Landau Spectrum and Line Broadening in Real Metals*

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The purpose of this investigation was to determine the natural width or broadening of the Landau levels of the conduction electrons in a perfect crystal when a uniform magnetic field is present. The eigenvalues and eigenfunctions of the effective-Hamiltonian equation have been found in the WKB approximation. Connection formulas good for all energies (including the region near the top of the barrier) were used to connect the nearly degenerate solutions in adjacent zones. The energy levels were found to be essentially discrete except in the immediate vicinity of open orbits. The effective-Hamiltonian solutions have been related to the solutions of the exact Hamiltonian. We have demonstrated that the effective-Hamiltonian formalism omits no source of level broadening (except for interband effects) since our solutions are completely consistent with the requirements of a group-theoretical treatment of the exact Hamiltonian.

I. INTRODUCTION

In 1930, the classic work of Landau[1] appeared in which he found the energy levels of a free electron in a magnetic field. Shortly thereafter, Peierls,[2] within the framework of the tight-binding approximation, carried out the first analysis of a Bloch electron in a magnetic field. In 1952, Onsager[3] showed how to quantize the allowed areas in k space of the electron orbits and, hence, how to determine the energy levels.

Kohn[4] and Blount[5] have demonstrated the validity of the effective-Hamiltonian formalism, which has been one of the most useful methods of studying the Landau levels of Bloch electrons. Blount,[5] Zil'berman,[6–8] and Azbel'[9] have discussed the solutions of the effective-Hamiltonian equation (the equivalent of the Schrödinger equation)

$$E\left(-i\nabla+\frac{e}{\hbar c}\mathbf{A}\right)\psi(\mathbf{r})=E\psi(\mathbf{r}). \tag{1.1}$$

It seems reasonable to conclude that the position of the energy levels is well established by the Onsager rules,[3] but the question of the natural width or broadening of the energy levels has not been clearly answered.

A completely different approach has been tried by Brown[10] and by Zak.[11–14] Brown found the irreducible representations of the exact Hamiltonian,

$$\mathcal{H}=\frac{1}{2m}\left(\mathbf{p}+\frac{e}{\hbar c}\mathbf{A}\right)^2+V(\mathbf{r}), \tag{1.2}$$

whereas Zak treated the lattice potential $V(\mathbf{r})$ as a perturbation using the proper symmetry-adapted wave functions. The perturbation approach, however, fails for a real metal because the matrix elements of the lattice potential exceed $\hbar\omega_c$, the separation of the unperturbed levels. But, group theory can establish the general nature of the solution.

The purpose of this work is to examine in detail the eigenvalues and eigenfunctions of the effective-Hamiltonian equation (1.1), with particular emphasis on determining the broadening of the Landau levels.

II. EFFECTIVE-HAMILTONIAN FORMALISM

We shall give a brief summary of the effective-Hamiltonian formalism and justify its use in the present problem. Let us first define the magnetic or modified Wannier functions for the band n as[10,15]

$$u_n(\mathbf{r},\mathbf{R}_j)=e^{(i/2)\mathbf{b}\times\mathbf{r}\cdot\mathbf{R}_j}a_n(\mathbf{r}-\mathbf{R}_j), \tag{2.1}$$

where $\mathbf{b}=e\mathbf{H}/\hbar c$, $a_n(\mathbf{r})$ is the zero-field Wannier function, and $\mathbf{R}_j$ is a vector of the direct lattice. We take as our basis functions

$$B_n(\mathbf{k},\mathbf{r})=\sum_{\mathbf{R}_j} e^{i\mathbf{k}\cdot\mathbf{R}_j}u_n(\mathbf{r},\mathbf{R}_j). \tag{2.2}$$

We restrict $\mathbf{k}$ to the first Brillouin zone (BZ). If we expand the Schrödinger wave function $\Phi(\mathbf{r})$ as

$$\Phi(\mathbf{r})=\sum_n \int_{\mathrm{BZ}} d^3k\, f_n(\mathbf{k})B_n(\mathbf{k},\mathbf{r}), \tag{2.3}$$

