Floquet's Theorem and Band Theory in One Dimension

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Floquet's theorem, and the general qualitative features of the band structure, are described in the one-dimensional case. The discussion includes a little-known unstable state at band edges that is not a Floquet function. This "band edge state" can in certain cases play a role in a thin crystalline layer, analogous to the role of a surface state in a semi-infinite crystal. Some incorrect and misleading statements about Floquet's and Bloch's theorems, which are widespread in expository accounts of the subject, are pointed out.

I. INTRODUCTION

A great many elementary accounts in the physics literature of the basic theory of Floquet's theorem and band theory contain incorrect or misleading statements. Statements of the form, "all solutions of Schrödinger's equation with a periodic potential are Floquet functions" are common but incorrect. Some of these statements are presented and corrected in Sec. VII.

It is convenient to give first a discussion of Floquet's theorem. This is done in Sec. III. The theory includes the unstable as well as the stable solutions; the treatment also deals carefully with the special situation which arises at a band edge (i.e., an energy separating an "allowed" band of stable solutions from a "forbidden" band of unstable solutions). At the band edge there are as usual two linearly independent solutions, but there is only one solution of Floquet form.

In this paper the analysis of a periodic potential on the real line ($-\infty \leq x \leq \infty$) is named after Floquet,[1] and the analysis using cyclic boundary conditions is named after Bloch.[2] In the physics literature either analysis is usually named after Bloch. Bloch's analysis is described and compared with Floquet's in Sec. VI.

II. THE EQUATION

In the one-electron approximation, the stationary states $\psi(x)$ of an electron in a crystal lattice are solutions of the time-independent Schrödinger equation in a periodic potential

$$(d^2\psi/dx^2)+Q(x)\psi=0,$$

where

$$Q(x)=(2m/\hbar^2)[E-V(x)]. \qquad (1)$$

We consider only the one-dimensional case and neglect spin. m is the mass of the electron, and E is the energy of the stationary state. We take E real, as this corresponds to physical solutions. (One can learn more by studying the analytic properties of the solutions with complex E,[3] but we do not do this here.)

$V(x)$ is the potential due to the lattice. $V(x)$ is periodic with minimum period a:

$$V(x)=V(x+a).$$

All the following results hold if $V(x)$ is finite and twice differentiable everywhere.[4] Most of the results hold under less restrictive conditions. In the problem of an electron moving in a crystal, a potential $V(x)$ with no lower bound at the positions of the nuclei is often indicated.[5–7] Such a potential is arrived at by a self-consistent one-electron approximation, such as the Hartree–Fock method. However the nearly free electron model (NFEM), based on a weak potential is found to give band structure results in good agreement with experiment for many crystals (particularly simple metals). The NFEM is justified by the theory of the pseudopotential.[8] In this theory it is found that there are a pseudopotential and a pseudowavefunction for a conduction electron which satisfy a one-electron Schrödinger equation.

The energy eigenvalue E of this pseudoequation is the same as that of the self-consistent equation. The advantage of this method is that the pseudopotential can be chosen to be small, so E can be found quite accurately by second-order perturbation theory. In general, the pseudopotential is a nonlocal potential $V(x, x')$, meaning that the potential term $V(x)\psi(x)$ in the one-electron Schrödinger equation is replaced by

$$\int dx' V(x, x')\psi(x').$$

Sometimes the pseudopotential can be approximated by a local potential, in which case the pseudoequation is formally the same as Eq. (1).

In what follows we will consider the mathematical nature of the solutions of Eq. (1). For our purpose there is no need to specify the origin of Eq. (1); we merely note that the one-electron approximation, and the results of band theory, are applicable to electrons in crystals in many cases.

III. STABLE AND UNSTABLE SOLUTIONS; FLOQUET'S THEOREM

Equation (1) is a second-order, linear, ordinary differential equation, so it has two linearly independent solutions for each value of E, and any linear combination of these two solutions is also a solution with the same E. For some values of E however, the solutions are not *stable*. We define a solution ψ to be stable if it is bounded, i.e., if there exists a constant M such that $|\psi|<M$ for all x. Otherwise the solution is *unstable*. (In the theory of differential equations, and its various fields of application, there exist many nonequivalent definitions given the name stability.) Under the assumptions about $V(x)$ made in Sec. II, the solutions of Eq. (1) are continuous,[9] so they can only be unstable by becoming infinite at $x=+\infty$ or $-\infty$, or both.

