

**Physics 221A**  
**Fall 2005**  
**Notes 6**  
**Bloch's Theorem and Band Structure**  
**in One Dimension**

### 6.1. Introduction

In these notes we examine Bloch's theorem and band structure in problems with periodic potentials, as a part of our survey of one-dimensional problems in quantum mechanics. Our purpose in studying such systems is two-fold. First, periodic potentials are important in solid state physics, and the band structure of the energy levels in crystals is fundamental to understanding the behavior of insulators, conductors, and semiconductors. Of course, real solids are three-dimensional, so the one-dimensional problems examined in these notes are only simplified models. Second, periodic potentials will give us our first examples of Hamiltonian systems with symmetry, and they will serve to illustrate certain general principles of such systems.

### 6.2. Bloch's Theorem

We wish to solve the one-dimensional Schrödinger equation,

$$-\frac{\hbar^2}{2m}\psi'' + V(x)\psi = E\psi, \tag{6.1}$$

where the potential is assumed to be spatially periodic,

$$V(x + a) = V(x). \tag{6.2}$$

Here  $a$  is the lattice spacing or spatial period of the one-dimensional lattice. We make no assumptions about the behavior of  $V(x)$  within any period, only that it be periodic.

For most of the following discussion, we will assume that the lattice goes on forever, so there is an infinite number of periods. Of course, in real solids the lattice has to end at the edge of the crystal, and there will be boundary conditions at the edge which will modify and complicate the problem. One reason we will assume an infinite lattice is to avoid such complications. In some problems, however, the variable  $x$  itself is periodic, and there are only a certain number  $N$  of lattice spacings in the period of  $x$ . For example, in

the internal rotations of the ethane molecule,  $\text{CH}_3\text{CH}_3$ , which was discussed in class, the potential energy goes through three periods when the angle  $\phi$  of rotation goes from 0 to  $2\pi$ . In this case, the coordinate  $x$  is identified with the angle  $\phi$ , and the lattice spacing is  $a = 2\pi/3$ . Below we will make some comments on cases such as this, where there are  $N$  lattice spacings within the period of the variable  $x$ .

We introduce the translation operator with a displacement equal to the lattice spacing,

$$T(a) = e^{-iap/\hbar}, \quad (6.3)$$

where  $p$  is the momentum operator. This operator has the usual action on wave functions,

$$[T(a)\psi](x) = \psi(x - a), \quad (6.4)$$

which causes the wave function  $\psi$  to be pushed down the  $x$ -axis by the lattice spacing  $a$ . This operator commutes with the kinetic energy,

$$\left[T(a), \frac{p^2}{2m}\right] = 0, \quad (6.5)$$

since both operators are functions of the momentum. It also commutes with the potential energy, because of the periodic condition (6.2). We see this if we compute the action of the product of  $T(a)$  and  $V(x)$  in the two different orders on a wave function  $\psi$ ,

$$\begin{aligned} [T(a)V(x)\psi](x) &= V(x - a)\psi(x - a), \\ [V(x)T(a)\psi](x) &= V(x)\psi(x - a), \end{aligned} \quad (6.6)$$

which are equal by Eq. (6.2). Therefore  $T(a)$  commutes with the entire Hamiltonian,

$$[T(a), H] = 0. \quad (6.7)$$

More generally,  $H$  commutes with any power of  $T(a)$ ,  $T(a)^n = T(na)$ , which is to say that it commutes with the entire group of symmetry operations generated by  $T(a)$ .

Since  $H$  and  $T(a)$  commute, they possess simultaneous eigenfunctions. This leads to a strategy for finding the eigenfunctions of  $H$  which is very common in cases of symmetry. Usually it is hard to find the eigenfunctions of  $H$ , but much easier to find the eigenfunctions of the symmetry operator. Therefore we find the eigenfunctions of the symmetry operator first, and then use them to simplify the search for the eigenfunctions of  $H$ . For example, suppose the eigenfunctions of the symmetry operator are nondegenerate. Then by Theorem 1.4, these functions are automatically the eigenfunctions of  $H$ , with no extra work. Even if the eigenfunctions of the symmetry operator are degenerate (as they usually

are), nevertheless the search for the eigenfunctions of  $H$  is simplified, because we only need to search in the various eigenspaces of the symmetry operator, which are smaller spaces than the whole Hilbert space we started with. For example, we may be forced to set up a matrix and to diagonalize it numerically to find the eigenfunctions of  $H$ . But if we can do this within one of the eigenspaces of the symmetry operator, then we will have a smaller matrix than if we did it in the entire Hilbert space. We will have more to say about this procedure when we discuss symmetry in quantum mechanics later in the semester, but these introductory comments will do for now.

