Bloch functions— general properties 11 h 15 In this chapter we discuss a number of general properties of eigen-functions in infinite periodic lattices and in applied electric and magnetic fields. The discussion is presented largely in the form of theorems. BLOCH THEOREM THEOREM 1. The Bloch	Hàm Bloch-các tính chất chung Trong chương này, chúng tôi sẽ đề cập đến một số tính chất tổng quát của các hàm riêng trong mạng tuần hoàn vô hạn dưới tác dụng của các trường điện và từ. Nội dung được trình bày chủ yếu thông qua các định lí. ĐỊNH LÝ BLOCH [redacted]

theorem states that if F(x) is periodic with the periodicity of the lattice, then the solutions <p(x) of the wave equation

(1) Hv(x) = v* + V(^i) r(x) = are of the form

(2) ^k(x) = e*‘xwk(x),

where uk(x) is periodic with the periodicity of the direct lattice.

Analytical proofs of this central theorem are found in the standard elementary texts on solid state theory. The most direct and elegant proof utilizes a little group theory.

Proof: With periodic boundary conditions over a volume of N3 lattice points, the translation group is abelian. All operations of an abelian group commute. If all operations of a group commute, then all the irreducible representations of the group are one-dimensional.

Consider the lattice translation operator T defined by

(3) Tx = x + tmnp = x + ma + nb + pc,

where m, n, p are integers; then

(4) Tmnpcpk(x) = ^(x + ma + nb + pc).

The operations T form a cyclic group; because the representations are

only one-dimensional,

(5) T'mnpipk(x) = Cmnp<Pk(x),

where Cmnp is a constant. Because

(6) T 10(HPk(x) = ¥>k(x + a) = Cioo^k(*),

we must have in particular for a

lattice having N lattice points on a side

(7) Tjtooiftix) = ^k(x + iVa) = (cmo)*Vk(x).

But with periodic boundary conditions

(8) *k(* + N&) = ^(x), so that

(9) (cioo)* - l; thus Cioo must be one of the N roots of unity:

(10) cioo - eUiilN; { = 1, 2, 3, • * • N.

This condition is satisfied generally by the function

(11) Vk(x) = e*‘xwk(x), if wk(x) has the period of the lattice and

(12) iVk = £a* + nb* + fc*, (£, f integral)

is a vector of the reciprocal lattice. For a lattice translation t,

(13) <pu(x + t) = e<k’(x+t)Mk(x + t) = eik'te*k‘*wk(x) = e**VkOO _ e<2*(f»i|+n,+j>r)/iV ,pk(x)i

as required by (5) and (10).

In other language, e**1® is the eigenvalue of the lattice translation operator Ta:

(14) Tn^(x) = e<k’t»^k(x),

where ^ is a lattice translation vector; ^(x) is an eigenvector of T„.

THEOREM 2. The function wk(x) of the Bloch function ^(x) = e*k‘xwk(x) satisfies the equation

(15) ^ (p + k)2 + P(x)) wk(x) = €kWk(x).

This is equivalent to a gauge transformation.

Proof: Note that, using p = —

iV, we have the operator equation

(16) petk'x =>= e*k*x(p -f k).

Thus

(17) P¥>k(x) = e<k'x(p + k)wk(x), and

(18) pVk(x) = elk'x(p + k) V(x),

from which (15) follows directly.

We may rewrite (15) as

(19) (V2 -i- 2tk ■ V) + F(x)^ uk(x) = \kwk(x), with

(20) Xt = £k - k\
2m

where £k is the eigenvalue of (15). If F(x) = 0, a solution of (19) is

(21) uk(x) = constant; Xk = 0, and

(22) £k = fc2; ^(x) = eik'x,
2m

the usual plane wave. At the point k = 0 the equation for UQ(X) is simply

(23) (- ^ V2 + F(x)^ u0(x) = £0w0(x);

thus the equation for u0(x) has the symmetry of F(x), which is the symmetry of the crystal space group.

Spin-Orbit Interaction. The hamiltonian with spin-orbit interaction has the form (Schiff, p. 333)

(24) H = + F(x) + x gradyw-p>

where d is the pauli spin operator, with the components

(25) = (l o); = (i ~o); = (o -l)

The hamiltonian (24) is invariant under lattice translations T if F(x) is

invariant under T. The eigenfunctions of (24) will be of the Bloch form, but they will not in general correspond to the pure spin states a or fi for which aza = a; <?2j8 = —(3. In general

(26) <pk t (x) = Xk t (x)« + 7k t (x)l8 = eik'*uk t (x),

where the arrow | on the Bloch function (x) denotes a state with the spin generally up in the sense that (^kt^^kt) ^ positive. In the absence of spin-orbit interaction <pT involves only a; and <p± only 0. The arrows on Xkt and 7kj are labels to indicate their association with <pk |.

THEOREM 3. With spin-orbit interaction the function uk(x) satisfies

are often treated as perturbations for small k or small changes in k from a special wavevector ko.

The quantity

(29) 7t = p + o' X grad V

has many of the properties for the problem with spin-orbit interaction which p has for the problem without spin-orbit interaction.

TIME REVERSAL SYMMETRY

The time reversal transformation K takes x into x; p into — p; d into— d.

The hamiltonian (24) is invariant under time reversal; thus [H,K] = 0. For a system of a single electron the result of Kramers (Messiah, Chapter 15, Section 18) for the time

reversal operator is

K = —iavKr

where Ko in the Sehrodinger representation is the operation of taking the complex conjugate. Thus Ko has the property for any two states ip and \p that

(31) M) = (K0t,K0<p).