Only stable solutions are acceptable as quantum mechanical states in a perfectly periodic potential. Nevertheless, we consider all solutions, stable and unstable, because the mathematical theory has a more complete form if all solutions are studied, and because the unstable solutions are useful in related problems (e.g., surface and size effects).

Since $Q(x)$ in Eq. (1) is real, the two independent solutions can be taken real. Nevertheless, it is convenient to consider linear combinations of solutions with complex coefficients. This is because we wish to find solutions with specially simple properties, which amounts to reducing a certain matrix to canonical form. The theory of the canonical form of matrices takes its most natural form if the matrix elements are complex numbers.

Suppose $\psi_1(x)$ and $\psi_2(x)$ are two independent solutions of Eq. (1). Then $\psi_1(x+a)$ and $\psi_2(x+a)$ are also solutions since Eq. (1) is unchanged by replacing x with $x+a$.

We write

$$\mathbf{v}(x)=\begin{pmatrix}\psi_1(x)\\ \psi_2(x)\end{pmatrix}.$$

Then

$$\mathbf{v}(x+a)=T\mathbf{v}(x), \tag{2}$$

where T is a 2×2 matrix whose elements are in general complex numbers. T is the operator of translation by a. Equation (2) holds because any solution can be written as a linear combination of two independent solutions.

A different pair $\mathbf{v}'=L\mathbf{v}$ of independent solutions [where L is any linear transformation, subject to $\det(L)\neq0$], translates according to

$$\mathbf{v}'(x+a)=T'\mathbf{v}'(x)$$

with

$$T'=LTL^{-1}. \tag{3}$$

The theory of the canonical form of matrices is concerned with the simplest form T' to which T can be reduced by the similarity transformation (3). The canonical form of the matrix T depends on its eigenvalues τ, i.e., the solutions of

$$\det(T-\tau I)=0, \tag{4}$$

where I is the 2×2 identity matrix. The eigenvalues are unaltered by similarity transformations. Since Eq. (4) is quadratic in τ, there are three cases[10–12]:

Canonical type I: If the eigenvalues of T are distinct ($\tau_1\neq\tau_2$), the canonical form is

$$T'=\begin{pmatrix}\tau_1 & 0\\ 0 & \tau_2\end{pmatrix}$$

(which is diagonal).

Canonical type II: If the solution of Eq. (4) is a double root ($\tau_1=\tau_2$) and

$$T\neq\begin{pmatrix}\tau_1 & 0\\ 0 & \tau_1\end{pmatrix},$$

then the canonical form is

$$T'=\begin{pmatrix}\tau_1 & 0\\ 1 & \tau_1\end{pmatrix}.$$

Canonical type III: If

$$T=\begin{pmatrix}\tau_1 & 0\\ 0 & \tau_1\end{pmatrix},$$

T is already in canonical form. (In this case $T'=T$ for all L.)

There are two restrictions on the canonical forms of T', which follow from the fact that T is a translation operator for solutions of Eq. (1).

First, $\det(T)=1$. Proof: From any two independent solutions ψ_1, ψ_2 construct the matrix

$$W=\begin{pmatrix}\mathbf{v} & \dfrac{d\mathbf{v}}{dx}\end{pmatrix}=\begin{pmatrix}\psi_1 & d\psi_1/dx\\ \psi_2 & d\psi_2/dx\end{pmatrix}.$$

Since ψ_1 and ψ_2 are solutions of Eq. (1),

$$\psi_1(d^2\psi_2/dx^2)-\psi_2(d^2\psi_1/dx^2)=0,$$

which is integrated to give

$$\det(W)=\psi_1(d\psi_2/dx)-\psi_2(d\psi_1/dx)=\text{const}$$

(independent of x). $\det(W)$ is called the Wronskian of the solutions ψ_1, ψ_2.

Differentiating Eq. (2),

$$(d/dx)\mathbf{v}(x+a)=T(d/dx)\mathbf{v}(x),$$

and thence,

$$W(x+a)=TW(x).$$

Therefore

$$\det[W(x+a)]=\det(T)\det[W(x)].$$

But we just saw that $\det[W(x)]$ is independent of x; therefore $\det(T)=1$. QED.

Now the determinant of a matrix is unaltered by similarity transformations (3), so $\det(T')=1$, which gives $\tau_1\tau_2=1$ for canonical type I, and $\tau_1^2=1$ (i.e., $\tau_1=\pm1$) for canonical types II and III.