In the present case, we begin by finding the eigenfunctions of the translation operator  $T(a)$ . We write

$$[T(a)\psi](x) = \tau\psi(x), \quad (6.8)$$

where  $\psi$  is an eigenfunction of  $T(a)$  and  $\tau$  is the eigenvalue. Since  $T(a)$  is unitary, the eigenvalue  $\tau$  must be a phase factor,

$$\tau = e^{-i\theta}. \quad (6.9)$$

The angle  $\theta$  characterizes the eigenvalues of  $T(a)$ , and may be restricted to the range  $-\pi < \theta \leq \pi$ . It is conventional to write this angle in the form,

$$\theta = ka, \quad (6.10)$$

where  $a$  is the lattice spacing as above, and  $k$  is a quantity with dimensions of wave number which characterizes the eigenvalue. Because of the range on  $\theta$ , the range on  $k$  can be taken to be

$$-\frac{\pi}{a} < k \leq \frac{\pi}{a}. \quad (6.11)$$

This range of  $k$  is called the *first Brillouin zone* in  $k$ -space.

We may now use these conventions and Eq. (6.4) to write Eq. (6.8) in the form

$$\psi_k(x - a) = e^{-ika}\psi_k(x), \quad (6.12)$$

where we attach a  $k$  subscript to  $\psi$  to indicate that it is an eigenfunction of  $T(a)$  with eigenvalue  $e^{-ika}$ . We may also write this equation in the form,

$$\psi_k(x + a) = e^{ika}\psi_k(x), \quad (6.13)$$

which makes it clear that  $\psi_k(x)$  becomes known everywhere on the  $x$ -axis once it is known in the fundamental period  $0 \leq x < a$ . Furthermore,  $\psi_k$  must satisfy boundary conditions on the first period,  $\psi_k(a) = e^{ika}\psi_k(0)$ . There are functions  $\psi_k$  which satisfy Eq. (6.13) for

any value of  $k$ , so the spectrum of  $T(a)$  is the entire unit circle in the complex plane (it is a continuous spectrum). Furthermore, the number of such functions (that is, the number of linearly independent eigenfunctions) for any value of  $e^{-ika}$  is infinite, so the eigenvalues are infinite-fold degenerate and the eigenspaces of  $T(a)$  are infinite-dimensional. This is because Eq. (6.13) places no restriction on what  $\psi_k$  does in the interior of the first period  $0 \leq x < a$ , apart from the boundary condition  $\psi(a) = e^{ika}\psi(0)$ .

In the case that the  $x$  variable is periodic after  $N$  lattice spacings, the single-valuedness of the wave function requires

$$\psi(x + Na) = \psi(x), \quad (6.14)$$

so the eigenvalues of  $T(a)$  are phase factors of the form  $e^{-2n\pi i/N}$ , for  $n = 0, \dots, N - 1$ . In this case, the spectrum of  $T(a)$  is discrete, although each eigenvalue is still infinite-fold degenerate. Since  $T(a)$  is a normal operator, its eigenspaces are orthogonal. For example, in the case of the internal rotations of ethane ( $N = 3$ ), the eigenvalues of  $T(a)$  are 1 and  $e^{\pm 2\pi i/3}$ , and the Hilbert space is broken up into three orthogonal subspaces corresponding to these eigenvalues.

Rather than  $\psi_k(x)$ , it is often easier to work with a function  $u_k(x)$ , defined by

$$\psi_k(x) = e^{ikx}u_k(x). \quad (6.15)$$

The  $x$ -dependent phase  $e^{ikx}$  in this equation just interpolates the constant phase  $e^{ika}$  in Eq. (6.13) between  $x = 0$  and  $x = a$ . The result is that  $u_k$  is periodic,

$$u_k(x + a) = u_k(x), \quad (6.16)$$

as follows by computing  $\psi_k(x + a)$  from Eq. (6.15),

$$\psi_k(x + a) = e^{ik(x+a)}u_k(x + a), \quad (6.17)$$

and from Eq. (6.13),

$$\psi_k(x + a) = e^{ika}\psi_k(x) = e^{ika}e^{ikx}u_k(x). \quad (6.18)$$

The eigenfunction  $\psi_k$  of  $T(a)$  itself is not periodic, but  $u_k$  is.

