet Theorem in Appendix B.) Now the solution of the Schrödinger’s equation

\[
\frac{d}{dt}\phi(t) = H(t)\phi(t)
\]
at any moment can be expanded according to the eigenvectors at that moment, i.e.

$$\phi(t) = \sum_{j=0}^{\infty} c_j(t) \psi_j(t).$$

(7.3)

Put the last expression into the Schrödinger's equation, we have

$$\sum_{j=0}^{\infty} \left[ i \dot{c}_j(t) \psi_j(t) + c_j(t) i \dot{\psi}_j(t) \right] = \sum_{j=0}^{\infty} \left[ c_j(t) E_j(t) \psi_j(t) \right],$$

(7.4)

where $\dot{c}_j(t)$ is the time derivative of $c_j(t)$. Since the eigenvectors are orthonormal at any moment

$$\psi_k(t) \cdot \psi_j(t) = \delta_{kj},$$

(7.5)

if we make an inner product with a row eigenvector $\psi_k(t)$ on the left of Eq.(7.4), we get

$$i \dot{c}_k(t) = E_k(t) c_k(t) - i \sum_{j=0}^{\infty} c_j(t) \psi_k(t) \cdot \dot{\psi}_j(t).$$

(7.6)

Since the orthonormality gives us

$$\psi_k(t) \cdot \dot{\psi}_k(t) = \frac{1}{2} \frac{d}{dt} [\psi_k(t) \cdot \psi_k(t)] = \frac{1}{2} \frac{d}{dt} [1] = 0,$$

(7.7)

and the time-dependence through $q = p - t/\tau_B$ gives

$$\dot{\psi}_j(t) = -\frac{1}{\tau_B} \frac{d}{dq} \psi_j(q(t)),$$

(7.8)

we have

$$\dot{c}_k(t) = -i E_k(t) c_k(t) + \frac{1}{\tau_B} \sum_{j \neq k} g_{kj}(t) c_j(t),$$

(7.9)

where

$$g_{kj}(t) = \psi_k(q(t)) \cdot \frac{d}{dq} \psi_j(q(t))$$

(7.10)

describes interband interactions. For weak fields, $\tau_B \to \infty$, the interband term can be neglected. Notice that the sum is functionally determined by $q$ regardless of field, therefore is not divergent, so my perturbation is not singular. The definition of "weak
field" can be given by $\tau_B \gg \max\{\tau_A, \tau_C\}$. Now we have an analytical solution to the 0th order of the electric field

$$\phi(t) = \sum_{j=0}^{\infty} c_j(0) \exp\left[-i \int_0^t E_j(t) dt\right] y_j(t)$$

(7.11)

which is very similar to the Houston function (see §2.1.9), but is in momentum space.

The Bloch-Floquet Theorem (Appendix B) gives us two results of the shifting periodic Hamiltonian: (1) the eigenvalues $E_j(t)$ are periodic; (2) the eigenvectors $y_j(t)$ are shifting periodic. All of them are functionally determined by $q = \vec{p} - t/\tau_B$.

Since $E_j(q)$ is periodic in $q$ with period 1, and is symmetric about $q = 0$, it can be expanded as a Fourier series with only even terms

$$E_j(q) = E_j^{(0)} + \sum_{n=1}^{\infty} E_j^{[n]} \cos(2\pi n q).$$

(7.12)

The higher levels need more terms to approximate. The lowest discrete bands can be approximated as

$$E_j(q) = B_j + \frac{W_j}{2} \left[ 1 - \cos(2\pi q - j\pi) \right],$$

(7.13)

where $B_j$ is the bottom of the band, and $W_j$ is the width of the band. Since $2\pi q = 2\pi \vec{p} - \omega_B t$, we have the approximated analytical solution for weak field

$$\phi(t) = \sum_{j=0}^{\infty} c_j(0) \exp\left[-i(a_j + b_j t)\right] \exp\left[i r_j \sin(\omega_B t - \varphi_j)\right] y_j(t),$$

(7.14)

where

$$a_j = \frac{W_j}{2\omega_B} \sin(\varphi_j),$$

(7.15)

$$b_j = B_j + \frac{W_j}{2},$$

(7.16)

$$\varphi_j = 2\pi \vec{p} - j\pi,$$

(7.17)

$$r_j = \frac{W_j}{2\omega_B}.$$

(7.18)
This phase factor \( \exp[ir_j \sin(\omega_B t - \varphi_j)] \) can be expanded into Bessel’s functions and Harmonic oscillators

\[
\exp[ir_j \sin(\omega_B t - \varphi_j)] = \sum_{n=0}^{\infty} J_n(r_j) \exp[i n(\omega_B t - \varphi_j)]
\]

(7.19)

whose Fourier transform in time will have a ladder-like structure with level difference of \( \omega_B \).

### 7.2 Properties of the Shifting Periodic Basis

I choose the parameter range of \( \tau_A = \tau_C = 1, \tau_B = 10 \). Knowing that \( H_p(t) = H(q) \), where \( q = \bar{\rho} - t/\tau_B \), we can generally diagonalize the Hamiltonian \( H(q) \) to know all situations. The functional form of the eigenvalues and eigenvectors are independent of the electric field, and depends only on the relative strength of the barriers. We can see from the dispersion relation the periodicity of the eigenvalues.

![Figure 7.1. Periodicity of the eigenvalue of a shifting periodic Hamiltonian. Plotted for two BZ's. Two discrete bands exist.](image)

When the lattice potential gets weaker, the band-gaps get smaller till all states are the continuous states. When the lattice potential gets stronger, the band-gaps become larger. Figures 7.2 and 7.3 show the ground state's eigenvector at different \( q \)'s in the two BZ's.
Figure 7.2. The ground state's eigenvector for different acting reduced momentum $q$'s in the one BZ at the left of $q = 0$. 
Figure 7.3. The ground state’s eigenvector for different acting reduced momentum $q$’s in the one BZ at the right of $q = 0$. 
The vertical lines are drawn to remind that these values are at discrete positions in a wavefunction-vector, representing different BZ's. The connection lines were drawn to make the change of shape more visible.