The second restriction on T involves $\mathrm{Tr}(T)$ (trace of T, = sum of diagonal elements), which is also unaltered by transformation (3). As remarked earlier, Eq. (1) is real, so two independent solutions $\psi_1(x)$ and $\psi_2(x)$ can be taken which are real functions, i.e., their values are real for all x. Then $\psi_1(x+a)$ and $\psi_2(x+a)$ are also real (because the set of all $x+a$ is the same as the set of all x); so T in Eq. (2) is real (has real matrix elements) for this particular choice of ψ_1, ψ_2. Therefore $\mathrm{Tr}(T)$ is real. But $\mathrm{Tr}(T)=\mathrm{Tr}(T')$,

$$\therefore\quad \mathrm{Tr}(T')\text{ is real,}$$

i.e., $\tau_1+\tau_2$ is real (canonical type I), τ_1 is real (canonical types II and III).

Write τ in the form

$$\exp(i\kappa a)=\exp(ika)\exp(-\mu a),$$

where $\kappa=k+i\mu$ with k and μ real. Then the possible canonical forms of T and the associated values of k and μ are as given in Table I.

Floquet's theorem concerns the existence of solutions ψ having the property

$$\psi(x+a)=\tau\psi(x). \qquad (5)$$

Solutions having this property are called Floquet functions or solutions.

The theorem can be stated in various ways. One way is[13]

Floquet's Theorem (1): There is always at least one Floquet solution of Eq. (1).

This result is an immediate consequence of the canonical forms of T. However, Floquet's theorem is much more useful in those cases when there are

TABLE I. Canonical forms of the translation matrix T and associated wavefunctions. The superscript s is for "stable" and the superscripts $\pm$ are used when $\exp(ika) = \pm 1$, i.e., at the center (resp. boundary) of the Brillouin zone. n is an integer. All functions denoted u, v, U, or V have period a. u_μ means u_κ with $\mathrm{Im}(\kappa) = -\mu$.

Canonical type	Canonical form of T	k	μ	Canonical wavefunctions	Stability of solutions
I^s	$\begin{pmatrix} \exp(ika) & 0 \\ 0 & \exp(-ika) \end{pmatrix}$	$\neq n\pi/a$	0	$\psi_{1,2} = \exp(\pm ikx)\, u_{\pm k}(x)$	All solutions stable
I^+	$\begin{pmatrix} \exp(\mu a) & 0 \\ 0 & \exp(-\mu a) \end{pmatrix}$	$2n\pi/a$	$\neq 0$	$\psi_{1,2} = \exp(\pm \mu x)\, u_{\pm\mu}(x)$	All solutions unstable
I^-	$\begin{pmatrix} -\exp(\mu a) & 0 \\ 0 & -\exp(-\mu a) \end{pmatrix}$	$(2n+1)\pi/a$	$\neq 0$	$\psi_{1,2} = \exp[(\pm\mu + i\pi/a)x]\, u_{\pm\mu}(x)$	All solutions unstable
II^+	$\begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}$	$2n\pi/a$	0	$\psi_1 = u_0(x)$ $\psi_2 = v_0(x) + (x/a)\, u_0(x)$	ψ_1 stable ψ_2 unstable
II^-	$\begin{pmatrix} -1 & 0 \\ 1 & -1 \end{pmatrix}$	$(2n+1)\pi/a$	0	$\psi_1 = \exp(i\pi x/a)\, u_{\pi/a}(x)$ $\psi_2 = \exp(i\pi x/a)$ $\times [v_{\pi/a}(x) - (x/a)\, u_{\pi/a}(x)]$	ψ_1 stable ψ_2 unstable
III^+	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$2n\pi/a$	0	$\psi_1 = U_0(x)$ $\psi_2 = V_0(x)$	All solutions stable
III^-	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$(2n+1)\pi/a$	0	$\psi_1 = \exp(i\pi x/a)\, U_{\pi/a}(x)$ $\psi_2 = \exp(i\pi x/a)\, V_{\pi/a}(x)$	All solutions stable

two independent Floquet solutions, because two such solutions can be taken as basis solutions, and the general solution is a linear combination of these. So the following, stronger statement of Floquet's theorem [cf. Ref. 9] is more useful:

Floquet's Theorem (2): When T has two distinct eigenvalues (canonical type I) or $T = \pm I$ (canonical type III) there are two independent Floquet solutions of Eq. (1).