Since  $H$  commutes with  $T(a)$ ,  $H$  possesses eigenfunctions which are of the form of  $\psi_k(x)$ , that is,  $e^{ikx}$  times a periodic function  $u_k(x)$ . This is *Bloch's theorem*. It has the same mathematical content as Floquet's theorem, which is often used for functions in the time domain. If we wish to find the eigenfunctions of  $H$ , we only need to search within a class of functions  $\psi_k$  of the form (6.15), where  $u_k$  is periodic. We must do this for each value of  $k$ , that is, we must work within each eigenspace of the translation operator separately.

This may sound like a lot of work, but it is much easier to work with functions which are periodic than those which are not, since a periodic function is determined by its values on a single period, whereas an arbitrary function can do anything anywhere on the  $x$ -axis. Also, periodic functions can be expanded in discrete bases like Fourier series, which is convenient.

In the case that  $x$  itself is periodic with  $N$  lattice spacings  $a$  in a period of  $x$ , there are  $N$  eigenspaces of the translation operator, and we must search for the eigenfunctions of  $H$  within each of these.

It is easy to transform the Schrödinger equation (6.1) from  $\psi_k$  to the periodic function  $u_k$ . We find

$$-\frac{\hbar^2}{2m}u_k'' + \frac{i\hbar^2 k}{m}u_k' + V(x)u_k = \left[E - \frac{\hbar^2 k^2}{2m}\right]u_k. \quad (6.19)$$

If we find a periodic solution  $u_k$  of this equation, then by Eq. (6.15) we will have found an eigenfunction  $\psi_k$  of the original Schrödinger equation (6.1).

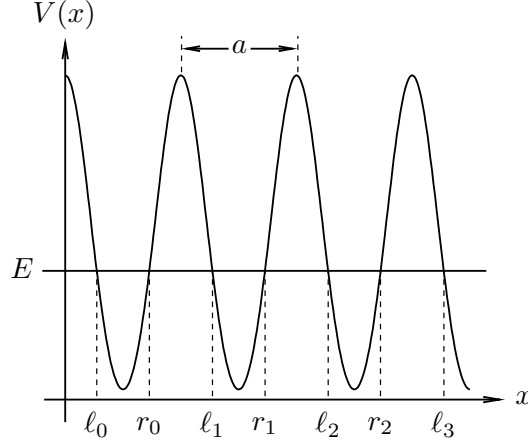
### 6.3. Band Structure

Bloch's theorem does not tell us about band structure, that is, the fact that in a periodic potential the energy levels lie in allowed energy bands, with gaps in between where there are no energy levels. In the case of an infinite lattice, the energy levels are continuous within the bands, whereas in the case of a finite lattice going around a periodic  $x$  coordinate, the energy levels within a band are discrete. In the latter case, the bands are really only meaningful if the separation between levels within a band is small compared to the band gaps.

To see the band structure it is necessary to take an example. Unfortunately, there are no simple examples of one-dimensional periodic potentials which are easy to solve and which are also physically realistic. One possibility is a periodic square well potential, which is not too hard to analyze. Another popular model is an infinite lattice of  $\delta$ -function potentials, which is called the Kronig-Penny model. Sakurai examines a tight-binding model, but his discussion is flawed by the fact that he uses a non-orthogonal basis (without telling you).

We will use WKB theory to analyze a periodic potential. We will assume that the potential has a single well in each period, as illustrated in Fig. 6.1. Let the wave function in the  $j$ -th classically allowed region have the form,

$$\psi(x) = \frac{1}{\sqrt{p(x)}} \left[ A_j \cos\left(\frac{S(x, \ell_j)}{\hbar} - \frac{\pi}{4}\right) + B_j \sin\left(\frac{S(x, \ell_j)}{\hbar} - \frac{\pi}{4}\right) \right], \quad (6.20)$$



**Fig. 6.1.** A periodic potential with lattice spacing  $a$ . The left and right turning points in the  $j$ -th region are  $\ell_j$  and  $r_j$ , respectively.

where  $\ell_j$  is the leftmost turning point in the  $j$ -th classically allowed region, and where

$$S(x, \ell_j) = \int_{\ell_j}^x p(x') dx'. \quad (6.21)$$

The other notation is as in Notes 5. We write the WKB wave function using real sines and cosines instead of complex exponentials, because in the limit that tunnelling can be neglected, the exact solution is given by the cosine wave alone (i.e., with  $B_j = 0$ ).