When the lattice is weak, i.e. $V_0 \rightarrow 0$, the eigenvector is very localized around one BZ. The stronger the barrier becomes, the more extended the wavefunctions is in momentum space.

The center of the localized wave-packet moves one site when the "acting reduced momentum" $q$ increases one BZ length. This is the shifting, the result of the acceleration effect.

The shape of the packet undergoes a periodic change around the accelerated center, if we can imagine the change to be on a continuous axes. This is a result of the lattice' periodicity. The packet is symmetric at the stable point of a band (center of the BZ for the ground state), and is anti-symmetric at the unstable point (the boundary of BZ for the ground state). It restores its shape after $q$ changes one (BZ), or time changes one $\tau_B$, but changes a sign (without affecting the probability density). A total restoration happens after $q$ changes two (BZ's), or time changes two $\tau_B$'s.

As the packet wiggles around its accelerating center, the average momentum will have an oscillating factor coupled to the acceleration. This confirms Bloch's physical intuition, but that effect is only in the average.

If we try to separate the two effects, by approximating the wave-packet to be a localized oscillating packet, around the accelerating center, then one can get the basis for Houston function in Eq.(2.4), after a Fourier transform to the real-space representation.
7.3 Analysis of the Analytical Solution at Weak Fields

Since the weak-field approximation was not applied when we derive Eq.(7.11) until the last step, and I also have checked that this approximation is not singular. So if Eq.(7.11), therefore Eq.(7.18) contains WSL and BO, then I can claim that we have derived WSL and BO without encountering the specific theoretical difficulties stated in §1.2, especially the first eight of them.

There are several points that can be observed in Eq.(7.18):

(1) There are two ways for the periodicity with time $\tau_B$ to appear in the solution: One is in the periodic phase factor, which I denote as the first kind, and will show that it determines the WSL; another is in the shifting periodic basis function $\psi^{(3)}_p(t)$ which oscillates around an accelerating center, which I denote as the second kind, and will show that it determines the BO.

(2) Since the first way $\tau_B$ appears is in a phase factor, if the initial condition is set that the electron was on one band only, e.g. $c_j(0) = \delta_{j0}$, then it has no physical effect, even if in numerical calculations, a time Fourier transform of the time series of the wavefunction shows the ladder-oscillation structure. It will have to be the time Fourier transform of the probability density. Our numerical result on Chapter 6 was a Fourier transform of the wave function, therefore only shows the existence of a ladder-oscillation structure in the wavefunction, but didn’t prove its physical reality.

(3) If the initial wave packet initially occupies more than one band, then the interband quantum interference will have a ladder-oscillation caused by this phase factor. So the physical Stark-ladder is not only a multizone phenomenon as I pointed out in Chapter 6, but also has to be a multiband phenomenon. As I had set the initial condition to be a Gaussian in Chapter 6, it had multiple band occupations in the beginning, and therefore the ladder was physical.

(4) If the field is strong enough that the interband interactions cannot be ne-
glected in order to get Eq.(7.11), then the first kind ladder-oscillation is more than a phase factor. It could either be destroyed, or show a distorted ladder with distance not equal to the Wannier value.

(5) The time Fourier transform of the wavefunction $\psi(t)$ convolutes the first kind ladder-oscillation structure in the phase factor with the time-evolution of the shifting periodic bases $v_j(t)$ of the second kind, thus will smear the ladders and give no clear-cut discrete levels.

(6) For the discrete bands like the ground state, the shifting periodic bases $v_j(t)$ have nonzero values on only a few neighboring elements. It is periodically evolving in shape but the center is moving to higher index elements (higher momentum BZ's) at a constant rate determined by the free-electron acceleration caused by the electric field. Since the shape of the wave packet wiggles periodically around the accelerating center, the average momentum will have a periodic oscillation around the acceleration value by the frequency of $\omega_B$. In other words, the average canonical momentum will oscillate during acceleration

$$<p> = eE_0 + c\cos \omega_B t.$$  \hspace{1cm} (7.20)

Thus the average of the mechanical momentum $\pi = p - eE_0$ is

$$<\pi> = c\cos \omega_B t.$$ \hspace{1cm} (7.21)

This is BO as Bloch had described. There is no physical acceleration for electrons on a discrete band. The nature of this oscillation is purely quantum, as may be seen in §8.1.

(7) Ehrenfest's theorem is satisfied by the interband term that destroys a solution in the form of Eq.(7.11). For any nonzero field, as time goes on, the electron will be influenced by the interband term in Eq.(7.9) to move up into a higher band.
If the next band is still a discrete band, BO continues with a different band width and oscillation magnitude, and still no physical acceleration exits. The stronger the field is, the shorter time it takes for the electron to move up. When it moves into a continuous band, like the third band and above in Figure 7.1., the wavefunction take a fundamental change and become extended like the free-electrons plane wave. The average of the canonical momentum is thus a constant, and the average of the mechanical momentum is thus increasing with time

\[ \pi = \pi_0 - e\mathcal{E}t, \]  

and physical acceleration appears, opposite to the direction of the electric field. Erenfest’s theorem is satisfied by electrons in the near-classical states (the continuous states), but not by electrons in the purely quantum states (discrete bands). If the lattice strength is approaching zero (free-space limit), then there is no discrete bands, then no effects like BO exist.

(8) More study into the role of the interband term in Eq.(7.9) may give us the time it takes for the electron to go the continuous band form a discrete band, thus give us the intrinsic lifetime of BO.

(9) The periodic signal cannot be detected by a time Fourier transform of one element of the vector \( \varphi^{(j)}(t) \) (wavefunction in one BZ), because when that period finishes, the shifting (acceleration) caused by the electric field has already moves the nonzero part out of that BZ (damping too fast). Thus what causes BO does not cause WSL.