When T has a double eigenvalue ($\tau_1 = \tau_2 = \pm 1$) and is $\neq \pm I$ (canonical type II) there is one Floquet solution ψ_1 of Eq. (1), and an independent solution ψ_2 with the property

$$\psi_2(x+a) = \tau_1 \psi_2(x) + \psi_1(x). \qquad (6)$$

Notes on Floquet's Theorem (2):

(i) The result is an immediate consequence of the canonical forms of T.

(ii) In canonical type I the general solution

$$g(x) = \alpha\psi_1(x) + \beta\psi_2(x)$$

has the property

$$g(x+a) = \tau_1\alpha\psi_1(x) + \tau_2\beta\psi_2(x) \qquad (\tau_1 \neq \tau_2).$$

In canonical type II g has the property

$$g(x+a) = \tau_1 g(x) + \beta\psi_1(x).$$

In neither type is the general solution a Floquet solution. This is so only for canonical type III.

(iii.a) A Floquet solution can be written in the form

$$\exp(i\kappa x)u(x)$$

with

$$u(x+a)=u(x).$$

The u and κ required to satisfy Eq. (5) are not unique:

$$\kappa'=\kappa+(2\pi n/a), \qquad (n=0, \pm 1, \pm 2, \cdots),$$
$$u'=\exp(-2\pi inx/a)u,$$

will do just as well. It follows that k can be restricted to the interval $-\pi/a \leq k \leq \pi/a$, the values $\pm\pi/a$ being equivalent to each other (reduced zone scheme).

(iii.b) If ψ_2 in Eq. (6) is written in the form

$$\psi_2(x)=\phi_2(x)+(x/a\tau_1)\psi_1(x), \tag{7}$$

then property (6) is equivalent to

$$\phi_2(x+a)=\tau_1\phi_2(x).$$

[Note ϕ_2 is not a solution of Eq. (1).]

(iii.c) From (iii.a) and (iii.b) one readily finds the expressions for ψ_1 and ψ_2 in terms of periodic functions given in Table I.

(iv) The Floquet solutions are stable if and only if $\kappa=k+i\mu$ is real, because $\exp[(ik-\mu)x]u(x)$ is unbounded as $x\to\mp\infty$ if $\mu\gtrless 0$.

The solution (6) is unstable at $x=+\infty$ and at $x=-\infty$ [because of the linear factor x in Eq. (7)]. So the canonical solutions are classified with regard to stability as indicated in Table I.

(v) From Table I, the general canonical type II solution

$$g=\alpha\psi_1+\beta\psi_2$$

can be written in terms of periodic functions as

$$\exp(ikx)\{[\alpha u_k(x)+\beta v_k(x)]+\beta\exp(ika)(x/a)u_k(x)\}$$
$$k=0 \text{ or } \pi/a. \tag{8}$$

An example of such a solution is shown in Fig. 1.

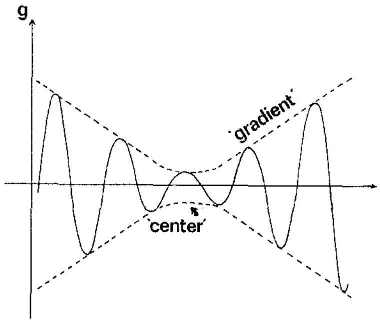

Fig. 1. A sketch of a canonical type II (or band edge) solution $g=\alpha\psi_1+\beta\psi_2$ [see Eq. (8), or Table I]. For simplicity we have chosen α and β real, and $k=0$, so g is real. The "gradient" and "center" depend on α and β.

IV. BAND STRUCTURE

So far we have discussed a classification of the solutions of Eq. (1) in terms of the properties of the matrix T. But T is a transformation property of the solutions ψ, so one has to find the solutions before classifying them. It would be nice if the classification could be related directly to the function $Q(x)$ in Eq. (1), so that one could say certain things about the solutions without having to solve Eq. (1) completely. A limited amount of progress has been made in this direction (Liapounov type results[14]). But more generally useful qualitative results can be gotten, which do not refer to $V(x)$ explicitly, but consider the way the solutions depend on the energy E which can be regarded as a parameter varying from $-\infty$ to $+\infty$. We summarize these results informally with an E-κ diagram (Fig. 2) and comments. These results are all proved in Ref. 15.

The following are comments on Fig. 2.