A straightforward analysis based on the WKB connection rules given in Notes 5 leads to a relation between the coefficients in one well and the next,

$$\begin{pmatrix} A_{j+1} \\ B_{j+1} \end{pmatrix} = \begin{pmatrix} 2e^\kappa \cos(\Phi/2) & 2e^\kappa \sin(\Phi/2) \\ -\frac{1}{2}e^{-\kappa} \sin(\Phi/2) & \frac{1}{2}e^{-\kappa} \cos(\Phi/2) \end{pmatrix} \begin{pmatrix} A_j \\ B_j \end{pmatrix}. \quad (6.22)$$

Here  $\Phi$  is the total Bohr-Sommerfeld phase around the orbit of energy  $E$  in the classically allowed region,

$$\Phi = \Phi(E) = \frac{1}{\hbar} \oint p dx = \frac{2}{\hbar} S(\ell_j, r_j), \quad (6.23)$$

where  $r_j$  is the right turning point in the  $j$ -th classical region, and  $\kappa$  is the dimensionless tunnelling action through the classically forbidden region,

$$\kappa = \frac{1}{\hbar} \int_{r_j}^{\ell_{j+1}} |p| dx. \quad (6.24)$$

In the following we will assume that  $\kappa$  is large enough that  $e^{-\kappa}$  is small. This means we are considering energies sufficiently below the top of the barrier.

Let us first look at the limit in which the tunnelling can be neglected. For example, we could raise the potential in the classically forbidden region to create an impenetrable barrier, which would make  $\kappa \rightarrow \infty$  while not changing  $\Phi$ . In this limit, Eq. (6.22) loses meaning, but it is easy to see what the wave functions are, since the wave function in each well is decoupled from those in all other wells. The wave functions in each well are quantized according to the Bohr-Sommerfeld rule,

$$\Phi = \Phi_n = (n + \frac{1}{2})2\pi, \quad (6.25)$$

where  $n = 0, 1, \dots$ , and they have energies  $E_n$ , where  $\Phi_n = \Phi(E_n)$ . We will call these the *nominal* Bohr-Sommerfeld levels (the levels we would have if tunnelling could be neglected). Also, let us denote the eigenfunctions in well  $j = 0$  by  $\tilde{\phi}_n(x)$ ; inside well  $j = 0$ , these are functions of the form (6.20) with  $A_0 = 1$  and  $B_0 = 0$ , but we will take them to vanish outside the well  $j = 0$ . The tilde means that these are eigenfunctions in the limit  $\kappa \rightarrow \infty$ . However, if we shift one of the  $\tilde{\phi}_n(x)$  by some integer number of lattice spacings, we will get another function of the same energy  $E_n$ , because the physics is the same in each well. The shifted function will have the form  $\tilde{\phi}_n(x - ja)$ , which is nonzero only in well  $j$ . Obviously, each energy eigenvalue  $E_n$  is infinite-fold degenerate, because the function  $\tilde{\phi}_n(x)$  can be shifted to any well. (If the lattice were periodic after some number  $N$  of lattice spacings, then the energy levels would be  $N$ -fold degenerate.) As we will see, this degeneracy is mostly lifted when we take tunnelling into account.

Any linear combination of degenerate eigenfunctions is also an eigenfunction. The following are interesting linear combinations, because they are not only energy eigenfunctions (in the limit  $\kappa \rightarrow \infty$ ), but they are also eigenfunctions of the translation operator  $T(a)$  with eigenvalue  $e^{-ika}$ :

$$\tilde{\psi}_{kn}(x) = \sum_{j=-\infty}^{+\infty} e^{ijk a} \tilde{\phi}_n(x - ja). \quad (6.26)$$

Here  $k$  lies in the Brillouin zone,  $-\pi/a < k \leq \pi/a$ , and the energies depend only on  $n$  (not on  $k$ ). Of course, we expect that the energy eigenfunctions can be written as eigenfunctions of the translation operator, even when tunnelling is taken into account; in that case, as we will see, the energies depend on both  $k$  and  $n$ .