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the eigenvalue equation for the exact Hamiltonian $\mathcal{H}$ is

$$\sum_n \int_{BZ} d^3k\, e^{i\mathbf{k}\cdot\mathbf{R}_j}[H_{mn}(\mathbf{k}+\tfrac{1}{2}\mathbf{b}\times\mathbf{R}_j) - EN_{mn}(\mathbf{k}+\tfrac{1}{2}\mathbf{b}\times\mathbf{R}_j)]f_n(\mathbf{k})=0. \quad (2.4)$$

We define the matrix elements $H_{mn}(\mathbf{k})$ and $N_{mn}(\mathbf{k})$ as

$$H_{mn}(\mathbf{k})=\sum_{\mathbf{R}_j} e^{i\mathbf{k}\cdot\mathbf{R}_j}W_{mn}(\mathbf{R}_j), \qquad N_{mn}(\mathbf{k})=\sum_{\mathbf{R}_j} e^{i\mathbf{k}\cdot\mathbf{R}_j}N_{mn}(\mathbf{R}_j), \quad (2.5)$$

where

$$W_{mn}(\mathbf{R}_j)=\int a_m^*(\mathbf{r}+\mathbf{R}_j)e^{(i/2)\mathbf{b}\times\mathbf{r}\cdot\mathbf{R}_j}\mathcal{H}a_n(\mathbf{r})d^3r, \qquad N_{mn}(\mathbf{R}_j)=\int a_m^*(\mathbf{r}+\mathbf{R}_j)e^{(i/2)\mathbf{b}\times\mathbf{r}\cdot\mathbf{R}_j}a_n(\mathbf{r})d^3r. \quad (2.6)$$

We choose the symmetric gauge for the vector potential

$$\mathbf{A}=(1/2)\mathbf{H}\times\mathbf{r}. \quad (2.7)$$

Consider the following eigenvalue equation, to which we presume to know the solution:

$$\sum_n [H_{mn}(-i\nabla+\tfrac{1}{2}\mathbf{b}\times\mathbf{r}) - EN_{mn}(-i\nabla+\tfrac{1}{2}\mathbf{b}\times\mathbf{r})]\psi_n(\mathbf{r})=0. \quad (2.8)$$

Let us write

$$\psi_n(\mathbf{r})=\int d^3k\,\psi_n(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}}, \quad (2.9)$$

where the integration is over all $\mathbf{k}$. Substituting (2.9) into (2.8), we obtain

$$\sum_n \int d^3k\, e^{i\mathbf{k}\cdot\mathbf{r}}[H_{mn}(\mathbf{k}+\tfrac{1}{2}\mathbf{b}\times\mathbf{r}) - EN_{mn}(\mathbf{k}+\tfrac{1}{2}\mathbf{b}\times\mathbf{r})]\psi_n(\mathbf{k})=0. \quad (2.10)$$

Since (2.10) must hold for all $\mathbf{r}$, it surely holds for $\mathbf{r}=\mathbf{R}_j$. Clearly, then, if we let

$$f_n(\mathbf{k})=\sum_{\mathbf{K}_i}\psi_n(\mathbf{k}+\mathbf{K}_i), \quad (2.11)$$

where the sum is over all reciprocal lattice vectors $\mathbf{K}_i$, we have solved the eigenvalue equation (2.4). If we substitute (2.11) and (2.2) into (2.3), we obtain on taking account of (2.9)

$$\Phi(\mathbf{r})=\sum_{\mathbf{R}_j,n}\psi_n(\mathbf{R}_j)u_n(\mathbf{r},\mathbf{R}_j). \quad (2.12)$$

We have, therefore, established that the effective-Hamiltonian equation (2.8) is equivalent to the exact Schrödinger equation. Equation (2.8) or its equivalent has also been obtained by a number of authors[4,5,15,16] several different ways, including Chambers,[15] who straightforwardly derived it using the Wannier representation and ignoring the question of replacing $\mathbf{R}_j$ by a continuous variable $\mathbf{r}$.