(10) Physical WSL has to be a multiband phenomenon, but physical BO exist for both one and multiband situation. We always have BO, but not always have WSL, depending on the initial condition. The reason that former theories were so incoherent may be because that they were talking about two different things, that
seemingly are caused by the same origin, but actually have different mechanisms.
An "obvious" fact that is very important to the understanding of BO and WSL is the conservation of probability density for a fixed reduced momentum.

8.1 The Meaning of Bloch Oscillations

The semi-classical picture of BO is a localized wave-packet whose center oscillates in both momentum space and real space while the packet is basically kept together in a reasonably short time. It is this picture that drew criticism when people tried to match it to various limiting cases. Some authors had included the acceleration regime into their picture of BO, but still think that BO is intra-BZ with some inter-BZ motion. I show that even this is not accurate.

I've noticed that in my multizone model, the Schrödinger's equation

\[ i \frac{d}{dt} \phi_p(t) = \mathbf{H}_p(t) \phi_p(t) \tag{8.1} \]

is dependent on the reduced momentum \( \bar{p} \), which gives position in the BZ, and enters Eq.(8.1) as a parameter. All wavefunctions at the same position in different BZ's evolve according to this equation. I have always noticed that since the Hamiltonian matrix is Hermitian, there is no dissipation for wave functions at \( \bar{p} \). But what is the meaning of this "no dissipation"?

The solution of Eq.(8.1) can be symbolically written as

\[ \phi_p(t) = T_p(t) \phi_p(0) \tag{8.2} \]
where the time-evolution operator is

\[ T_p(t) = \exp[-iH_p(t_n)\Delta t] \exp[-iH_p(t_{n-1})\Delta t] \ldots \exp[-iH_p(t_1)\Delta t], \tag{8.3} \]

where \( t_n = n\Delta t, \ n = 1, 2, \ldots N, \) and \( \Delta t = t/N, \ N \to \infty. \) Since \( H_p(t) \) is Hermitian, we have

\[ T_p(t) = I, \tag{8.4} \]

where \( I \) is the unit matrix. Therefore the total probability density of the electron at the reduced momentum \( \tilde{p} \) is

\[ \sum_n |\phi_{\tilde{p},n}(t)|^2 = \phi_{\tilde{p}}(t)^* \phi_{\tilde{p}}(t) \tag{8.5} \]

\[ = \phi_{\tilde{p}}(0)^* T_p(t)^\dagger T_p(t) \phi_{\tilde{p}}(0) \tag{8.6} \]

\[ = \phi_{\tilde{p}}(0)^* \phi_{\tilde{p}}(0) \tag{8.7} \]

\[ = \sum_n |\phi_{\tilde{p},n}(0)|^2. \tag{8.8} \]

In other words, the total probability density of the electron at the reduced momentum \( \tilde{p} \) is conserved. It never leaks to or absorbs from the wavefunctions at other \( \tilde{p} \)'s. As a matter of fact, wavefunctions at different \( \tilde{p} \)'s never mix with each other. If initially an electron is localized in the (canonical) momentum space in a certain BZ at certain \( \tilde{p} \), it never moves to other positions in the same BZ! What it does is quantum mechanically tunnel to similar positions in other BZ's, governed by the Schrödinger's equation. After one \( \omega_B \), the wavefunction shifts one BZ in canonical momentum, but the mechanical momentum is not chanched. The wavefunction's wiggling around the accelerating center in canonical momentum space results in the wavefunction's oscillating up-and-down in the same position in mechanical momentum space. The average mechanical momentum thus oscillates without acceleration, and the wavefunction has the appearance of moving left-and-right in the mechanical momentum space, but the quantum nature determines the interaction is not between different
canonical momentum in the same BZ (left-and-right), but only for the same $\bar{p}$ (up-and-down in mechanical momentum space). So the semiclassical picture of BO as a wave packet oscillating in one BZ is right in appearance and wrong in nature. That is why it contradicts the physical cases at the field-free limit, the free-space limit, and the semiclassical limit, as rightly criticized by the Critical School in the last half century (See Chapter 2 §2.2).

The meaning of BO is that an electron initially localized in momentum space, at a certain position in a BZ, quantum mechanically tunnels to the same position in other BZ’s. It oscillates around the average center which keeps moving to BZ’s of higher canonical momentum, one BZ at a $\tau_B$, but the mechanical momentum is not changed. In the canonical momentum space, BO is totally inter-BZ motion, not the intra-BZ motion as the classical picture tells, not even intra-BZ plus some inter-BZ motion. In the mechanical momentum space, BO is a left-and-right motion by average (semiclassical), but the nature is up-and down (quantum).

When the field is zero, the periodic symmetry is restored, and all BZ’s fold together into the first BZ, therefore no cross-BZ tunnellings happen, and Bloch functions take over. When the barriers are weak, there’s almost no oscillation as the electron wave packet simply tunnels exactly to the next BZ, and a physical acceleration according to the field happens. In the semiclassical limit, no quantum tunnelings will happen, and no oscillations exist, too.

Another factor that may affect the lifetime of BO is of microscopic nature, if the measured phenomena depend on the coherence of the exciton package being preserved. The electric field will cause the electron and the hole both to accelerate, in the opposite directions, if they have moved to the continuous bands. When the field is weak, the Coulomb interaction between the electron and the hole may keep them together. But when the field is strong, they will be separated in space till they
lose coherence. The experiments [180] show that the dephasing rate increases for high electric field. Higher field makes the electron reach the continuous band faster, it also splits the exciton quicker.