(i) The energy E is divided into *bands* by the values $E_0^+<E_1^-\leq E_2^-<E_1^+\leq E_2^+<E_3^-\leq E_4^-<E_3^+\leq E_4^+<\cdots$. The canonical type of the solution for each value of the energy is indicated in Fig. 2. An energy value separating a band of solutions of type I^s from a band of solutions of type I^+ or I^- is called a band edge. In Fig. 2, E_0^+, E_1^-, E_2^-, E_1^+, E_2^+, E_3^+, E_4^+, E_5^-, E_6^- are band edges, but $E_3^-=E_4^-$ and $E_5^+=E_6^+$ are not. We denote the interval or band $E_a<E<E_b$ by (E_a, E_b). A band (E_a, E_b) is said to be stable (resp. unstable) if all the solutions in (E_a, E_b) are stable (resp. unstable). The band $(-\infty, E_0^+)$ is unstable. It never vanishes. The bands (E_0^+, E_1^-), (E_2^-, E_1^+), $\cdots$, are stable. They never vanish. The bands (E_1^-, E_2^-), (E_1^+, E_2^+), $\cdots$, are unstable if they do not vanish. If, e.g., $E_3^-=E_4^-$, as in Fig. 2, the

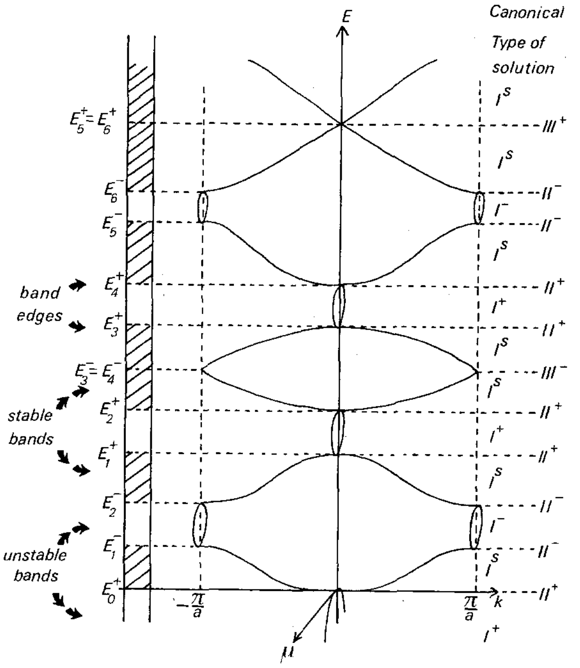

FIG. 2. The band structure in one dimension: E as a function of $\kappa(=k+i\mu)$; μ can be $\neq 0$ only when $k=0$ or $\pm\pi/a$. The superscript s is for "stable," and the superscripts $\pm$ are used when $\exp(ika) = \pm 1$.

related unstable band vanishes, and there is a stable band (E_2^+, E_3^+). [If $V(x) = \text{const}$ (free electron model), all unstable bands except $(-\infty, E_0^+)$ vanish. Less trivial cases occur in three-dimensional crystals in which certain unstable bands vanish due to screw or glide symmetry elements.[16]] This subsection [IV(i)] contains the main results of the oscillation theorem.[4]

(ii) For each value of E within a stable band, there are two independent stable Floquet solutions.

For each value of E within an unstable band there are two independent unstable type I Floquet solutions. These unstable Floquet solutions have $k[=\text{Re}(\kappa)]=0$ or $\pm\pi/a$.

For each value of E at a band edge the solutions are of canonical type II. Moreover type II solutions occur only at band edges, so we can refer to type II solutions as band edge solutions. At a band edge there is only one independent Floquet solution; it is stable. There is also an independent unstable solution, namely ψ_2 in Eqs. (6) and (7); a linear combination of the stable and unstable solutions is unstable.

(iii) $E(\kappa)$ is a continuous function of κ.

(iv) $E(\kappa) = E(-\kappa)$. [This follows from the results of Sec. III; see Table I. The result does not require $V(x) = V(-x)$.]

(v) $dE(k)/dk = 0$ at a band edge. [When the unstable band vanishes, as at $E_3^- = E_4^-$ in Fig. 2, there is no band edge, so $dE(k)/dk$ need not vanish.]

(vi) There are not more than two κ values corresponding to any energy. So a curve like that shown in Fig. 3 is not possible. [This follows from the facts that Floquet solutions with different κ (modulo $2\pi/a$) are linearly independent, and that Eq. (1) has only two linearly independent solutions.]