When the field vanishes ($\mathbf{b}=0$), $u_n(\mathbf{r},\mathbf{R}_j)=a_n(\mathbf{r}-\mathbf{R}_j)$, and

$$H_{mn}(\mathbf{k})=E_n(\mathbf{k})\delta_{mn}, \qquad N_{mn}(\mathbf{k})=\delta_{mn}. \quad (2.13)$$

$E_n(\mathbf{k})$ is the energy-band function for the band n in the absence of a field. When the energy gaps between the bands are not so small as to allow magnetic breakdown,[4,5] we can diagonalize (2.8) to any order of b by a unitary transformation of the form[4,5,15,16]

$$H'=S^\dagger HS, \qquad N'=S^\dagger NS. \quad (2.14)$$

To lowest order and for all practical purposes, H' and N' are given by (2.13).

Dropping the band index n (we consider a single band) and letting

$$E(\mathbf{k})=\sum_{\mathbf{R}_j}W(\mathbf{R}_j)e^{i\mathbf{k}\cdot\mathbf{R}_j}, \quad (2.15)$$

[$W(\mathbf{R}_j)$ is given by (2.6) with $m=n$ and $b=0$] we have then the eigenvalue equation

$$E\left(-i\nabla+\frac{e}{\hbar c}\mathbf{A}\right)\psi(\mathbf{r})=\sum_{\mathbf{R}_j}W(\mathbf{R}_j)e^{(i/2)\mathbf{R}_j\cdot(\mathbf{b}\times\mathbf{r})}T(\mathbf{R}_j)\psi(\mathbf{r}) =E\psi(\mathbf{r}). \quad (2.16)$$

The translation operator $T(\mathbf{R}_j)$ is defined by

$$T(\mathbf{R}_j)=e^{i\mathbf{R}_j\cdot(-i\nabla)}.$$

We write $\psi(\mathbf{r})$ in such a form as to reduce (2.16) to an equation in one variable,

$$\psi(\mathbf{r})=e^{ik_zz+ik_xx-i(b/2)xy}\phi(y-k_x/b). \quad (2.17)$$

We choose the z axis to be along $\mathbf{H}$, so that k_z is a good quantum number. For convenience, the y axis is chosen to be along the shortest reciprocal lattice vector $\mathbf{K}_1$ in the plane perpendicular to $\mathbf{H}$.

Substituting (2.17) into (2.16) and shifting the origin of y to k_x/b, we can show that $\phi(y)$ satisfies the one-dimensional equation

$$\sum_j W(\mathbf{R}_j)e^{ik_zZ_j-i(b/2)X_jY_j-ibyX_j}T(Y_j)\phi(y)=E\phi(y), \quad (2.18)$$

where $\mathbf{R}_j=(X_j,Y_j,Z_j)$ and

$$T(Y_j)\phi(y)=\phi(y+Y_j). \quad (2.19)$$

As in the free-electron case,[14] the eigenvalue is independent of k_x. [We shall see in Sec. VI that for each solution $\phi(y)$ only a discrete set of values for k_x is allowed. Therefore, the degeneracy of the solutions in k_x is not as large as one might expect at first sight.]

It should be noted that the solutions to (2.16) must

[16] L. M. Roth, J. Phys. Chem. Solids 23, 433 (1962).

be of the Bloch form (in one dimension) because the differential operator on the left-hand side is periodic in y with period $r_1=K_1/b$. As a consequence, we can label $\phi(y)$ with a continuous index Q, where

$$\phi_Q(y+r_1)=e^{iQr_1}\phi_Q(y). \tag{2.20}$$

In general, we must also label $\phi(y)$ with a discrete index n which corresponds to a particular Landau level. The dependence of the energy on Q corresponds to the broadening of the levels.

III. WKB SOLUTIONS

Zil'berman[7] and Blount[5] have shown that the WKB solutions to (2.16) are of the form

$$\phi(y)=\frac{1}{\sqrt{V}}\exp\left[\pm i\int^y k(y')dy'\right], \tag{3.1}$$

where $k(y)$ is given implicitly by

$$E[-by, k(y),k_z]=E \tag{3.2}$$

and

$$V=\frac{1}{\hbar}\left|\frac{\partial E}{\partial k_y}\right|_{k_y=k(y)}. \tag{3.3}$$