Further, with <rv2 = 1,

(32) (Kf,Kv) = (K^,^KW) =

also,

(33) K%<p = (—iav)(—icry)<p = — tp.

An important application of time-reversed pairs of states has been made by P. W. Anderson [Phys. Chem. Solids 11, 26 (1959)]. He shows that in very impure superconductors we must consider pairs defined by the time reversal operation, rather than Bloch function pairs.

THEOREM 4. If p is a one-electron eigenstate of H, then K<p is also an eigenstate with the same energy eigenvalue in the absence of external magnetic fields. Further, K<p is orthogonal to <p. This is the Kramers theorem.

Proof: The hamiltonian commutes with K; therefore K<p must be an eigenstate if y> is an eigenstate, and the eigenvalues are the same. Now by (32) and (33)

(34) (*,*„) = ~(K2<p,K<p) = — (<p,K<p) = 0,

so that and are linearly independent.Q.E.D.

THEOREM 5. The states and belong to wavevector — k, so

that ekT = e_kl and eki = e_kt.

Proof: Ktpki — —WyKo^ = e-** X (periodic function of x) j, so that

(35) T =

apart from a phase factor. We recall that <rv reverses the spin direc-tion. We assign opposite spin arrows to <p and K<p because

(<Pkt>°'z¥'kT) = (^ff*<Pkt»^Pkf) = —

using oyr* = —<Tt<Ty. From (35) and Theorem 4 we have

(36) £kt = e-ki > Sk| = £-kf-

Q.E.D.

The bands have a twofold degeneracy in the sense that each energy occurs twice, but not at the same k. A double degeneracy at the same energy and k occurs only if other symmetry elements are present; with the inversion operation J the energy surface will be double at every point in k space.

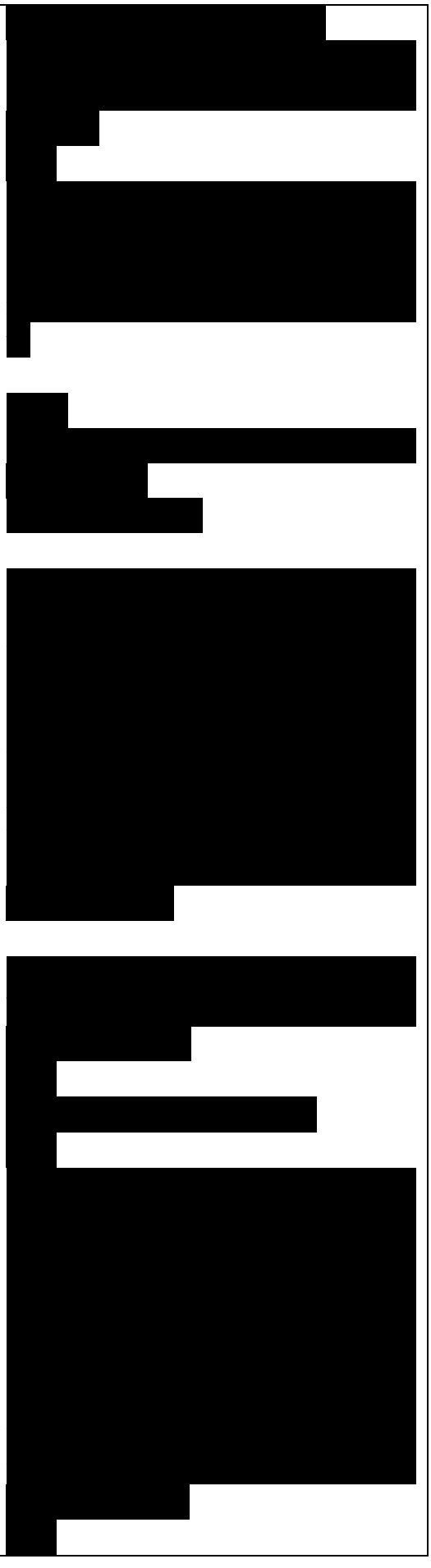
THEOREM 6. If the hamiltonian is invariant under space inversion, then

(37) *kT(x) = <p_kt(-x),

apart from a phase factor, and

(38) ekT=e_kT.

Proof: The space inversion operator J sends x into — x; p into —p; and d into d. The reason d does not change sign is that it is an angular momentum and transforms as an axial vector. Thus if JT(x) = F(x), then the hamiltonian including spin-orbit interaction is invariant under J. Then J^(x) is degenerate with (x). But



(39) Jipk t (x) = e_ik'X T(-x)
is a Bloch function belonging to — k, because the eigenvalue of J<pk | under a lattice translation operator T is e~ik'tn. We may call w_k| (x) = wkf (—x), whence
(40) ^_kT(x) =
and
(41) ekf = e_kT. Q.E.D.
It is simple to show directly, if one wishes, that w_kf (x) satisfies the same differential equation as wkf (—x).
We recall that J commutes with <rz, so that the expectation value of <rz over <pk | and ^_kT is the same. Therefore, using (36), the com¬bined symmetry elements K and J have the consequence that
(42) eki = ekA,
where
(43)
apart from a phase factor.
The product operation
(43) C = KJ = ~i<rvK0J = JK
will be called conjugation. Conjugation reverses the spin of a Bloch state, but does not reverse its wavevector:
(44) CVfct = <pki,
apart from a phase factor. A number of theorems involving the opera¬tions K and C are given as exercises at the end of the chapter.
THEOREM 7. In the momentum representation, with G a reciprocal lattice vector,
(45) *(*) = e*"2f0(k)
where the /o(k) are c-numbers, the wave equation without

spin-orbit interaction is

(46) in (k + G)2/o(k) + | F(G ~ e)f‘(k) = Sk/o(k)’

where g is a reciprocal lattice vector and V(G) is the fourier trans-form of V(x) between plane wave states:

(47) 7(G) = f d3x eiG'*V(x).