8.2 The Meaning of Wannier-Stark-Ladders

Physical intuition tells us that when a periodic lattice is tilted (biased), the originally coherent states in neighboring wells become less coherent, as the originally aligned "bands at different sites" (if such a concept of local bands are legal, since band should be a global concept) become shifted. Then the originally globally extended states become less extended or more localized, and as the lattice is tilted more they become more localized until totally independent from each other. These concepts had helped the experimentalists greatly as they try to design what to observe. (see Chapter 3 §3.2.3). But there are also rigorous theoretical results that the states should all be extended, because no discrete state exists, and therefore no square-integrable localized states exist. (see Chapter 2 §2.2.3). Can these two ideas be reconciled?

I noticed in Eq.(7.6) that given the index of BZ to be \( n \), as time increases infinitely, the solution of the Schrödinger's equation in that BZ become fast oscillating in time, and does not carry the BO information any more. Now look at the same solution at a given time \( t \), as \( n \) increases or decreases so that the diagonal element in \( H_p(t) \) is much larger than the off-diagonal ones, then the solution at the nth BZ becomes fast oscillating with \( n \), therefore with momentum \( p = p_0(\hat{p} + n) \).

\[
\phi(p, t) = \text{const } \exp[i\left(\frac{\tau_B}{3\tau_A}\right)(\frac{P}{P_0} - \frac{t}{\tau_B})^3] \\
\approx \text{const } \exp\left(\frac{ip^3}{6\hbar meE}\right), \quad (p \to \pm\infty). \tag{8.10}
\]

Now if we do the Fourier transform to get the real space wavefunction

\[
\psi(x, t) = \frac{1}{\sqrt{2\pi\hbar}} \int \phi(p, t) \exp(ipx/\hbar) dp, \tag{8.11}
\]
the integration will suppress the contributions from the fast oscillating part. The contributing wavefunction is around the momentum $p_c$ and the extension range is $1/\sigma$, where

$$p_c(t) = e\mathcal{E}t,$$

$$\frac{1}{\sigma} = p_0(3\tau_A/\tau_B)^{1/3} = (6me\mathcal{E}\hbar)^{1/3}.$$  

If we use a travelling Gaussian centered at $p_c(t)$ to represent the contributing part

$$\phi(p, t) = \exp\left[-\frac{\sigma^2}{\hbar^2}(p-p_c(t))^2\right] \exp(ip_{c}(t)/\hbar),$$

we see that $\psi(x, t)$ is a localized traveling wave of momentum $p_c(t)$

$$\psi(x, t) = \exp\left[-\frac{(x-x_c)^2}{2\sigma^2}\right] \exp[ip_{c}(t)(x-x_c)/\hbar].$$

The probability density of the above wavefunction will be

$$|\psi(x, t)|^2 = \exp\left[-\frac{(x-x_c)^2}{\sigma^2}\right],$$

where

$$\sigma = (6me\mathcal{E}\hbar)^{-1/3}.$$  

In other words the time-average of the wavefunction is localized in a region whose size is inversely proportional to the cubic root of the electric field. So the real space wave function is actually localized to a range determined by the electric field. The stronger the field is, the more localized the wavefunction becomes, just like the semiclassical picture tells. As a localized state in real space moves one III site, it changes an energy difference of $e\mathcal{E}d = \hbar\omega_B$, which is the Wannier-Stark-Ladder. So the semiclassical picture for WSL is basically right. However, the WS states are travelling wave-packets that will not always be localized in the same place. The time average is zero except at points $x = x_c$, where $x_c$ is an arbitrary number. The position and energy of WS electrons can take arbitrary numbers with continuous spectra, only having “resonance states” with relative energy level spacing of $\hbar\omega_B$. 

8.3 Time-dependent Fields

8.3.1 The Harmonic Field

The current method can readily be extended to the case of harmonic electric fields, which is of important interest since the excitation of the excitons in which WSL and BO are to be observed was done by lasers which is composed of harmonic electromagnetic fields.

For a harmonic electric field (uniform but not static) in the direction of super-lattice growth, (thus the problem is reduced to be one-dimensional)

\[ E(t) = E_0 \sin(\omega t), \] (8.18)

it can be represented by a vector potential

\[ A(t) = -\int^t E(t) dt = \frac{E_0}{\omega} [\cos(\omega t) - 1]. \] (8.19)

Under the same a priori choices of (1) Momentum representation, (2) Vector potential gauge, (3) Mathieu-type potential, (4) Constant-mass model, and define the same time scales \( \tau_A, \tau_B, \tau_C, \) and the reduced momentum \( \tilde{p}, \) we get the same form of dynamics in the Schrödinger's equation

\[ i \frac{d}{dt} \phi_p(t) = H_p(t) \phi_p(t), \] (8.20)

where the Hamiltonian matrix \( H_p(t) \) is the matrix

\[ H(q) = \frac{1}{\tau_C} I + \begin{pmatrix}
\frac{1}{2\tau_C} & \frac{1}{\tau_A} (q - 1)^2 & \frac{1}{2\tau_C} & 0 \\
\frac{1}{2\tau_C} & \frac{1}{\tau_A} (q + 0)^2 & \frac{1}{2\tau_C} & \frac{1}{\tau_B} (q + 1)^2 \\
\frac{1}{2\tau_C} & \frac{1}{\tau_A} (q + 1)^2 & \frac{1}{2\tau_C} & \cdot \\
0 & \cdot & \cdot & \cdot 
\end{pmatrix}, \] (8.21)

in which the "acting reduced momentum" \( q = q_p(t) \) is

\[ q_p(t) = \tilde{p} + \frac{1}{\omega \tau_B} [\cos(\omega t) - 1] \] (8.22)
where \( \tau_{B_0} = \hbar/eE_0d \). Since \( q_p(t) \) is itself periodic with time, so is the Hamiltonian matrix, whose eigenvalues and eigenvectors should also be periodic with time. The conservation of the probability density at any reduced momentum still hold, the electrons tunnel into the same position in other BZ's then tunnel back in the period of the external field. Therefore the average position in the momentum space has a continuous oscillation with the frequency of the external period.

