Sec. III seem to indicate that Ham's result is nevertheless at least qualitatively correct for n-type silicon.

In the calculations of Maxwellian averages of relaxation times in this paper, impurity scattering has been added to lattice scattering according to the usual rule,

$$\frac{1}{\tau_\alpha}=\frac{1}{\tau_{L\alpha}}+\frac{1}{\tau_{I\alpha}}, \tag{9}$$

where the subscript α refers to the direction with respect to a spheroid axis, either $\parallel$ or $\perp$. These calculations have had to be carried out numerically. The $\tau_{L\alpha}$, which includes acoustic and intervalley scattering, is given by an expression of the form presented by Herring.[4] The $\tau_{I\alpha}$ depends on energy as,

$$\tau_{I\alpha}=A_\alpha\epsilon^{\frac{3}{2}}, \tag{10}$$

where A_α includes the various parameters in the Brooks-Herring formula, which one obtains by averaging $\tau_{I\alpha}$ according to the usual Maxwellian prescription. The magnitude of $A_\perp$ to be used in calculating $\tau_\perp$ for a particular sample at a particular temperature is determined by the obvious requirement that the ratio of the mobility calculated from Eq. (10) and $A_\perp$ to the total mobility calculated from Eq. (9) must be the same as the ratio of the mobility calculated from the Brooks-Herring formula to the observed mobility. Then, $A_\parallel=4A_\perp$. We have neglected the logarithmic function of ϵ which should really be included in the expression for τ_I simply because its presence would make the calculations much too difficult.[10] The resultant error is not important in our cases of weak ion scattering.

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Dispersion Relations for Bloch Functions

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It is shown that the Floquet factor $e^{ik(E)a}$ is analytic in the upper half complex energy plane, thus enabling a set of four dispersion relations to be derived from this expression as a direct result of the application of Cauchy's theorem. These relations are characterized by their ability to relate the wave number k at one energy to the wave number at all others. In particular, the imaginary part of the wave number k_i in the forbidden gap may be equated to an integral of a function of the real part of the wave number k_r over allowed energies. As an application of these dispersion relations a theorem regarding the location of the branch points has been established.

I. INTRODUCTION

THE physical concept of causality has been exploited in many areas of physics and in the majority of cases has shed valuable light on problems hitherto impossibly difficute to calculate.[1] The statement of microscopic causality alone is usually sufficient to guarantee that the scattering amplitude is analytic in the upper half complex energy plane, so that a direct application of Cauchy's theorem enables relations between the real and imaginary parts of the scattering amplitude to be established. For this reason, we have been motivated to extend a similar technique to the problem of a one-dimensional Schrödinger equation possessing a periodic potential. This equation in its three-dimensional form is essentially the starting point for a large class of problems in solid-state physics; however, exact solutions, even in the one-dimensional case are virtually impossible to obtain, except for a very limited class of periodic potentials (e.g., square well, delta function, sinusoidal, etc.). For this reason, it would be desirable to make some statements about the properties of wave functions in solids without recourse to the details of the actual potential other than its periodicity, causal nature, and general mathematical properties.

In problems involving single potential scattering, the outgoing wave function is related to the incoming wave function by the scattering matrix S, defined by the relation $\psi_{\text{out}}=S\psi_{\text{in}}$. Hence, by analogy it is almost obvious that the Floquet factor $[\lambda(E)=e^{ik(E)a}]$ defined by $\psi(x+a)=\lambda\psi(x)$ plays a similar role for periodic potentials. This immediately tempts us to investigate the analytic properties of $\lambda(E)$ with the aim of being able to derive a set of dispersion relations for this quantity. Unfortunately, causality alone is not sufficient to guarantee that $\lambda(E)$ is analytic in the upper half plane, since it appears that a knowledge of the zeros of the corresponding single potential S matrix is also required.[2] However, it is shown in the Appendix, using a direct approach, that $\lambda(E)$ is analytic in the upper half complex energy plane for a large class of potentials; more-

[1] E.g., M. Gell-Mann and M. Goldberger, Phys. Rev. 96, 1433 (1954).