The result (47) follows on operating on (46) with H = T + 7 and taking the scalar product with etk'VG‘x.

It follows from the representation (46) that the expectation value of the velocity v satisfies

(48) (k|v|k) = (k|p/m|k) = m_1 J (k + G)|/G(k)|2

6

= gradk e(k).

The proof of the last step is left to the reader. An alternate deriva-tion is given as Theorem 11.

It also follows that the effective mass tensor defined by

(49) (£),.-££•«

is equal to (Problem 8):

(50) &ir^+%G<il,a(kr)

THEOREM 8. The energy ek is periodic in the reciprocal lattice; that is,

(51) sk = sk+G-

Proof: Consider a state <pk of energy ek; we may write

(52) <pk = eik‘%(x) = ei(k+G)'x«k+G(x) = <pk+G, where

(53) Wk+o(x) = e-lG‘*wk(x)

has the periodicity of the lattice. Thus may be constructed from <pk; it follows that Bk = ek+G.

We now develop an important theorem related to the effective mass tensor (1 /TO)MV defined by (50), which is equivalent to

e,, = k,k, + ■ • • .
2m \m*/py

THEOREM 9. If the state <pk at k = 0 in the band y is nondegenerate, except for the time reversal degeneracy, the effective mass tensor at this point is given by

where 8, y are band indices and the zeros stand for k = 0. Without spin-orbit interaction p replaces tc, and usually it is sufficiently accurate to write p for «. The result (56) is referred to also as the /-sum rule for k = 0.

Proof: In the equation (27) for uk(x) we treat

(57)

as a perturbation, with the hamiltonian for k = 0 treated as the unperturbed hamiltonian. We could equally expand about any other wavevector, say k0.

Let us consider first the diagonal matrix elements of H'. If the crystal has a center of symmetry, then

(58) (y0*\°y) = 0

by parity; further

(59) <TO|X|C7) = 0,

by Exercise 5, with | Cy) denoting the conjugate state to |Oy). The spin indices are not shown in our present notation. If the crystal does not have a center of symmetry, we must

consider the matrix elements for the particular symmetry involved. Thus at the point T in the zinc-blende structure the twofold representations r6 and r7 of the double group satisfy the selection rules (see Chapter 10)

(60) r6 X Tv = r7 + r8; r7 x rv = r6 + r8,

where IV is the vector representation. These rules are given by G. Dresselhaus, Phys. Rev. 100, 580 (1955), along with the character table. Because * transforms as a vector, the rules tell us that * does not have diagonal matrix elements within the twofold representations. Thus the first-order energy correction from H* vanishes. In Problem (14.4), we have a situation in which the first-order energy does not vanish.

The energy to second order is

(61) *00 - *(0) +f + -tl'

v 2m m t Sy0 — 2a o

where on the right-hand side we have included the kinetic energy associated with the elk x modulation. The result (56) is obtained if we write (61) in the form

(62) e?(k) = e7(0) + —) kjc, +

By going to higher orders in the perturbation theory we may construct the entire energy surface. The method is referred to as k • p perturba¬tion theory. The eigenfunction to first order in k is

(63) +

If further degeneracy exists at the point k = 0, we must apply degen¬erate perturbation theory, as in Schiff, pp. 156-158. The valence band edge in important semiconductor crystals is degenerate; the form of the energy surfaces is considered in a later chapter on semiconductor bands, but an example will be given below.

We can draw some immediate conclusions from the form of (61). If one e70 — £«o is very small, the form of the band y near k = 0 will be determined largely by the matrix elements connecting it with the band 8; and, vice versa, 8 will be determined by y. Further, if the energy denominator is very small, the effective mass ratio m*/m will be very small. An extreme example may be cited: It is believed that the energy gap in the semiconductor crystal Cd^Hgi^Te (x = 0.136) is less than 0.006 ev, and the experiments suggest also that m*/m ^ 4 X 10-4 at the bottom of the conduction band.