### 8.3.2 Mixture of Harmonic with Uniform Fields

A harmonic electric field superposed over a uniform static field

\[
E(t) = E + E_0 \sin(\omega t)
\]

(8.23)
can be represented by a vector potential

\[
A(t) = -\int_0^t E(t)dt = -Et + \frac{E_0}{\omega} \left[ \cos(\omega t) - 1 \right].
\]

(8.24)

we get the same Schrödinger's equation with a different "Acting Reduced Momentum" \( q \)

\[
q_p(t) = \bar{p} - \frac{1}{\tau_B} t + \frac{1}{\omega \tau_{B_0}} \left[ \cos(\omega t) - 1 \right],
\]

(8.25)

where \( \tau_B = \hbar/eEd \), and \( \tau_{B_0} = \hbar/eE_0d \). The Hamiltonian matrix is both shifting-periodic with the "dc Bloch frequency" \( \omega_B = eEd/\hbar \) determined by the static field, and also periodic with the "ac Bloch frequency" \( \omega_{B0} = eE_0d/\hbar \) determined by the alternating field. The first effect makes the electron tunnel to the same position in other BZ's, with the average position in momentum space moving, and the wavefunction has a phase factor with a ladder-oscillation structure that depends on the band widths. If the electron was initially on more than one band, then it oscillates between these bands. And the time-average of the wavefunction are localized around each well in a range that decreases with stronger field, and it displays a Wannier-Stark-Ladder
between these bands. However if the electron was on one band only, then no physical effect is expected. When there is an interband Bloch Oscillation, as time goes on, the average momentum is increasing. When the total average energy is high enough that the electron is in the continuous states, it loses this ladder-oscillation information and simply accelerates to infinity. That is one reason why BO should have a finite lifetime. The second effect makes the electron tunnel to other BZ's and then tunnel back, therefore makes the average position in the momentum space oscillate between different BZ's. It wouldn't have any effects on oscillation between bands, because the oscillation between BZ's are the same for all bands. When the driving frequency $\omega$ (not the ac Bloch frequency $\omega_{B0}$) is the multiple of the dc Bloch frequency $\omega_B$

$$\omega = n\omega_B, \quad (n = 1, 2, 3, \ldots) \tag{8.26}$$

some coherent enhancement to the BO was expected. Since the mechanism of WSL is interband oscillation, and the ac effect is interzone oscillation, no enhancement to WSL is expected from this author. More work could be done to make this matter clearer.

### 8.3.3 Turning on the Uniform Field

If the electric field has a turning-on process

$$\mathcal{E}(t) = \mathcal{E}[1 - \exp(-t/\tau)], \quad (8.27)$$

then the gauge can be chosen that $\varphi = 0$, and

$$A(t) = -\mathcal{E}t + \mathcal{E}\tau[1 - \exp(-t/\tau)]. \quad (8.28)$$

The dynamics is determined by the same Hamiltonian matrix with functional dependence on the acting reduced momentum

$$q = \tilde{p} - \frac{1}{\tau_B}[t - \tau(1 - \exp(-t/\tau))]. \quad (8.29)$$
Now the initial state can be taken as a Bloch function, which is an eigenstate when there is no field present.

8.4 Reflections and Perspectives

The major purpose of this dissertation has been to derive WSL and BO without encountering the problematic theoretical difficulties as stated in §1.2. This is also my major contribution.

Knowing that claiming that I have overcome all these technical problems is inviting criticism, I do believe that I have solved the first eight out of the ten problems stated. Our approach provides a coherent platform for the full-Hamiltonian independent-electron model for the study of WSL and BO.

Let us examine those points that has been resolved:

(1) The remaining symmetry after the symmetry breaking by the presence of an electric field is identified as the shifting periodicity, and this symmetry was utilized through the Bloch-Floquet theorem, and a non-perturbative approach relative to the electric field is taken. (No claim of discovering this symmetry is given by the current author, but stating it clearly and utilizing it to simplify the problem for WSL and BO appears to be original.) Until the last step before getting Eq.(7.11) I didn’t require any restrictions on the field strength, and even the last step approximation was checked to be sure that it is not singular.

(2) By using the momentum representation, I have avoided using any boundary conditions in the real space. Using the momentum representation doesn’t require a periodic boundary condition in configuration space, only that the magnitude of the wavefunction approaches zero at infinity.

(3) By starting from the time-dependent Schrödinger’s equation from the beginning, and using other choices of gauge, representation and basis etc, I get both a
band structure and a continuous energy spectrum.

(4) By using a multi-BZ basis, the Ehrenfest's theorem was built into the basis, and the acceleration scheme is included in the theory.

(5) By using a sinusoidal model for the potential and being open to any other potential functional forms, my theory is not sensitive to the functional form of potential. The weak-barrier (free-space) limit is also checked so that correspondence principle is fulfilled.

(6) By using the vector potential gauge, and identifying the Hamiltonian to be the energy operator of the electron plus the lattice, excluding the field, the instantaneous spatial periodicity was kept and translated into the shifting periodicity in momentum representation. The confusion about the status of the band was also removed.

(7) By using a full-Hamiltonian model, and then identifying WSL as a multiband phenomenon and BO as existing for both single and multiband situations, former apparent controversies may be resolved, if more work is done to identify them individually.

(8) By solving a full-Hamiltonian independent-electron model free form problematic analytical approximations, I have built a platform for more developments in microscopic models.

(9) The initial condition from a Bloch state is a problem that I didn't totally solve, but layed out as a perspective in §8.3.3. However for the purpose of excitons as initial conditions, the current setting of Gaussians is fully legitimate and enough for simulation of the physical situation. The turning-on process is theoretically interesting because it describes the symmetry breaking process.

(10) For the lifetime problem now I only have a qualitative argument that agrees with the experiment, but more work on the interband term in Eq.(7.9) will give us
an intrinsic lifetime of BO.