[2] This statement is almost self-evident as a consequence of the work by D. S. Saxon and R. A. Hutner, Philips Research Repts. 4, 81–122 (1949).

over, it can also be shown that this factor is still analytic for those cases which can be solved exactly and for which the proof given in the Appendix does not apply (e.g., delta function and square well potentials), suggesting that $\lambda(E)$ is probably analytic for all simple periodic potentials.

In Sec. II, four dispersion relations are derived treating the energy as a variable, and one of these relations is then transformed to a more physically appealing form so that the wave number becomes the variable of integration.

In Sec. III the dispersion relations are extended to the nth power of the Floquet factor and a condition for locating the branch points in the forbidden gaps is derived as an example.

II. DEVELOPMENT

The normalized Schrödinger equation for a one-dimensional lattice has the form

$$[\partial^2/\partial x^2+\kappa^2]\psi(x)=-eV(x)\psi(x), \qquad (1)$$

where

$$\kappa^2=E, \quad V(x)=V(x+na), \qquad (2)$$

and $(2m/\hbar^2)$ has been set equal to unity. The solutions of Eq. (1) have the usual form

$$\psi(k,x)=e^{ikx}u(k,x), \qquad (3)$$

where $u(k,x)$ has the periodicity of the lattice. The wave number k is usually restricted to real values by boundary conditions at infinity and the allowed energies are characterized by the corresponding values of $E(k)$. Nevertheless, by relaxing these conditions it is possible to investigate the properties of complex k solutions, which are of importance in connection with many aspects of solid-state physics. For example, "forbidden solutions" provide asymptotic forms for localized states in crystals[3]; they give information necessary for the calculation of transition probabilities in direct and indirect tunnelling processes.[4,5] Moreover, a study of the analytic properties of k as a function of E leads to exponentially damped Wannier functions[6] and may have important bearing on the theory of allowed (real k) bands. In this paper, we shall derive dispersion relations which relate the wave number at one energy to the wave number at all others.

It is evident from Eq. (3) that a Bloch function has the property

$$\psi(k,\,x+a)=e^{ika}\psi(k,x), \qquad (4)$$

where a is the lattice constant. As mentioned previously, we shall be concerned with the analytic properties of the function

$$\lambda(E)=e^{ika}=\mu(E)+i\eta(E), \qquad (5)$$

TABLE I. Properties of $\mu(ka)$, $\eta(ka)$, and $\lambda(ka)$ in allowed and forbidden energy regions.

Allowed energies	Forbidden energies
$\mu_r=\cos k_r a$	$\mu_r=(-1)^N\cosh(k_i a)$
$\mu_i=0$	$\mu_i=0$
$\eta_r=\sin k_r a$	$\eta_r=0$
$\eta_i=0$	$\eta_i=(-1)^N\sinh(k_i a)$
$\lambda_r=\cos k_r a$	$\lambda_r=(-1)^N e^{-k_i a}$
$\lambda_i=\sin k_r a$	$\lambda_i=0$
$\lambda=e^{ik_r a}$	$\lambda=(-1)^N e^{-k_i a}$

where

$$\mu(E)=\cos k(E)a, \qquad (6a)$$

$$\eta(E)=\sin k(E)a, \qquad (6b)$$

and

$$k=k_r+ik_i.$$

For real energies the wave number k is either real for allowed energies or the real part k_r is some integral multiple N of π/a for forbidden energies. From this it follows that on the real E axis $\mu(E)$ is always real and $\eta(E)$ is either real or pure imaginary. The function $\lambda(E)$, therefore, is either complex on the unit circle for allowed energies or real for forbidden energies. These statements can be summarized in detail with the aid of Table I.

The asymptotic values of $\lambda(E)$ on the positive and negative real energy axes may be deduced immediately from well-known properties of $\mu(E)$.[7]

$$\lim_{E\to+\infty}\mu(E)=\cos(E)^{\frac{1}{2}}a, \qquad (7a)$$

$$\lim_{E\to-\infty}\mu(E)=+\infty. \qquad (7b)$$

However, since $\lambda(E)$ is a double valued function of the energy with simple branch points at those real values of the energy corresponding to $E_n(n=1,\,2,\,\cdots)$ when $\lambda=\pm1$,[6] we shall define a single valued function $\lambda^{(+)}(E)$ which is the value of $\lambda(E)$ corresponding to the choice of both positive real and imaginary parts of the wave number k_r and k_i (i.e., the first quadrant of unreduced k space). This choice then guarantees that