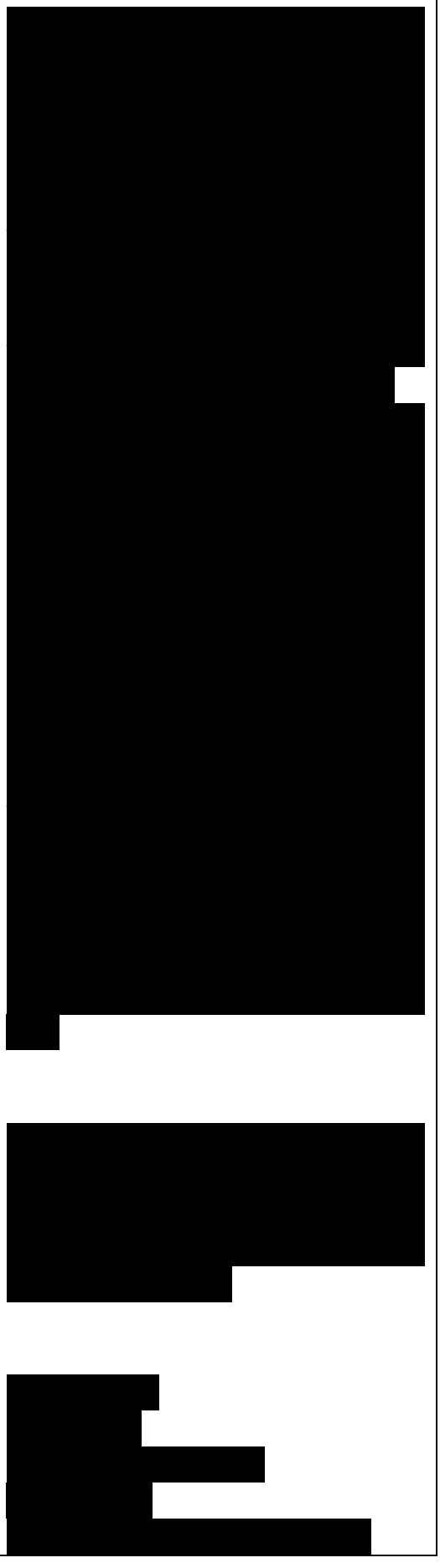
According to calculations by F. S. Ham, Phys. Rev. 128, 82 (1962), the effective masses at k = 0 in the conduction bands of the alkali

values:

Na	K	Rb	Cs
3s	4s	5s	6s
0.965	0.86	0.78	0.73

Metal Li

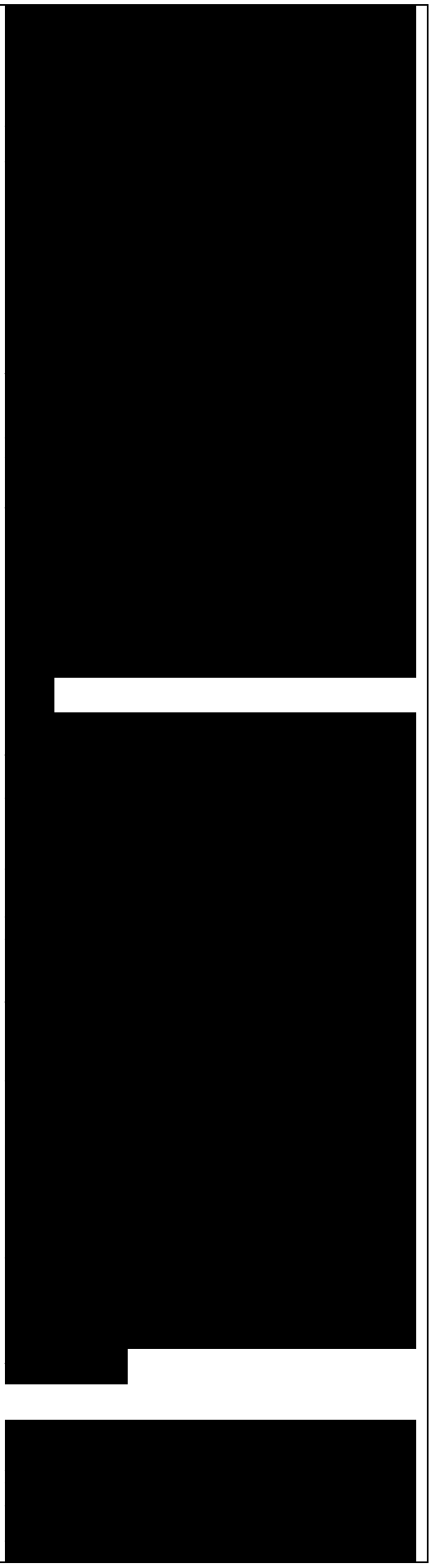
Band index 2s m*/m %, 33



Suppose that the order of the bands near k = 0 in an alkali metal is the same as the order of the states in a free atom. Then in Li all the perturbations on the 2s conduction band will come from p levels higher in energy than 2s, as there is no 1 p level; for Li es0 — £Po < 0, so that m < m*. For Na the 3s conduction band is perturbed about equally, but in opposite directions, by the 2p levels below and the 3p levels above 3s in energy, and thus m* = m. As we go further along in the alkali series, the perturbations from below increase in effect relative to those from above, and m* < m.

Degenerate k • p Perturbation Theory. The simplest example of k • p perturbation theory for degenerate bands occurs in uniaxial crystals with a center of symmetry. Suppose we have a band of s-like symmetry at k = 0 lying above by an energy Eg a pair of bands degenerate at k = 0 and transforming at this point like x and y. The symmetry axis is along the z direction. The state which is z-like at k = 0 will be neglected implicitly: we assume that the crystal potential splits z off from the other states by an energy large in com¬parison with Eg. We neglect spin-orbit interaction in this example.

We note that the first-order energy correction vanishes from the perturbation (l/w)k • p, by parity. The second-order



energy involves the matrix elements

(64) <s|tf"|x> = —J (s|k • p|j>0'|k • p|z> = 0,

m Eg 7

also by parity; here j = x, y. Further,

(65) (x\H"\x) = (x\k • p|s)(s|k • p|x) = -]<z|px|s>|2;

(66) (x\H"\y) = (x\k • p|s)(s|k • p|y) = - <*|p*IsXsWz/>-

By symmetry (slpjj?/) = (s|px|z); thus we may write, for i, j = x or y,

(67) (i\H"\j) = —Akikj-, A =

The secular equation for the three states is

Eg+ A(kx2 + ky2) -X 0
0
0 —Akx2 — X — Akxky
0 — Akykx —Aky2 — X

which is also the value of <y|k * p\yz)(yz\k • p|y). The contributions of the d states to the off-diagonal elements vanish. Thus (71) becomes, in general,

Akx2 -f- Bk2 -f- X
Akxk
Akykx Aky2 + Bk2 + X

x,,; = — Bk2;

Xk = - Bk2 - A{k2 + ky2).