V. PHYSICAL APPLICATIONS OF STABLE AND UNSTABLE SOLUTIONS

In the quantum mechanics of a system with a perfectly periodic potential, the stable solutions correspond to physical solutions. The unstable solutions do not correspond to physical solutions, because they diverge as $x \rightarrow +\infty$, or $-\infty$, or both.

Unstable solutions of canonical type I diverge like $\exp(\mu x)$ as $x \rightarrow \pm\infty$ with $\mu \gtrless 0$. However, these unstable solutions do have a physical role in the theory of *surface states*. Consider a semi-infinite crystal with a surface (Fig. 4), in which the potential has the periodic form $V(x)$ only for $x \leq 0$. In the region $x > 0$ there is a surface potential which becomes constant a short distance outside the boundary.

The unstable solution of canonical type I has energy E in an unstable band (or energy gap) of the unbounded crystal. In suitable circumstances a solution of energy E in $x \geq 0$ can be matched (continuity of ψ and $d\psi/dx$ at $x=0$) to a solution $\exp(\mu x)u(x)$ or $\exp[(\mu + i\pi/a)x]u(x)$ with $\mu > 0$

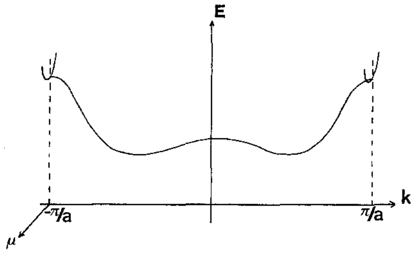

FIG. 3. This kind of $E(\kappa)$ curve, with $\kappa(E)$ more than two valued in places, is not possible in one space dimension.

of energy E in $x \leq 0$.[17] If so a surface state exists whose wavefunction decreases exponentially as it penetrates into the crystal. Such states are important in connection with electronic surface effects.

Now the unstable solution of canonical type II [Eq. (7)] diverges like x both as $x \to +\infty$ and as $x \to -\infty$. So it cannot have a physical role in a semi-infinite crystal. This solution is not generally included in physical treatments of band theory, although it was recognized by Kramers,[18] and it also appears in some mathematical treatments.[19,20]

It is possible however for this solution to have a role in a thin crystalline layer analogous to the role of the unstable solutions $\exp(\mu x)u(x)$ and $\exp[(\mu + i\pi/a)x]u(x)$ in a semi-infinite crystal. Such a solution has to be matched at two boundaries ($x=0$ and L, Fig. 5). Since the energy of a band edge state cannot be varied continuously (it must be at a band edge of the infinite crystal), this matching is only possible for special values of L, or for special forms of surface potential.

The band edge state can also be considered in the following way: A surface state with energy near the band edge has small μ, and extends a long way into the crystal. The band edge state is a limiting case (energy→band edge, $\mu \to 0$) of two surface states each associated with one of the two surfaces of a finite layer.

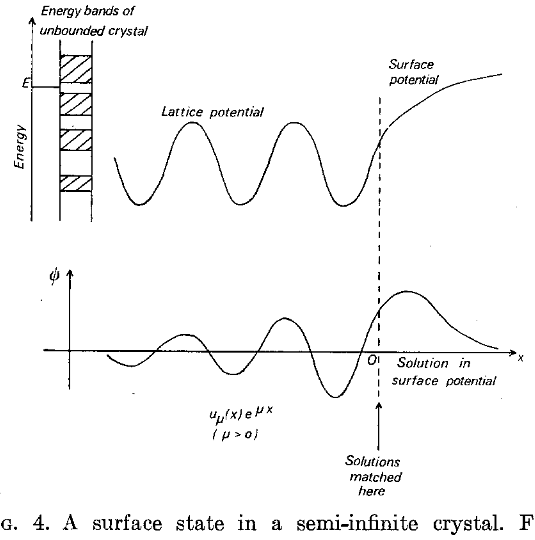

FIG. 4. A surface state in a semi-infinite crystal. For $x \leq 0$ the potential is periodic, and the solution is an unstable Floquet solution. E lies in an energy gap (unstable band) of the unbounded crystal.