$$\lim_{E\to\infty}\lambda^{(+)}(E)=\exp[i(E)^{\frac{1}{2}}a]. \qquad (7c)$$

Extending $\lambda^{(+)}(E)$ into the upper half complex energy plane and defining $\lambda^{(+)}(E)$ on the real axis as the limit of approaching the real axis from above, we see that this requirement leads automatically to

$$\lim_{E\to-\infty}\lambda^{(+)}(E)=0, \qquad (7d)$$

provided that we remain on the first Riemann sheet characterized by $0\leqslant\theta\leqslant2\pi$.

Using the analyticity of λ (where we have dropped the

[3] P. Kaus, Bull. Am. Phys. Soc. 3, 400 (1958).
[4] P. Kaus, Bull Am. Phys. Soc. 4, 181 (1959).
[5] E. O. Kane (to be published).
[6] W. Kohn, Phys. Rev. 115, 809 (1959).
[7] H. A. Kramers, Physica 2, 483 (1935).

plus superscript for convenience) which essentially follows from the work of Kohn[6] and which is derived in a different manner in the Appendix, we are now in a position to make a direct application of Cauchy's Theorem and write

$$\lambda(E)=\frac{1}{2\pi i}\oint_c \frac{\lambda(E')}{E'-E}dE' \tag{8a}$$

$$=(1/\pi i)\,\mathrm{P}\int_{-\infty}^{\infty}\frac{\lambda(E')}{E'-E}dE', \tag{8b}$$

where the contour is taken along a line just above the real E axis and around the semicircle at infinity in the upper half plane, on the first Riemann surface. Using Eq. (7c) it is clear that the contribution to the integral around this infinite semicircle vanishes.

Equating real and imaginary parts, and replacing the contour integral by an integral along the real E axis, we obtain the relations

$$\lambda_i(E)=-\left(\frac{1}{\pi}\right)\mathrm{P}\int_{-\infty}^{\infty}\frac{\lambda_r(E')}{E'-E}dE', \tag{9a}$$

$$\lambda_r(E)=\left(\frac{1}{\pi}\right)\mathrm{P}\int_{-\infty}^{\infty}\frac{\lambda_i(E')}{E'-E}dE'. \tag{9b}$$

Starting with infinite negative energy we note that every energy for which $\lambda(E)$ changes from real to complex is the bottom of an allowed band and every energy where it changes from complex to real is the top of an allowed band and the bottom of a forbidden gap. Let us designate these limiting energies as E_n in ascending order ($E_0=-\infty$). An allowed band is now seen to extend from E_{2N-1} to E_{2N} and a gap from E_{2N} to E_{2N+1} with increasing energy. We may now write our dispersion relations in a more physically appealing form:

$$\lambda_i(E)=-\left(\frac{1}{\pi}\right)\sum_{N=1}^{\infty}\mathrm{P}\int_{E_{2N-1}}^{E_{2N}}\frac{\lambda_r(E')}{E'-E}dE' -\left(\frac{1}{\pi}\right)\sum_{N=0}^{\infty}\mathrm{P}\int_{E_{2N}}^{E_{2N+1}}\frac{\lambda_r(E')}{E'-E}dE', \tag{10a}$$

$$\lambda_r(E)=\left(\frac{1}{\pi}\right)\sum_{N=1}^{\infty}\mathrm{P}\int_{E_{2N-1}}^{E_{2N}}\frac{\lambda_i(E')}{E'-E}dE'. \tag{10b}$$

The first sum of integrals in each case corresponds to allowed zones and the second sum in the first equation to forbidden gaps; in addition, we have made use of the fact that in forbidden gaps $\lambda(E)$ is real.

These relations may now be written in terms of the wave number k, by substituting from the definition of $\lambda(E)$, Eqs. (5) and (6).[8] It is now useful to distinguish two distinct possibilities.

[8] Provided that we remain in the region characterised by the first quadrant in complex unreduced k space.