Since $E(\mathbf{k})$ is periodic in reciprocal space, $k(y)$ is not uniquely defined by (3.2). Let us take $\mathbf{K}_2$ to be the shortest reciprocal lattice vector in the k_y direction. (For an arbitrary field direction, K_2 may be exceedingly long.[5]) For any $k(y)$ which satisfies (3.2), we see that $k(y)=mK_2$ also satisfies (3.2), where m is an integer. The most general solution to (2.16) would then be

$$\phi(y)=\sum_m \frac{A_m}{\sqrt{V}}\exp\left[i\left(mK_2y+\int^y k(y')dy'\right)\right]$$
$$+\sum_m \frac{B_m}{\sqrt{V}}\exp\left[i\left(mK_2y-\int^y k(y')dy'\right)\right], \tag{3.4}$$

where we choose a particular solution or branch of $k(y')$ as defined by (3.2).

IV. A SIMPLE MODEL

In view of the absence of experimental data concerning the details of the Landau spectrum (energy spectrum) and level broadening, it does not seem worthwhile at this point to worry about complicated Fermi-surface topology, but rather to emphasize only certain basic features. Therefore, we shall make a number of simplifying assumptions to obtain a model which demonstrates the important ideas involved.

For our model, we assume that the basis vectors $\mathbf{a}_i$ of the direct lattice form an orthogonal set (i.e., $\mathbf{a}_i\cdot\mathbf{a}_j=0$, $i\neq j$) and that $\mathbf{H}$ is directed along $\mathbf{a}_3$. This means that $\mathbf{K}_1$ and $\mathbf{K}_2$ coincide with the basis vectors of the reciprocal lattice. Furthermore, we assume, for a given

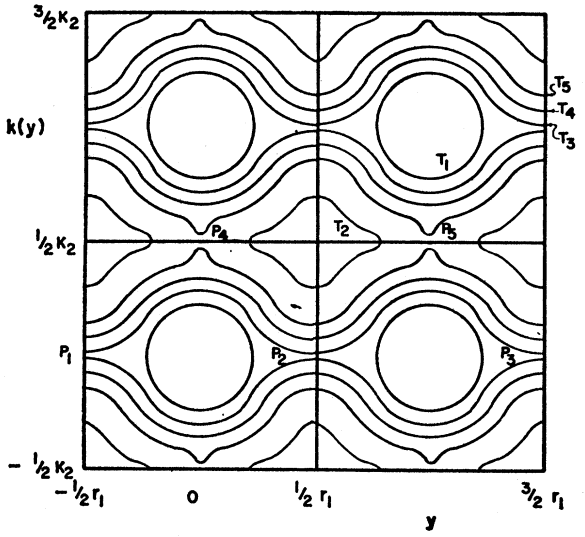

FIG. 1. Contours of constant energy in the $k(y)$-y plane $[E(-by, k(y))=E]$. T_1: closed electron orbit; T_2: closed hole orbit; T_3, T_4, and T_5: open orbits. P_1, P_2, P_3, P_4, and P_5: saddle points in $E(-by, k(y))$.

k_z, that $E(k_x,0)$ and $E(0,k_y)$ (k_z is fixed and will be suppressed) are simple functions with maxima W_1 and W_2 at the zone boundaries ($\pm\frac{1}{2}K_1$ and $\pm\frac{1}{2}K_2$). We take $W_2>W_1$ so that the curves of constant energy in the $k(y)$-y plane appear as in Fig. 1.

Under the assumptions of our model, saddle points in $E(k_x,k_y)$ occur at two types of points (in reciprocal space), $(\pm\frac{1}{2}K_1,0)$ and $(0,\pm\frac{1}{2}K_2)$ or the equivalent points in other zones. In Fig. 1, the saddle points of the first type have been denoted by P_1, P_2, and P_3, while those of the second type have been denoted by P_4 and P_5. Near these points, the orbits appear as in Fig. 2. In our model, the $k(y)-y$ coordinates coincide with the principal axes of the saddle points.

Near the saddle point at $y=\frac{1}{2}r_1$ [in the $k(y)y-$ plane], for example, when $E<W_1$, there is no real value of $k(y)$ which satisfies (3.2) for $y_1<y<y_2$ [see Fig. 2(a)]. In this region between the turning points y_1 and y_2, the WKB solutions behave as if a potential barrier is present. Similarly, the WKB solutions behave as if there is a potential barrier at $(0,\frac{1}{2}K_2)$.