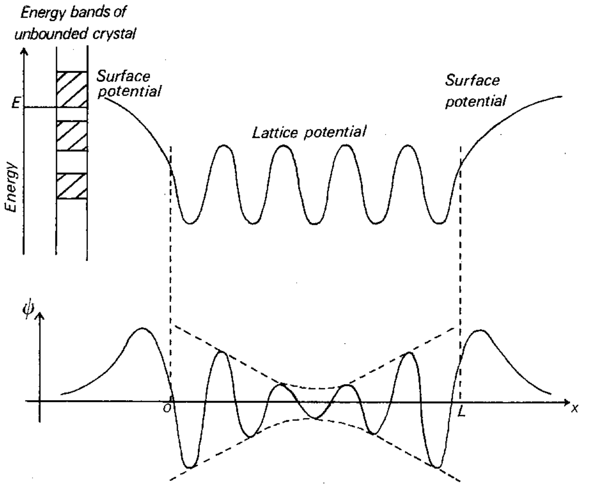

FIG. 5. A band edge state in a finite crystal: It is matched at $x=0$ and L to solutions with energy E in the surface potential.

To find the possible electron states in a finite crystalline layer one can proceed by finding the states in the infinite crystal for all energies (stable bands, unstable bands, and band edges), and then picking out those solutions which fit the boundary conditions at the two surfaces ($x=0$ and L). This will lead to a discrete spectrum of energy levels. A band edge state occurs when one of these energy levels coincides with a band edge.

These considerations are relevant for the theory of the "quantum size effect."[21] This effect concerns the oscillations with thickness of the electronic properties (e.g., electrical conductivity) of layers of semiconductor or semimetal whose thickness is comparable with the effective de Broglie wavelength of the conduction electrons and holes.

VI. CYCLIC BOUNDARY CONDITIONS; BLOCH'S THEOREM

We now consider a finite length Na of the crystal (where N is a large but finite integer) and suppose it bent into a circle and the ends joined. This finite periodic system is mathematically much simpler than the infinite system. The wavefunctions must have the period Na (since $x+Na$ is the same point as x), i.e.,

$$\mathbf{v}(x+Na) = T^N \mathbf{v}(x) = \mathbf{v}(x)$$

[cf. Eq. (2)]. Such boundary conditions are called *cyclic.* Equation (1) subject to cyclic boundary conditions does not possess nontrivial solutions $[\mathbf{v}(x)\not\equiv 0]$ for all energy E. For a nontrivial solution

$$T^N = I. \tag{9}$$

Now canonical type I, with

$$T=\begin{pmatrix}\exp(i\kappa a) & 0\\ 0 & \exp(-i\kappa a)\end{pmatrix},$$

is compatible with Eq. (9) only if κ is real and equal to $2\pi m/Na$ (m=integer). Canonical type II, with

$$T=\begin{pmatrix}\pm 1 & 0\\ 1 & \pm 1\end{pmatrix},$$

is not compatible with Eq. (9).

In canonical type III, $T=I$ is compatible with Eq. (9) for all N, and $T=-I$ is compatible with Eq. (9) if N is even.

Thus all the canonical solutions compatible with cyclic boundary conditions are stable Floquet solutions. The basis set of solutions can be taken in canonical form without loss of generality, so we have:

Bloch's Theorem: The general nontrivial solution of Eq. (1) subject to cyclic boundary conditions is a linear combination of two stable Floquet solutions.

The use of cyclic boundary conditions is essential to Bloch's theorem, because Sec. III showed that for a noncyclic lattice $(-\infty \le x \le \infty)$ only one of the two independent solutions at a band edge is a Floquet solution.

In group theoretical terms Bloch's argument[2] is that the translations $T, T^2, T^3, \cdots, T^N = I$ of a crystal, subject to cyclic boundary conditions form a finite Abelian group, and all the irreducible matrix representations of such a group are one dimensional. If cyclic boundary conditions are not applied, the translations form an *infinite* Abelian group, and the irreducible representations of an infinite Abelian group are *not* all one dimensional.

In the application of cyclic boundary conditions one does, of course, suppose that N is very large. Nevertheless, there are some solutions in the infinite lattice which are not obtained from the cyclic lattice, even when $N\rightarrow\infty$. The theory with cyclic boundary conditions is strikingly simple. A specially valuable feature is that this theory holds for the three-dimensional case in almost as simple a form.[2] However, one does see more by including the unstable solutions, and they are essential in the study of surface effects.