Case (1) when the energy E is allowed ($E_{2M-1}<E<E_{2M}$).

$$\sin k_r(E)a=-\left(\frac{1}{\pi}\right)\sum_{N=1}^{\infty}\mathrm{P}_M\int_{E_{2N-1}}^{E_{2N}}\frac{\cos k_r(E')a}{E'-E}dE' -\left(\frac{1}{\pi}\right)\sum_{N=0}^{\infty}\int_{E_{2N}}^{E_{2N+1}}\frac{(-1)^N e^{-k_i(E')a}}{E'-E}dE', \tag{11a}$$

$$\cos k_r(E)a=\left(\frac{1}{\pi}\right)\sum_{N=1}^{\infty}\mathrm{P}_M\int_{E_{2N-1}}^{E_{2N}}\frac{\sin k_r(E')a}{E'-E}dE'. \tag{11b}$$

Case (2) when the energy E is forbidden ($E_{2M}<E<E_{2M+1}$).

$$\sum_{N=1}^{\infty}\int_{E_{2N-1}}^{E_{2N}}\frac{\cos k_r(E')a}{E'-E}dE' =-\sum_{N=0}^{\infty}\mathrm{P}_M\int_{E_{2N}}^{E_{2N+1}}\frac{(-1)^N e^{-k_i(E')a}}{E'-E}dE', \tag{12a}$$

$$e^{-k_i(E)a}=(-1)^M\left(\frac{1}{\pi}\right)\sum_{N=1}^{\infty}\int_{E_{2N-1}}^{E_{2N}}\frac{\sin k_r(E')a}{E'-E}dE', \tag{12b}$$

where the notation P_M means that the principal value is to be taken in the Mth member of the sum of integrals, which is the only member where a singularity will occur.

The dispersion relations can also be written as integrals over k space. For example, the relation (12b) becomes:

$$e^{-k_i(E)a}=(-1)^M\left(\frac{\hbar}{\pi}\right) \times\sum_{N=1}^{\infty}\int_0^{\pi/a}\frac{\sin k_r a}{E_N(k_r)-E}v_N(k_r)dk_r, \tag{13}$$

where

$$v_n(k)=(1/\hbar)dE_N(k)/dk, \tag{14}$$

and $E_N(k)$ is the energy-wave number relationship in the Nth allowed band.

It should perhaps be mentioned that we could have written a dispersion relation for the quantity $\lambda(E)/E$ in a completely analogous fashion. This function would have the advantage of a more rapid convergence so that the contribution to the integrals from higher energies would become less important. However, in order to write such a relation we would require knowledge of the subtracted quantity $\lambda(0)$. It is possible, however, that $\lambda(E)$ could be experimentally determined at some given energy. For example, the top of the valence band and the bottom of the conduction band are both amenable to experimental observation. Thus, by a suitable choice of the zero point of the energy scale, we have effectively determined $\lambda(0)$, and are in a position to make use of these modified dispersion relations.

III. EXTENSION OF THE DISPERSION RELATIONS AND LOCATION OF BRANCH POINTS

The wave functions at the point x and at the point $(x+na)$ are related by the nth power of the Floquet factor, i.e.,

$$\psi(x+na)=\lambda^n(E)\psi(x), \quad n\geqslant 1. \tag{15}$$

Thus it is possible to write dispersion relations for the quantity $\lambda^n(E)$ for the same reasons that the relations for $\lambda(E)$ are valid. For the fourth relation corresponding to Eq. (13) we obtain:

$$e^{-nk_i(E)a}=(-1)^{Mn}\left(\frac{\hbar}{\pi}\right)\times\sum_{N=1}^{\infty}\int_0^{\pi/a}\left[\frac{v_N(k_r)}{E_N(k_r)-E}\right]\sin nk_r a\,dk_r. \tag{16}$$

Letting

$$Q(k_r,E)=\sum_{N=1}^{\infty}\left[\frac{v_N(k_r)}{E_N(k_r)-E}\right], \tag{17}$$

we have

$$\left(\frac{\hbar}{2}\right)Q(k_r,E)=\sum_{n=1}^{\infty}a(-1)^{Mn}e^{-nk_i(E)a}\sin nk_r a. \tag{18}$$