The surfaces of constant energy are figures of revolution about the z axis. One surface (that with the + sign) describes heavy holes; the other surface describes light holes.

ACCELERATION THEOREMS

THEOREM 10. In a steady applied electric field E the acceleration of an electron in a periodic lattice is described by

k = eE,
and the electron remains within the same band. We suppose that the band is nondegenerate.
First proof: If the electric field is included in the hamiltonian in the usual way as a scalar potential <p = — eE • x, the nonboundedness of x causes some mathematical difficulty. The simplest approach to the problem is to establish the electric field by a vector potential which increases linearly with time. We set
A = —cEt;
thus
_ 1 dA ^ E = — grad <p — =
E,
C dt
as required. The one-electron hamiltonian is

It is useful to become familiar with the classical motion of free electrons in the vector field A = — cEt:
H = r— (p + eE t)2;
the hamiltonian equations are
(82) p = —dH/dx — 0; - x = dH/dp = (p + eEt)/m.
On quantum theory for a free electron
(83) ip = [p,tf] =0; ix — [x,H] = z‘(k0 + eEt)/m,
where k0 is the eigenvalue of p, which is a constant of the motion.
Observe that the hamiltonian (80) has the periodicity of the lattice, whether or not E is present. Therefore the solutions are precisely of the Bloch form:

<Pk(x,E,0 = eik'xuk(x,E,t),
where uk(x,E,t) has the periodicity of the lattice; here the time t is viewed as a parameter. The functions «rk(x,E,£) for band y can be expanded as a linear combination of uak(x,0)—the eigenfunctions of all bands for E = 0. We see that bands can be defined rigorously in the electric field and k is a good quantum number: in this formula-tion k is not changed by the electric field!

We now treat the time t as a parameter and compare the kinetic energy term (p + eEt + k)2/2m in the effective hamiltonian for «k(E,2) with the kinetic energy term (p + eEt' -f k')2/2m in the hamiltonian for uk'(E,t'). The two hamiltonians will be identical if

(85) eEt + k = eEt' + k',

so that the state and the energy at k,£ are identical with those at k', t' if (85) is satisfied. Thus an electron which stays in a given state k will appear to change its properties in terms of the states classified in k at t = 0 as if

k = eE.

That is, an electron in ** at t = 0 will at a later time t be in a state having the original k, but with all the other properties (including the energy) of the state originally at k — eEt. The current in the state k is related

to the expectation value of p — (e/c)A; the current will tend to increase linearly with time because A cc t.

Because eE(t — t') is invariant under spatial translation, it will not cause k to change. We must still show that an electron at k in band y will at time t still be in the same band. That is, we need the adiabatic theorem, which states that a transition between states a and 7 is unlikely to occur if the change in the hamiltonian during the period l/o)ay is small in comparison with the energy difference ioay:

(87)

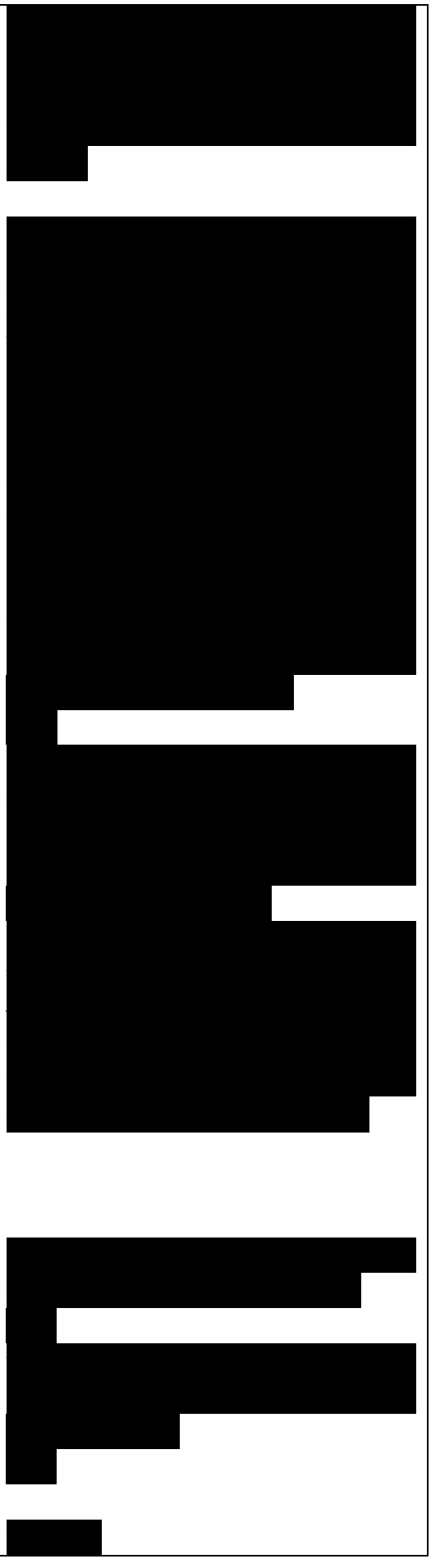
Our states a and y are states of the same k, but in different bands. The condition (87) is very easily satisfied—it is difficult to violate over an extended volume of a crystal. The argument of the present theorem is due to Kohn and to Shockley. The vector potential A = —cM can be established in a ring-shaped crystal by changing magnetic flux at a uniform rate through an infinite solenoid running through the inside of the ring.