VII. SOME COMMON IMPERFECTIONS IN EXPOSITIONS OF FLOQUET'S AND BLOCH'S THEOREMS

The following imperfections in expositions of Floquet's and Bloch's theorems and band theory have been noted to be quite widespread:

(i) In most physics and some mathematics expositions, the possibility of the band edge solution ψ_2 in Eqs. (6) and (7) is overlooked. The statement[22–24] that the general solution of Eq. (1) is a linear combination of two Floquet solutions is not completely correct; it is not true at a band edge.

(ii) Statements of Bloch's theorem equivalent to the following are quite common in physics books[25–38]:

Statement I: "The solutions of Eq. (1) are Floquet functions." The weakness of such statements, in expositions for the novice to the subject, lies in the uncertainty as to what is meant by "the solutions." The most natural interpretation is that "the solutions" means "all solutions." Indeed some books[39–48] make statements like

Statement II: "All solutions of Eq. (1) are Floquet functions." We saw in Sec. III that statement II is incorrect, and insofar as statement I is most naturally interpreted to mean the same as statement II, statement I is misleading.

(iii) Some treatments[25–27,37,49] give the two Floquet solutions of energy E (again valid only for canonical types I and III) as

$$u_\kappa(x)\exp(\pm i\kappa x).$$

As shown in Sec. IV the two solutions are

$$u_\kappa(x)\exp(i\kappa x) \quad \text{and} \quad u_{-\kappa}(x)\exp(-i\kappa x),$$

which do not amount to the same thing.

VIII. CONCLUSION

Certain deficiencies are quite common in expositions of Floquet's and Bloch's theorems. One defect is that the status of the Floquet solutions is not often made clear.

In physical problems involving an unbounded crystal, so that only stable solutions are used, the stable Floquet solutions form a basis set. It is this property that makes them so useful, and it would seem to be pedagogically important to stress this property. No generality is lost by starting with Floquet solutions in an unbounded crystal problem. The general stationary state is a superposition of two Floquet functions—except at a band edge, where there is only one Floquet function that is itself the most general stable stationary state. The most general time dependent state can be gotten by superposing Floquet functions with different energies E [with the time-dependent factors $\exp(-iEt/\hbar)$ included]. In this way one can, for example, construct a wavefunction that is initially localized; as time proceeds the wavefunction spreads out.

Floquet's and Bloch's theorems and band theory are rightly considered to be so important that the student of physics should understand them as early as possible. The real difficulties to the student of this material are often made greater by inadequate statements of the central theorem. Even the correct statements are not often accompanied by an elementary explanation of the status of the Floquet functions. It is true that the nature and status of the Floquet functions is implicit in the derivation of Floquet's and Bloch's theorems, but the beginning student is not usually able to appreciate such implicit consequences. Expository accounts should help the student by an explicit statement of the status of the Floquet functions. Some of the best expositions in this respect are to be found in Refs. 50–53, although only the first of these is at an elementary level.

It is not suggested that the unstable solutions should necessarily be presented in elementary expositions, because the analysis of the stable solutions only is so much simpler, and the stable solutions are so much more important than the unstable ones. But it is suggested that elementary expositions should stress the feature that the Floquet functions are a basis set, i.e., the general stable solution is a linear combination of Floquet functions.

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Expulsion of Free Electronic Charge from the Interior of a Metal*

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Using the frequency dependent conductivity, we show that electronic charge is expelled from the interior of a metal by setting up an oscillation driven by the Coulomb repulsion at the plasma frequency. This oscillation damps out in a time on the order of an electronic collision time. The usual textbook derivation does not obtain this result because it discusses this high-frequency phenomenon in terms of the zero-frequency conductivity. In the case of poorer conductors which do not support plasma oscillations the usual treatment is valid.

I. INTRODUCTION

It is generally accepted that electronic charge is expelled from the interior of a conducting material within a very short time.[1] The derivation of this result, which is based upon Gauss' law, charge conservation, and Ohm's law, gives an exponential decay time of $\tau_r = (4\pi\sigma)^{-1}$, where σ is the dc conductivity in esu units. However, in the case of metals one finds that this relaxation time is much shorter than a typical electronic collision time τ. This treatment of the problem is therefore not self-consistent since one should use the conductivity appropriate to the frequency $\omega \approx \tau_r^{-1}$, and this is very different from the dc conductivity. At low frequencies collisions occur so frequently that the charge carriers are moving as if within a viscous medium, whereas at high frequencies the charge carriers behave almost as if they were free.

These two frequency regimes are well-known in the transverse electromagnetic response of metals. Radio waves do not penetrate metals because they are damped out within a skin depth