This sum can be performed and yields

$$Q(k_r,E)=a[(-1)^M/\hbar]\sin k_r a/[\cosh k_i a-(-1)^M\cos k_r a]. \tag{19}$$

Substituting from (17) and solving for $\cosh k_i(E)a$ we finally obtain,

$$\cosh k_i(E)a=(-1)^M\{\cos k_r a+[(\hbar/a)\sum_{N=1} v_N(k_r)/(E_N(k_r)-E)]^{-1}\sin k_r a\}. \tag{20}$$

The significance of Eq. (20) lies in the observation that the imaginary part of k in the Mth gap can be obtained from knowledge of $E(k_r)$ and its derivative at only *one arbitrary point* of reduced k space for all bands. This was achieved by using an infinity of dispersion relations.

The left-hand side of Eq. (20) is not a function of k_r, so that differentiation with respect to k_r, leads to relations involving the energy and wave number in allowed bands alone, except for the forbidden reference energy E. As an example, the extended dispersion relation given by Eq. (16) may be used to locate the branch points in the forbidden gaps. These branch points are defined by the energy in each gap at which it is a single valued function and thus lie at the maximum values of $k_i(E)$ in each gap. Hence, the condition for E being a branch point is given by

$$dk_i(E)/dE=0. \tag{21}$$

From (16) we can see that this is equivalent to

$$dQ(k_r,E)/dE=\sum_N v_N(k_r)[E_N(k_r)-E]^{-2}=F(k_r,E)=0, \tag{22}$$

for all k_r between 0 and π/a. But this condition is equivalent to

$$(d/dk_r)\sum_N [E_N(k_r)-E]^{-1}=-\hbar F(k_r,E)=0, \tag{23}$$

for all k_r or

$$\sum_N [E_N(k_r)-E]^{-1}=C(E),$$

where $C(E)$ is independent of k_r.

Therefore, if E is a branch point, then

$$\sum_N \{1/[E_N(k_1)-E]-1/[E_N(k_2)-E]\}=0, \tag{24}$$

where k_1 and k_2 are any two wave numbers between 0 and π/a. Choosing in particular $k_1=0$ and $k_2=\pi/a$, we obtain the following simple equation determining the energy of the branch points

$$G(E)=\sum_N\{1/[E_N(0)-E]-1/[E_N(\pi/a)-E]\}=0. \tag{25}$$

Thinking of $G(E)$ as a function of E defined at all energies, it is easy to see that its zeros lie in the forbidden gaps, since in a gap

$$E_N(0)\leqslant E\leqslant E_{N+1}(0), \tag{26a}$$

for gap 2, 4, 6, $\cdots$ etc., or

$$E_N(\pi/a)\leqslant E\leqslant E_{N+1}(\pi/a), \tag{26b}$$

for gap 1, 3, 5, $\cdots$ etc. When $E_N(k_r)$ is the energy in the Nth allowed band,

$$E_N(0)\leqslant E\leqslant E_N(\pi/a), \tag{27a}$$

for band 1, 3, 5, $\cdots$ etc., or

$$E_N(\pi/a)\leqslant E\leqslant E_N(0), \tag{27b}$$

for band 2, 4, 6, $\cdots$ etc.

From (25), (26), and (27) we see that in a gap $G(E)$ goes continuously either from $+\infty$ to $-\infty$ or from $-\infty$ to $+\infty$ and therefore through zero.

This result of course is not new[6,7]; however, this technique has led in principle at least by means of Eq. (25) to determine the position of the branch points in terms of the energies at the edges of the bands.

Other choices of k_1 and k_2 are, of course, equally valid, but this particular choice demonstrates that Eq. (25) does indeed represent a condition for a branch point in every gap.