Second 'proof: We write H — HQ + H', where

(88) = Y(z); H' = —F • x, with F = eE as the force on an electron in the electric field. Now note that

(89) gradk ^(x) = ix^(x) + e*,x gradk e''ik'x<Pk7(x).

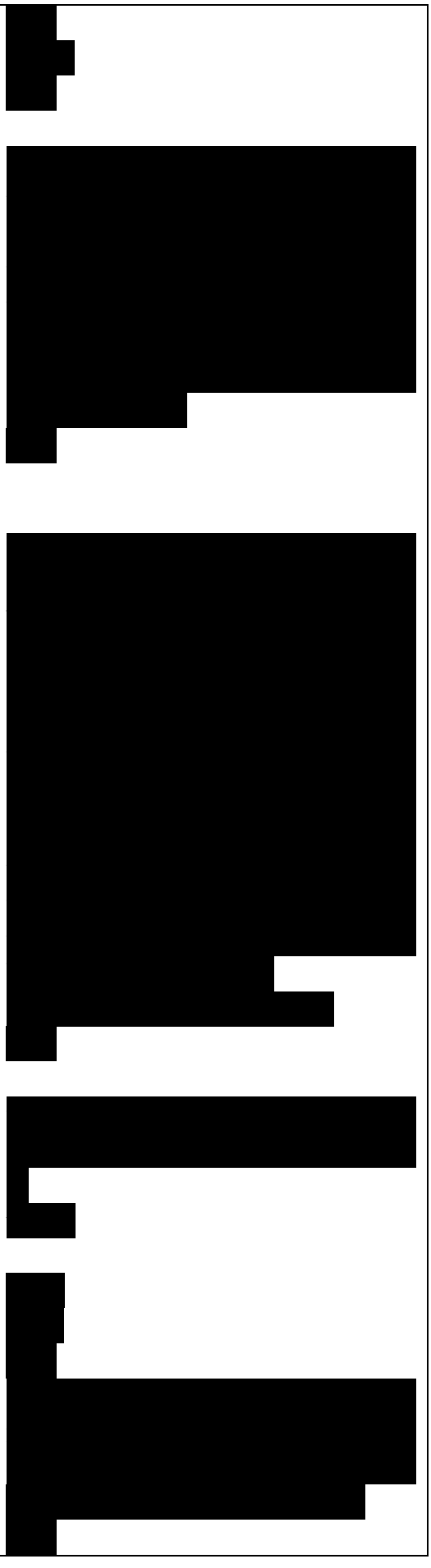
Then



(90) H = H* + iF • gradk)
where
(91) Hv = Ho- ieik'x¥ • gradk e"**
acts as invariant under a lattice translation because the term in F does not mix states of different k, but only of the same k of different bands. If <pk7(x) are the eigenstates of Hq, then
(92) -i(Sk'|e*-*F • gradk
= — i J dzx et(k-k')-* UytW * gradk uky,

which vanishes except for k = k' because the term u£s gradk ukr is invariant under a lattice translation. It follows that Hw gives interband mixing, but only the term iF • gradk in the hamiltonian (90) can cause a change of k. Notice that in the present formulation, unlike the earlier one with a time-dependent vector potential, k is not a constant of the motion.

Consider the problem of a free electron
(93) <Pk = etk‘xe-taW
in an electric field. The time-dependent Sehrodinger equation is
so that
da dk. 1
(96) Tt-Tt'* = ^nk
or
(97) ' § = F. w - —
The same argument applies in a crystal. We define a set of func-tions XkT(x) as the eigenfunctions of
(98) HpXky = £k7Xky



The time-dependent equation is

(99) i ^ = (H, + tF • gradk)Xk.
at

We try a solution with Xk confined to one band:

(100) xk = the derivative is

^ v ^Xk {da. , .dk \

(101) ’ *■ = \Tt +1 Jt ■gradV

or, on comparing (99) with (101),

dk , 0

(102) - = F. <wl

Thus the acceleration theorem is valid in the basis Xk-r of Bloch states for which the polarization effect of the electric field has been taken into account by the hamiltonian Hv.

For very short time intervals it can be shown that the motion of an electron in a crystal is governed by the free electron mass and not by the effective mass; see, for example, E. N. Adams and P. N. Argyres, Phys. Rev. 102, 605 (1956).

We give now a theorem which connects the expectation value of the velocity with the wavevector, thereby enabling us to use the accelera¬tion theorem to connect the change of velocity and the applied force; see also (49).

THEOREM 11. If (v) is the expectation value' of the velocity in a state |k7), then

(103) (v) = i([H,x]) = gradk Bky,

in the absence of magnetic

fields.

Proof; We consider the matrix element in the band y:

(104) <k|[tf,x]|k> = f d3x u$(x)e-*"[H,x]eik-*uw(x).

Now

(105) gradk (e“= — ie~ik'*xHeik'x + ie~{k’xHxelk'x — ie~ik'x[H,x]eik’x;

further, we have seen in (15) that

(106) H (p,x)eikx = eik‘xH{ p + k,x).