New approaches to solve known problems often reveal new problems. One weakness of this work is the lack of a rigorous mathematical proof of the convergence of the eigenvalues and eigenvectors of the truncated Hamiltonian matrix to the value from the infinite matrix. Now I have numerical evidence and qualitative argument for this convergence, but more rigorous work is needed to secure this result.

Some other minor contributions was also made during this work period, such as: (1) finding the field-induced changes of transmission spectrum; (2) finding the quantum meaning of BO to be purely inter-BZ in canonical momentum space, and “up-and-down” interaction in mechanical momentum space; (3) a simplified method to calculate one-dimensional band; (4) relating the normally considered pure mathematical decisions of choosing representation, gauge etc. to physical advantages; (5) a hint to the question of the status of energy band theory in the presence of an external field that breaks the periodic symmetry, that an extended momentum space representation, and a gauge that identifies the Hamiltonian as the energy operator of the electron plus the lattice, may keep the band structure present; (6) a clear presentation of the symmetry of shifting periodicity, a proof of the Bloch-Floquet Theorem in the new representation.

More accurate numerical works can be done by applying the high precision algorithm (the modified Cayley’s method) [205, 206] to calculate the time-evolution operator

\[
\exp\left[ -\frac{i}{\hbar} \mathbf{H}(t) \Delta t \right] \approx \left[ 1 + \frac{i}{2} \frac{\Delta t}{\hbar} \mathbf{H}(t) \right]^{-1} \left[ 1 - \frac{i}{2} \frac{\Delta t}{\hbar} \mathbf{H}(t) \right] \tag{8.30}
\]

whose error is in the order of \( \Delta t^3 \), to see the time-evolution of a wave-packet of a WS electron.
APPENDIX A

RESULT OF THE FIELD-FREE LIMIT
At the field-free limit, i.e. $\mathcal{E} \to 0$ or $\tau_B \to \infty$, the Hamiltonian $H_\beta$ becomes independent of time $t$

$$i \frac{d}{dt} f_\beta(t) = H_\beta f_\beta(t). \quad (A.1)$$

If we diagonalize $H_\beta$

$$H_\beta \gamma_\beta^{(j)} = E_\beta^{(j)} \gamma_\beta^{(j)}, \quad (A.2)$$

where $E_\beta^{(j)} = E_j(\beta)$ is the $j$th energy band at the momentum $\beta$, in other words, the dispersion relation, and put the column eigenvectors together as a matrix

$$\gamma_\beta = \{ \gamma_\beta^{(1)}, \gamma_\beta^{(2)}, \gamma_\beta^{(3)}, \ldots \}, \quad (A.3)$$

and the eigenenergies together as a diagonal "eigenenergy matrix"

$$E_\beta = \begin{pmatrix}
E_\beta^{(1)} & 0 & & \\
0 & E_\beta^{(2)} & & \\
& & E_\beta^{(3)} & \\
& & & \ddots
\end{pmatrix}, \quad (A.4)$$

then

$$H_\beta \gamma_\beta = \gamma_\beta E_\beta. \quad (A.5)$$

Because of the orthonormality or the eigenvectors of a Hermitian matrix

$$\gamma_\beta^T = \gamma_\beta^{-1}. \quad (A.6)$$

Here because the Hamiltonian matrix is real and symmetric (a special kind of Hermitian), its eigenvectors can be taken to be real, therefore the conjugal conjugate $\gamma_\beta^\dagger$ is its transpose $\gamma_\beta^T$. We have

$$H_\beta = \gamma_\beta E_\beta \gamma_\beta^T \quad (A.7)$$

and the evolution operator is

$$\exp(-iH_\beta t) = \sum_{n=0}^{\infty} \frac{1}{n!} (-it)^n H_\beta^n \quad (A.8)$$
where the "phase factor matrix" is

\[ P_{\bar{p}}(t) = \begin{pmatrix} \exp[-iE^{(1)}_{\bar{p}}t] & 0 \\ \exp[-iE^{(2)}_{\bar{p}}t] & \exp[-iE^{(3)}_{\bar{p}}t] \\ 0 & \end{pmatrix} \]  \hspace{1cm} (A.11)

The wavefunction for reduced momentum \( \bar{p} \) at any time will be

\[ \tilde{f}_\bar{p}(t) = \nu_\bar{p} P_{\bar{p}}(t) v^T_\bar{p} \tilde{f}_\bar{p}(0). \]  \hspace{1cm} (A.12)

or in familiar terms, the solution can be expanded as a sum of eigenfunctions of the Hamiltonian multiplied by the time-dependent phase factors at different eigenenergies

\[ \tilde{f}_\bar{p}(t) = \sum_{j=0}^{\infty} [v^{(j)}_{\bar{p}} \cdot \tilde{f}_\bar{p}(0)] v^{(j)}_{\bar{p}} \exp(-iE^{(j)}_{\bar{p}}t), \]  \hspace{1cm} (A.13)

where \( v^{(j)}_{\bar{p}} \) is the eigenvector, and the \( n \)th elements of which is the momentum-space wavefunction \( \phi_{n,\bar{p}}(t) \) in the \( n \)th BZ. If initially the particle was on one band only, say, the ground level, \( i.e. \)

\[ [v^{(j)}_{\bar{p}} \cdot \tilde{f}_\bar{p}(0)] = c_p \delta_{j1} \]  \hspace{1cm} (A.14)

then the wavefunction will be

\[ \tilde{f}_\bar{p}(t) = c_p v^{(1)}_{\bar{p}} \exp(-iE^{(1)}_{\bar{p}}t). \]  \hspace{1cm} (A.15)

It stays on the same band and oscillate harmonically with a lattice eigenfrequency.