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APPENDIX. PROOF OF THE ANALYTIC PROPERTIES OF $\lambda(E)$ FOR NONSINGULAR CLASS OF POTENTIALS

By considering the one-dimensional Schrödinger equation written in the form

$$d^2\psi/dx^2+(\pi/a)^2[E-V(x)]\psi(x)=0, \tag{A1}$$

we may expand the periodic part of the Bloch function and the periodic potential in reciprocal lattice units by allowing:

$$\psi(x)=e^{ikx}\sum_{-\infty}^{\infty} b_m e^{2\pi i m(x/a)},$$

$$V(x)=-\sum_{-\infty}^{\infty} C_n e^{2\pi i n(x/a)}, \tag{A2}$$

where

$$C_{-m}=C_m^*,$$

and

$$C_0=0.$$

Substituting (A2) into (A1) we obtain

$$-(k+2\pi m/a)^2 b_m+(\pi/a)^2\sum_{l=-\infty}^{\infty}(C_l+E\delta_{l0})b_{m-l}=0,$$

which is equivalent to

$$\textstyle\sum_n\{[(\pi/a)^2E-(k+2\pi n/a)^2]\delta_{mn}+(\pi/a)^2C_{m-n}\}b_n=0. \tag{A3}$$

We now divide the mth equation of the infinite set (A3) by the quantity

$$[(\pi/a)^2E-4(\pi/a)^2m^2],$$

giving a new set of equations

$$\sum_{n=-\infty}^{\infty}\Delta_{mn}(k,E)b_n=0, \tag{A4}$$

where

$$\Delta_{mm}=[E-(ak/\pi+2m)^2]/[E-(2m)^2],$$

and

$$\Delta_{mn}=C_{m-n}/[E-(2m)^2],\quad m\neq n. \tag{A5}$$

Nontrivial solutions to (A4) exist for (k,E) combinations which make the determinant of the infinite matrix Δ_{mn} vanish. This determinant, denoted by $\Delta(k,E)$ is immediately recognized to be Hill's determinant. The condition

$$\Delta(k,E)=0, \tag{A6}$$

obviously implies a relation between k and E for nontrivial solutions of the Schrödinger equation. Equation (A6) has been extensively treated in the literature.[9] For potentials such that the C_n series is absolutely convergent (A6) gives the very simple result:

$$\sin^2(ka/2)=\Delta(0,E)\sin^2(\pi E^{\frac{1}{2}}/2), \tag{A7}$$

where

$$\Delta(0,E)=|\Delta_{mn}(0,E)|,$$

and from (A5)

$$\Delta_{mm}(0,E)=1. \tag{A8}$$

From the point of view of solving the Schrödinger equation or even obtaining the energy versus momentum relationship, the solution (A7) essentially begs the question, since $\Delta(0,E)$ is an infinite determinant for which only approximate solutions can be obtained under certain circumstances.[9] However, for purposes of proving the analyticity of $\lambda(E)$, we are interested only in the singularities of $\Delta(0,E)$ in the upper half energy plane, including its asymptotic behavior as the energy approaches infinity. This question can be answered rigorously by direct inspection of the determinant.

It is clear that $\Delta(0,E)$ possessed singularities only on the real E axis for $E=0,\ 4,\ \cdots(2m)^2\cdots$; however, it is easily seen that the expression $\Delta(0,E)\sin^2(\pi E^{\frac{1}{2}}/2)$ remains finite at these points, thus the expression

$$\cos(ka)=1-2\Delta(0,E)\sin^2(\pi E^{\frac{1}{2}}/2) \tag{A9}$$

is analytic in the upper half E plane. Moreover, in the limit as the energy approaches infinity, $\Delta(0,E)$ goes to unity, i.e.,

$$\cos_{E\to\infty}(ka)\to\cos(\pi E^{\frac{1}{2}}). \tag{A10}$$

It follows, keeping the condition of footnotes 7 and 8 in mind, that $\lambda(E)=e^{ika}$ is analytic in the upper half plane and vanishes on the semicircle at infinity, justifying the direct application of Cauchy's Theorem to the quantity $\lambda(E)$.

The condition of absolute convergence for the C_n series is not a very serious limitation since a vast class of potentials meets this convergence condition, and even those which do not can be expressed by such a series, except at points where the potential or one of its derivatives has a singularity. In any case, for two highly artificial potentials (square well and delta function), which do not meet the convergence requirement but for which the corresponding Schrödinger equation can be solved completely, the analyticity of $\lambda(E)$ can be verified by inspection. This makes it very plausible that $\lambda(E)$ is analytic even in those cases for which the above proof does not hold.

[9] For example: E. T. Whittaker and G. N. Watson, ***Modern Analysis*** (Cambridge University Press, New York, 1958), Chap. XIX.