When W_2 is sufficiently larger than W_1 so that a sizeable region of open orbits exists, we expect that for orbits such as T_1 and T_3 (in Fig. 1) the WKB solutions will be inaccurate in the neighborhood of points such as P_1, P_2, P_3 (i.e., close to turning points). Likewise, for

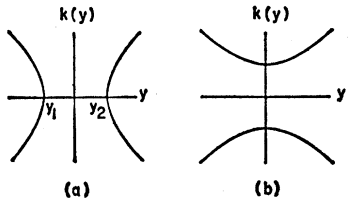

FIG. 2. Orbits in the region of saddle points. (a) Saddle point at $y=\frac{1}{2}r_1$ (P_2 in Fig. 1) for $E<W_1$. y_1 and y_2 are turning points. (b) Saddle point at $y=0$ (P_4 in Fig. 1) for $E<W_2$.

orbits such as T_2 and T_5, the WKB solutions will be inaccurate near P_4 and P_5. The open orbit T_4 will be described accurately everywhere by a WKB solution. On the other hand, when W_2 is nearly equal to W_1, all the WKB solutions with energies near W_1 or W_2 may be inaccurate in the neighborhood of both sets of saddle points.

V. CONNECTION FORMULAS

When the probability to tunnel through the barrier (at $\frac{1}{2}r_1$, for example) is negligible, each eigenstate can be thought of as being localized in some valley. When the coupling between the states in adjacent valleys is negligible, all states are degenerate, and the levels are discrete. When the tunneling probability or coupling is not negligible, the degeneracies are removed and the discrete levels are broadened. Such is the case whether the coupling is intraband coupling, as discussed above, or interband coupling as in magnetic breakdown.

Since the WKB connection formulas and transmission coefficient (tunneling probability) are not accurate for energies near the top of the barrier or above the barrier, it was desirable to have a better approximation in this region where all the interesting effects take place. Away from the turning points, the WKB solutions are certainly accurate enough for our purposes. It is in the neighborhood of the turning points where a more careful analysis is necessary in order to obtain the proper connection between the solutions in adjacent valleys.

Azbel'[9] gave a cursory treatment of the problem, but did not develop it enough to be of any help in the present investigation. The same type of barrier problem for the simpler kinetic-energy operator $-(\hbar^2/2m)\times(d^2/dy^2)$ has been solved by Miller and Good.[17] The additional complications introduced by the operator $E(-by, -i(d/dy))$ are, however, minor, and the analysis of Miller and Good will be useful.

For y near $\frac{1}{2}r_1$, we can expand $E(-by, k(y))$ about its local maximum:

$$E(-by, k(y))=W_1+\frac{\hbar^2k^2(y)}{2m_2^*}-\frac{\hbar^2b^2}{2m_1}(y-\tfrac{1}{2}r_1)^2+\cdots. \quad (5.1)$$

The effective mass m_1 is defined as positive, since the appropriate minus sign appears in (5.1), and the asterisk on m_2^* designates an effective mass at the bottom of the band.

In a restricted region around $\frac{1}{2}r_1$, then,

$$\frac{\hbar^2k^2(y)}{2m_2^*}+W_1-\frac{\hbar^2b^2}{2m_1}(y-\tfrac{1}{2}r_1)^2=E. \quad (5.2)$$

If we replace $k(y)$ by $-i(d/dy)$ in (5.2) and operate on $\phi(y)$, we obtain an equation which is correct for y near $\frac{1}{2}r_1$, and which can be solved exactly,

$$-\frac{\hbar^2}{2m_2^*}\frac{d^2\phi}{dy^2}-\frac{\hbar^2b^2}{2m_1}(y-\tfrac{1}{2}r_1)^2\phi=(E-W_1)\phi. \quad (5.3)$$