The real-space wavefunction at the field-free limit is gotten by the Fourier transform

\[ \psi(x, t) = \frac{1}{\sqrt{2\pi\hbar}} \int \phi(p, t) \exp(ipx/\hbar)dp \]  \hspace{1cm} (A.16)
It is a composition of Bloch-type wavefunctions, in which the function

\[ u_{\vec{p}}(x) = \frac{\sqrt{\hbar}}{d} \sum_{n=-\infty}^{\infty} \phi_{n,\vec{p}}(t) \exp\left(\frac{2\pi n}{d} - x\right) \]  

(A.20)

satisfies

\[ u_{\vec{p}}(x + d, t) = u_{\vec{p}}(x, t), \]  

(A.21)

and

\[ K_{\vec{p}} = \frac{2\pi \vec{p}}{d} \]  

(A.22)

is the pseudo-momentum. The above result is true with or without the electric field.

But when there is no electric field present, a periodic (Born-von Karman) boundary condition can be used (it can't be used at the presence of an electric field, as proven by Rabinovitch [52]), by requiring the total length of the lattice to be a multiple of half of the de Broglie wavelength

\[ Nd = l\frac{\lambda}{2}, \]  

(A.23)

where \( l \) is an integer, and \( N \) is the total number of lattice periods, therefore the reduced momentum

\[ \vec{p} = \frac{k}{k_0} = \frac{d}{\lambda} = \frac{l}{2N}. \]  

(A.24)

where \(-N \leq l < N\) refers to the reduced momentum in the first BZ. Replacing all the indexing by \( \vec{p} \) to be by \( l \), the real-space wavefunction is

\[ \psi(x, t) = \sum_{l=-N}^{N-1} u_l(x, t) \exp\left(iK_l x\right) \]  

(A.25)
is a general superpositions of Bloch-like wavefunctions, where $K_l = \pi l/Nd$ and $-\pi/d \leq K_l < \pi/d$, and

$$u_l(x, t) = \sum_{j=0}^\infty w_{lj}(x) \exp[-iE_l^{(j)} t]$$  \hspace{1cm} (A.26)

is an expansion by energy bands, in which

$$w_{lj}(x) = c_{lj} \sum_{n=-\infty}^\infty (v_l^{(j)})_n \exp(i\frac{2\pi n}{d} x)$$  \hspace{1cm} (A.27)

is the Wannier function, where

$$c_{lj} = \frac{\sqrt{\hbar}}{d} [v_l^{(j)} \cdot f_l(0)]$$  \hspace{1cm} (A.28)

is a coefficient determined by initial conditions. Since $(v_l^{(j)})_n$ is nonzero only around $n \approx j$, Wannier function is only a sum of a few terms, and it satisfies

$$w_{lj}(x + d) = w_{lj}(x).$$  \hspace{1cm} (A.29)

Thus my model reproduces the mainline thoughts of traditional solid-state physics on this topic in the field-free limit.
APPENDIX B

PROOF OF THE "BLOCH-FLOQUET THEOREM"
Since for a shifting periodic Hamiltonian

\[ H(t + T) = SH(t)S^{-1}, \]  \hspace{1cm} (B.1)

we can get from the eigenequation of \( H(t) \)

\[ H(t)\psi_j(t) = E_j(t)\psi_j(t), \]  \hspace{1cm} (B.2)

by multiplying \( S \) from the left and insert \( S^{-1}S \) in the middle

\[ [SH(t)S^{-1}] [S\psi_j(t)] = E_j(t) [S\psi_j(t)], \]  \hspace{1cm} (B.3)

in which we see that \([S\psi_j(t)]\) is an eigenvector of \( H(t + T) \) with the eigenvalue \( E_j(t) \).

In general

\[ H(t + T)\psi_j(t + T) = E_j(t + T)\psi_j(t + T). \]  \hspace{1cm} (B.4)

Since \( H(t + T) \) looks not different with \([SH(t + T)S^{-1}]\) except shifted down one row and right one column, we can expect the same structure of eigenvalues with the proper indexing, and eigenvectors that is shifted one row down, and possibly a difference of a phase factor. i.e.

\[ E_j(t + T) = E_j(t) \]  \hspace{1cm} (B.5)

\[ \psi_j(t + T) = [S\psi_j(t)] \exp[-i\omega_j(T; t)]. \]  \hspace{1cm} (B.6)

Define the operator of time-shift \( \hat{T}_T \) to be

\[ \hat{T}_T\psi_j(t) = \psi_j(t + T). \]  \hspace{1cm} (B.7)

we should have

\[ \hat{T}_T\hat{T}_T\psi_j(t) = \psi_j(t + T + T') = \hat{T}_T\hat{T}_T\psi_j(t). \]  \hspace{1cm} (B.8)
The left hand side gives

\[
LHS = S\{S_{y_j}(t) \exp[-i\omega_j(T'; t)]\} \exp[-i\omega_j(T; t + T')]
\]
\[= [S^2_{y_j}(t)] \exp[-i\omega_j(T'; t) - i\omega_j(T; t + T')].\]  

(B.9) \hspace{1cm} (B.10)

The right hand side gives

\[
RHS = S\{S_{y_j}(t) \exp[-i\omega_j(T'; t)]\} \exp[-i\omega_j(T; t + T')]
\]
\[= [S^2_{y_j}(t)] \exp[-i\omega_j(T'; t) - i\omega_j(T'; t + T')].\]  

(B.11) \hspace{1cm} (B.12)

To make \(LHS = RHS\) we must have

\[
\omega_j(T'; t) + \omega_j(T; t + T') = \omega_j(T; t) + \omega_j(T'; t + T').
\]  

(B.13)

For that to be true for all values of \(t, T,\) and \(T',\) we must have

\[
\omega_j(T; t) = \omega_jT,
\]  

(B.14)

so that

\[
LHS = \omega_j T' + \omega_j T = \omega_j T + \omega_j T' = RHS.
\]  

(B.15)