Thus

(107) (k|[if,x]jk) = —i j dzx wk(x)(gradk e~ik'xHeik'x)uk(x)

= -i j d3x wk (x)(gradk H(p + k,x))wk(x).

Now use the Feynman theorem, namely

(108) J- <k|H|k> = ^k| ^ |k),

where X is a parameter in the hamiltonian. Thus (107) becomes —i gradk £k, and

(109) <*> = gradk £k.

Q.E.D.

Further, as (x) is a function of k alone,

(H°) jt (±) = gradk gradk ek, or, by (55),

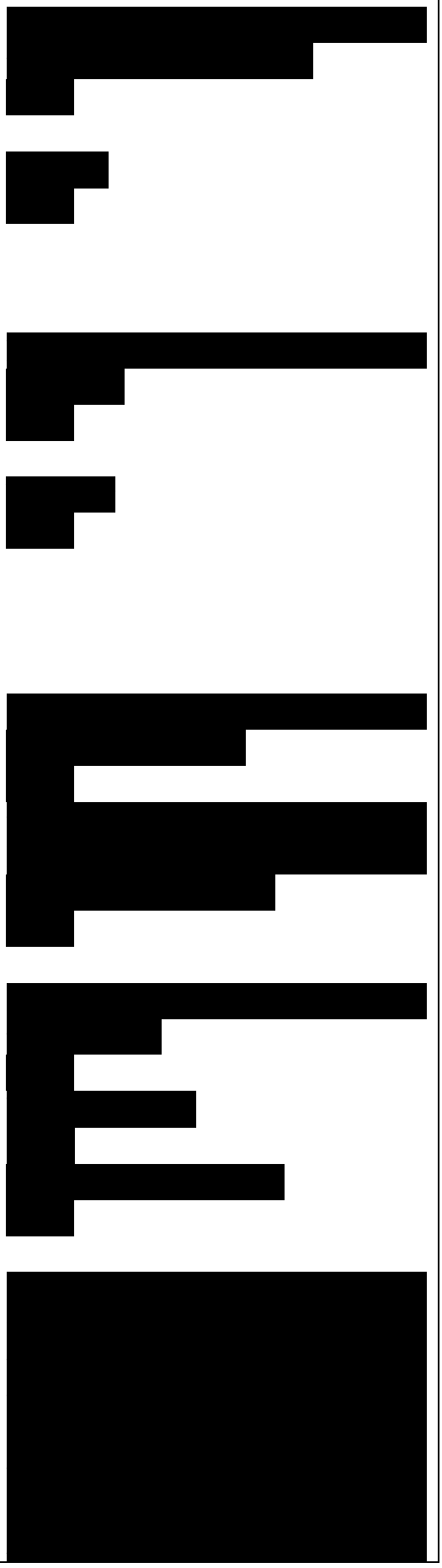
- <*> = F (1\ . dr^ dt \m*Jrfl

If £k = k2/2m*, then

(111) m* ~ (x) = F.

dt

It is more difficult to treat rigorously the motion of a lattice electron in a magnetic field. Particular problems are treated at several points in the text. For a general discussion and further references, see G. H. Wannier, Rev. Mod. Phys.



34, 645 (1962) and E. J. Blount in Solid state physics 13, 306. For electrons in nondegenerate bands and not-too-strong magnetic fields the result of the detailed calcula¬tions is that the equation of motion (111) may be generalized to

(112) F = e^E+|vx H^.

We now give several theorems concerning special functions—Wannier functions—which are sometimes used in discussions of the motion of lattice electrons in perturbed potentials and in electric and magnetic fields.

WANNIER FUNCTIONS

Let ^(x) be a Bloch function in the band y; the Wannier functions are defined by

(113) wy(z - x.) = AT» X e-^Wx),

k

where N is the number of atoms and xn is a lattice point.

THEOREM 12. The Bloch functions may be expanded in terms of Wannier functions as

(114) ^(x) = N~H X «<k'*ti>(x - x,,).

n

Proof: From the definition of w,

(115) *>k(x) N~» X X o-^'-NvW

n k'

= 2V-1 J ei(k~k,)'x"<pk'(x) = <pk(x).

k',n

THEOREM 13. Wannier functions about different lattice points are orthogonal, that is,

(116) j dzx w*(x)w(x — xn)

=0, xn 0.
Proof:
(117) f dzx w*(x)w(x - xn) = N~% J f dzx e“ik‘*»^(x)^k.(x)
J kk' J
= JV-* X = «0,. K

The Wannier functions tend to be peaked around the individual lattice sites xn. We examine this under the special assumption that
(118) <pk = e*'xM0(x),
where u0(x) is independent of k. Then
(119) w(x - xn) = N~Hu0(x) J e*-(*-*n).
In one dimension with lattice constant a,
2ir
(120) iVa’
where m is an integer between ±%N. Then
(122)
for Ny> 1, and
sin {T(X — xn)/a} W(x — xn)/a)

In three dimensions we have the product of three similar functions. Thus the Wannier function assumes its largest value within the lattice cell about xn, and it tails off as we go out from the central cell.
THEOREM 14. If s(k) is the solution of the unperturbed one-particle periodic potential problem for a nondegenerate energy band, then the eigenvalues with a slowly varying perturbation H'(x) are given by the eigenvalues X of the equation







(124) [e(p) + H'(x)]U(x) = \U(x),

where e(p) is the operator obtained on substituting p or — i grad for k in e(k) in the band y; U(x) has the property that

(125) x(x) = 2 U(xn)w(x - xn),
n

where %{x) is the solution of the Sehrodinger equation

(126) [Hq + H' (x)]x(x) = Xx(x).