Let us return to Eq. (6.22), and assume that  $\kappa$  is not infinite. Denote the matrix in that equation by  $M$ , and suppose that  $(A_0, B_0)$  is an eigenvector of  $M$  with eigenvalue  $\lambda$ .

We can normalize the eigenvector by taking  $A_0 = 1$ . Then we have

$$\begin{pmatrix} A_j \\ B_j \end{pmatrix} = \lambda^j \begin{pmatrix} A_0 \\ B_0 \end{pmatrix}. \quad (6.27)$$

Therefore if  $|\lambda| > 1$ , the solution will blow up as  $x \rightarrow \infty$ , and if  $|\lambda| < 1$ , the solution will blow up as  $x \rightarrow -\infty$ . Therefore we require  $|\lambda| = 1$  in order to obtain an acceptable solution, and  $\lambda$  must be a phase factor, say,  $e^{i\alpha}$ . Also, since  $\det M = \lambda_1 \lambda_2 = 1$ , if one of the eigenvalues is a phase factor, the other one must be too, and in fact they are complex conjugates of each other.

To find the eigenvalues of  $M$ , let

$$q = \text{tr } M = 2 \cos \frac{\Phi}{2} \left( e^\kappa + \frac{1}{4} e^{-\kappa} \right), \quad (6.28)$$

so the secular equation is

$$\lambda^2 - q\lambda + 1 = 0. \quad (6.29)$$

The roots are

$$\lambda = \frac{q \pm \sqrt{q^2 - 4}}{2} = \frac{q \pm i\sqrt{4 - q^2}}{2}. \quad (6.30)$$

If  $|q| > 2$ , then both roots are real, with  $|\lambda_1| > 1$  and  $|\lambda_2| < 1$ , or vice versa. This case does not lead to acceptable solutions. But if  $|q| \leq 2$ , then both roots are phase factors,  $\lambda = e^{\pm i\alpha}$ , with

$$\cos \alpha = \frac{q}{2} = \cos \frac{\Phi}{2} \left( e^\kappa + \frac{1}{4} e^{-\kappa} \right). \quad (6.31)$$

To find the wave functions, let  $(A_0 = 1, B_0)$  be an eigenvector of  $M$  with eigenvalue  $\lambda = e^{i\alpha}$ , and let  $\phi_n(x)$  be the wave in region  $j = 0$  of the form (6.20) which vanishes in all regions  $j \neq 0$ . This is just like the function  $\tilde{\phi}_n(x)$  introduced earlier, except now both  $A_0$  and  $B_0$  are nonzero. (In fact, as we will show,  $B_0$  is small, so functions  $\tilde{\phi}_n$  and  $\phi_n$  are almost the same.) Then in view of Eq. (6.27), the overall energy eigenfunction is

$$\psi_{kn}(x) = \sum_{j=-\infty}^{\infty} e^{ij\alpha} \phi_n(x - ja), \quad (6.32)$$

which is an eigenfunction of the translation operator with eigenvalue  $e^{-ika} = e^{-i\alpha}$ . In other words, WKB theory has automatically generated for us eigenfunctions of the translation operator.

To find the energies of the eigenfunctions  $\psi_{kn}(x)$ , we return to Eq. (6.28) and the condition  $|q| \leq 2$ , which is equivalent to

$$\left| \cos \frac{\Phi}{2} \left( e^\kappa + \frac{1}{4} e^{-\kappa} \right) \right| \approx e^\kappa \left| \cos \frac{\Phi}{2} \right| \leq 1. \quad (6.33)$$



Since  $e^\kappa$  is large, this condition can only be satisfied if  $\cos \Phi/2$  is small. Now  $\cos \Phi/2$  vanishes when  $\Phi$  is given by the Bohr-Sommerfeld condition (6.25), so we must assume that  $\Phi$  differs from  $\Phi_n$  by only a small amount  $\delta$ ,

$$\Phi = (n + \tfrac{1}{2})2\pi + \delta, \quad (6.34)$$

which implies

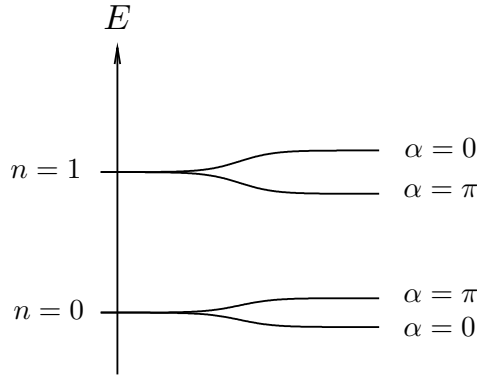
$$\begin{aligned} \cos \frac{\Phi}{2} &\approx (-1)^{n+1} \frac{\delta}{2}, \\ \sin \frac{\Phi}{2} &\approx (-1)^n. \end{aligned} \quad (6.35)$$