Thus we have

\[
y_j(t + T) = S_{y_j}(t) \exp(-i\omega T).
\]  

(B.16)

which is equivalent to writing

\[
y_j(t) = u_{j,\omega}(t) \exp(-i\omega t),
\]  

(B.17)

where the function \(u_{j,\omega}(t)\) satisfies

\[
u_{j,\omega}(t + T) = S_{u_{j,\omega}}(t).
\]  

(B.18)

Drop index \(j,\) then the eigenvector of a Shifting Periodic Hamiltonian can be written as

\[
x(t) = u_\omega(t) \exp(-i\omega t),
\]  

(B.19)
where the function $u_\omega(t)$ satisfies
\[ u_\omega(t + T) = S u_\omega(t), \] (B.20)

where $\omega$ is called pseudo-energy. Proof done.
APPENDIX C

PHYSICAL MEANINGS OF TWO GAUGES
It is well accepted that gauges are not physically measurable. The choice of a specific gauge is only for mathematical convenience. Any physically measurable quantity should be gauge-independent. Quantum mechanically both the Hamiltonian operator and the wavefunction are gauge-dependent, but the expectation value of any physical quantity is gauge-independent. Also the functional form of Schrödinger’s equation is gauge-independent [204]. The works of Kobe et al. [106, 109] shows that in general it’s not a Hamiltonian \( H \), but the “energy operator”

\[
\epsilon = H - (-e)\phi(x, t),
\]

where the electron’s charge is \(-e\), which satisfies

\[
\frac{d\epsilon}{dt} = \vec{v} \cdot \vec{F}_{ext},
\]

where \( \phi(x, t) \) is the scalar potential of the electromagnetic field, \( \vec{v} = \dot{x} \) is the velocity, and \( \vec{F}_{ext} \) is the external force that provides energy. The meaning of the last equation is that the rate of change of energy is equal to the power supply from the external field. So in general, the scalar potential should not be included in the energy operator. But a special case is taken when the external field is a uniform static field, whose scalar potential is considered a potential energy of the particle. In this case, the “natural Hamiltonian" for a WS electron is considered as

\[
H = \frac{p^2}{2m} + V(x) + e\mathcal{E}x,
\]

which is in a scalar potential gauge of \( \phi = -\mathcal{E}x \), and \( A = 0 \). By choosing a gauge transformation function \( \chi = -\mathcal{E}tx \) we change to a vector potential gauge \( \phi = 0 \), and \( A = -\mathcal{E}t \). The unitary operator related to the gauge transformation is \( T_\chi(t) = \exp[i\mathcal{E}\chi(x, t)] \) where \( \chi(x, t) \) is an operator that will have a specific form according to the
chosen representation. The Hamiltonian is transformed to

\[ H = \frac{1}{2m} (p - e \xi t)^2 + V(x), \quad (C.4) \]

which is not considered the "natural Hamiltonian". It is not regarded as the energy operator, therefore the band it creates, called the "Hamiltonian band" here, is not considered the same as the energy band. But the question is: Why is the problem so naturally simplified in an "unnatural gauge"? Is this special case necessary?

In the vector potential gauge,

\[ H = \frac{\pi^2}{2m} + V(x), \quad (C.5) \]

where \( \pi = p - e \xi t \) is the mechanical momentum, different from the canonical momentum \( p \). By applying the Hamilton's equations

\[ \dot{x} = \frac{\partial H}{\partial p} = \frac{\pi}{m} \quad (C.6) \]
\[ \dot{p} = -\frac{\partial H}{\partial x} = -V'(x), \quad (C.7) \]

we find

\[ \frac{dH}{dt} = \frac{\pi}{m} (-e \xi) = \nabla \cdot \vec{F}_{\text{ext}}, \quad (C.8) \]

i.e. the time derivative of \( H \) is equal to the power supply by the external field. That identifies \( H = \varepsilon \), i.e. the Hamiltonian is the energy operator, contrary to popular belief. This energy is the "internal energy" composed of the kinetic energy and the potential energy by conservative forces other than the external field. As the external field provides energy, the electrons "internal energy" increases with time as it accelerates.

In the scalar potential gauge, the canonical momentum is the same as the mechanical momentum. By applying the Hamilton's equations

\[ \dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m} \quad (C.9) \]
\[ \dot{p} = -\frac{\partial H}{\partial x} = -V'(x) - e\mathcal{E}, \]  
\[ \frac{dH}{dt} = 0. \]  

Therefore we find that

\[ \frac{dH}{dt} = 0. \]  

In other words, since the external field is now considered internal, by including the scalar potential as part of the electrons potential energy, the whole system is conservative in energy. However, if we separate the field form the environ of the particle, then

\[ \frac{d}{dt}(H - e\mathcal{E}x) = \frac{p}{m}(-e\mathcal{E}) = \nabla \cdot \vec{F}_{\text{ext}}, \]

or \( \epsilon = H - (-e)\phi(x,t) \) is the “internal energy”. By including the field into the system we get a conservation law which doesn’t tell us directly what’s happening to the particle. By specifying the field as “external” we can tell directly the physical change of the particle’s “internal energy”. Even though all gauges are equivalent in essence, there is one gauge in which the scalar potential is chosen to be zero, so that the dynamics-governing Hamiltonian operator has the physical meaning of being the same as the “internal energy” operator. That explains why my approach has greatly simplified the problem, because the gauge I’ve chosen is the most “natural”, and the “Hamiltonian band” is the “internal energy band”. This should be the general rule, no special case needs to be given to the uniform field case. The WS electrons have a band structure determined by the periodic lattice potential. Adding an external field did not make the periodicity disappear, and the band remains. The lattice is not considered “biased” because the field is not considered the ‘internal environ” of the WS electron. The field is considered “external”, so it provides a source for the “internal energy” of the electron, which grows in time, as the original oscillatory motion determined by the band continues, with a new interactive part called the BO.
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