Proof: A clear proof is given by J. C. Slater, Phys. Rev. 76, 1592 (1949). A treatment of a similar problem for weakly bound donor and acceptor states in semiconductors is given in Chapter 14; the method given there is the one most often used in practice when quantitative calculations are carried out.

In a magnetic field (124) becomes

U(i) = W(x),

as demonstrated by J. M. Luttinger, Phys. Rev. 84, 814 (1951). In the expansion of s(k) any product of k's is to be written as a symmetrized product before making the substitution k —> p — e/cA. An example of effects arising from the noncommutativity of the components of k in a magnetic field is given in Chapter 14.

PROBLEMS 3 h 30

1. If Oi has the property

(128) KOiK~l = 0i+,

show that

(129) {<p\Ox\K<p) = 0.

For Oi we may have a symmetrized product of an even number of momentum components, or any function of x.

2. For 0\ as defined in the first problem, show that

(130) (<P\OI\<P) = (K<p\0i\K<p).

3. If 02 has the property

(131) K02K-1 = -02+,

show that

(132) (^|02k> = -(K<p\Oz\K<p).

4. Show that the results of 1, 2, 3 hold if everywhere C = KJ is written for K; the states are now assumed to be eigenstates of a hamiltonian invariant under C.

5. If COC~l = 0+ show that

(133) <Tk|0|kJ,> = 0;

here 0 might be p, a symmetrized product of an even number of linear momenta, or the spin-orbit interaction; show further that

(134) <Tk|0|kt> - <|kiO|k|).

6. If COC~l = —0+, show that

(135) <tk|01kf) = -Uk|0|k.l>;

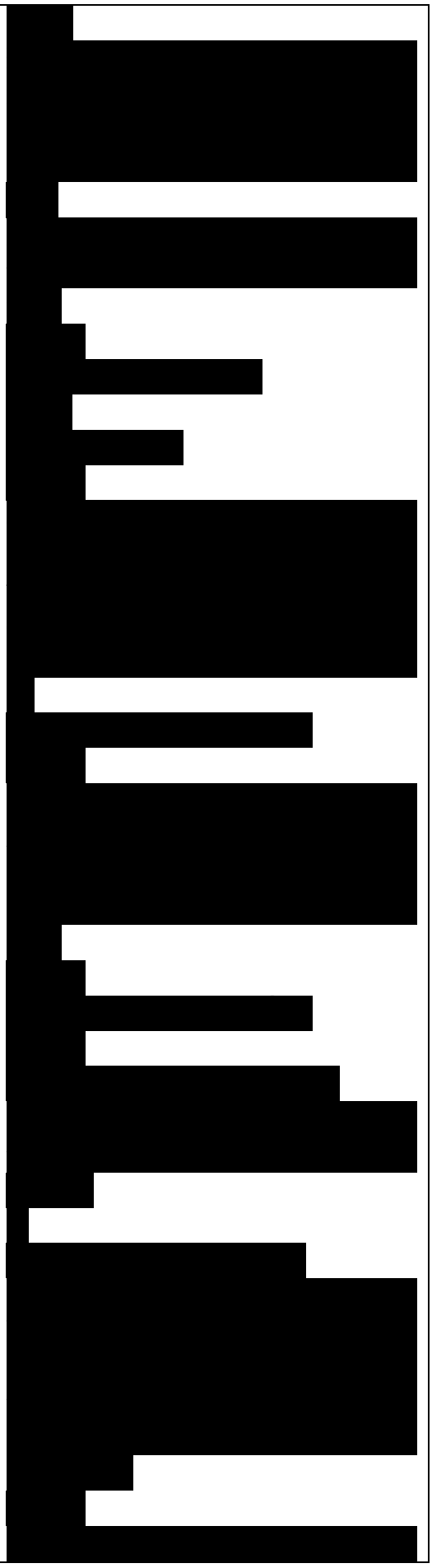
here 0 might be L or d.

7. Prove (49); use (47) and the normalization condition gradk ^ |/o(k)|2

8. Prove (51).

9. Evaluate the effective mass tensor (56), with p written for w, in the limit of separated atoms. The wavefunctions may be written in the tight binding form as

(136)



where v is an atomic function in the state y. It is assumed that t»'s centered on different lattice sites do not overlap. We find that <7k|p|k5) = (vt|p|t><«), where vy and % are different states of the same atom. Now

(137) ^(y\p\8) = (Bs - ey)(y\x\8), so that

(138) (-£) = [l - 2m X (S» - M(-»W*>I2] - 0,

\Jrl J xx j

on application of the atomic /-sum rule. Show that (136) satisfies the trans¬lational symmetry requirement (14).

10. (a) Show that an electron in a crystal in an electric field £ will oscillate according to

(139) e(x — x0) • £ = £(k0 + e£t) — E(k0),

from conservation of energy. The amplitude Ax of oscillation is Ax = As/e[£|, where Ae is the width of the band. (6) Estimate Ax for a reasonable electric field, (c) Estimate the frequency of the motion.

11. Consider a Bloch state which is nondegenerate at k = 0. Using <pk(x) as an expansion of ^o(x) to first order in k • p, show by direct calculation that

<kWk>-*•(£)./

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