On the other hand, from Eq. (6.31) we have (neglecting  $e^{-\kappa}$  in comparison to  $e^\kappa$ ),

$$\cos \frac{\Phi}{2} \approx e^{-\kappa} \cos \alpha. \quad (6.36)$$

Therefore  $\delta$  can be expressed as a function of  $\alpha = ka$  (which specifies the translation eigenvalue):

$$\delta = 2(-1)^{n+1} e^{-\kappa} \cos \alpha. \quad (6.37)$$



**Fig. 6.2.** The nominal Bohr-Sommerfeld energy levels  $E_n$  open up into energy bands when the tunnelling is turned on. The energy cycles once through the band, bottom to top or vice versa, as  $\alpha$  goes from 0 to  $2\pi$ , or, equivalently, as  $k$  covers the Brillouin zone.

We see that the Bohr-Sommerfeld phases  $\Phi = \Phi_n$  characterizing the quantized energies in the absence of tunnelling open up into small bands around  $\Phi_n$  of width

$$\Delta\Phi = 2\delta_{\max} = 4e^{-\kappa}, \quad (6.38)$$

when tunnelling is allowed. Also, from classical mechanics we have

$$\frac{d\Phi}{dE} = \frac{2\pi}{\hbar\omega}, \quad (6.39)$$

where  $\omega$  is the frequency of the classical orbit of energy  $E$ , so the nominal Bohr-Sommerfeld energies  $E_n$  in the absence of tunnelling open up into small bands of width

$$\Delta E = \frac{2\hbar\omega_n}{\pi} e^{-\kappa}, \quad (6.40)$$

when tunnelling is turned on. See Fig. 6.2. In Eq. (6.40),  $\omega_n$  is the classical period of the orbit with energy  $E_n$ . The energy within a band is a function of  $\alpha$ ,

$$E = E_n + \frac{\hbar\omega_n}{\pi} (-1)^{n+1} e^{-\kappa} \cos \alpha. \quad (6.41)$$

We see that for band  $n = 0$ , the bottom of the band (the ground state) is the wave function with  $\alpha = 0$ . This wave function is purely real, and has no nodes (as we expect for the ground state of a one-dimensional problem). As we increase the angle  $\alpha$ , the energy rises up to the top of the band at  $\alpha = \pi$  and produces a real wave function with one node per period. The energy then returns to the bottom as  $\alpha$  increases to  $2\pi$ . For the band  $n = 1$ , this pattern is reversed ( $\alpha = 0$  is at the top of the band).

To obtain the energy eigenfunctions explicitly, we need the eigenvector of the matrix  $M$  corresponding to  $\lambda = e^{i\alpha}$ . These are easy to obtain in the approximation  $e^{\kappa} \gg 1$ ; we use Eqs. (6.22) and (6.35), to obtain

$$A_0 = 1, \quad B_0 = \frac{1}{2} (-1)^{n+1} e^{-\kappa} e^{-i\alpha}. \quad (6.42)$$

As expected, the coefficient  $B_0$  is small. The energy eigenfunctions are purely real for  $\alpha = 0$  or  $\alpha = \pi$ , for which the phase  $e^{i\alpha} = \pm 1$ . These wave functions are nondegenerate. For all other values of  $\alpha$ , the wave functions are complex, and are two-fold degenerate. The degenerate wave functions are complex conjugates of each other, and are related by time-reversal.

The bands are exponentially small in the quantity  $\kappa$ , so in the energy range we are considering ( $E$  sufficiently below the top of the wells), we have small bands separated by large band gaps. However, as we raise  $E$  toward the top of the well,  $\kappa$  decreases, and the bands open up wider. Our WKB approximation breaks down as we approach the top of the well, but it can be shown that as we rise above the top of the well, the situation reverses, with large energy bands and exponentially small band gaps.