If we let

$$S=[(m_2^*/m_1)b^2]^{1/4}(y-\tfrac{1}{2}r_1)$$

and

$$a=2\frac{(m_1m_2^*)^{1/2}}{m}\left(\frac{E-W_1}{\hbar\omega_c}\right),$$

where $\omega_c=eH/mc$, and m is the free-electron mass, then (5.3) becomes

$$\frac{d^2\phi}{dS^2}+(a+S^2)\phi=0. \quad (5.4)$$

Equation (5.4) arises when the scalar Helmholtz equation is separated in parabolic coordinates.[18] For every value of a, there are two solutions[17]

$$\phi_1=D_{(1/2)(ia-1)}(\sqrt{2}Se^{-i\pi/4}) \quad (5.5)$$

and

$$\phi_2=D_{(1/2)(-ia-1)}(\sqrt{2}Se^{i\pi/4}). \quad (5.6)$$

The functions $D_n(z)$ are defined by Whittaker and Watson,[19] but only their asymptotic form will concern us.

The general WKB solution will be for $y>y_2$

$$\phi(y)=\frac{B_1}{\sqrt{V}}\exp\left(i\int_{y_2}^{y}kdy\right)+\frac{B_2}{\sqrt{V}}\exp\left(-i\int_{y_2}^{y}kdy\right), \quad (5.7)$$

and for $y<y_1$,

$$\phi(y)=\frac{A_1}{\sqrt{V}}\exp\left(i\int_{y}^{y_1}kdy\right)+\frac{A_2}{\sqrt{V}}\exp\left(-i\int_{y}^{y_1}kdy\right). \quad (5.8)$$

[For convenience, the argument y in $k(y)$ and the primes on the variable of integration have been dropped.] When $E>W_1$, we take $y_1=y_2=\frac{1}{2}r_1$.

In the region where the solutions (5.5) and (5.6) join onto the WKB solutions (5.7) and (5.8), it is reasonable to use the asymptotic form of ϕ_1 and ϕ_2. From Miller and Good,[17] we have for S large and positive (with an appropriate normalization),

$$\phi_1\rightarrow\frac{e^{(1/2)a\pi}}{\sqrt{V}}\exp\left(i\int_{y_2}^{y}kdy\right), \quad (5.9)$$

and for S large and negative,

$$\phi_1\rightarrow\frac{Ce^{(1/4)a\pi}}{\sqrt{V}}\exp\left(-i\int_{y}^{y_1}kdy\right)-\frac{i}{\sqrt{V}}\exp\left(i\int_{y}^{y_1}kdy\right), \quad (5.10)$$

[17] S. C. Miller, Jr., and R. H. Good, Jr., Phys. Rev. **91**, 174 (1953).

[18] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953), pp. 1398–1405.

[19] E. T. Whittaker and G. N. Watson, *Modern Analysis* (The University Press, Cambridge, England, 1915), p. 347.

where

$$C=\left(\frac{2}{\pi}\right)^{1/2}\left(\frac{|a|}{2e}\right)^{-(1/2)ia}\Gamma(\tfrac{1}{2}+\tfrac{1}{2}ia)\cosh\tfrac{1}{2}a\pi. \quad (5.11)$$

The second solution ϕ_2 gives the complex conjugate of (5.9) and of (5.10). The solution (5.9) corresponds to a wave traveling to the right, away from the barrier in the region $y>y_2$ (since the phase is increasing as y increases), whereas (5.10) is the sum of two terms, the first being a wave traveling to the right, toward the barrier in the region $y<y_1$, and the second being a wave traveling to the left and away from the barrier ($y<y_1$). Symbolically, we have

$$\begin{matrix} A_1 & B_1 \\ \leftarrow & \rightarrow \end{matrix}$$

$$\begin{matrix} A_2 & B_2 \\ \rightarrow & \leftarrow \end{matrix}.$$

Let us now use the notation that Pippard[20] used in the analogous situation in magnetic breakdown. First, assume that B_2 is zero so that we have only a transmitted wave for $y>y_2$. We write

$$B_1=pA_2, \quad (5.12)$$

and

$$A_1=qA_2, \quad (5.13)$$

where A_2 is the amplitude of the incoming wave for $y<y_1$, A_1 is the amplitude of the reflected wave, and B_1 is the amplitude of the transmitted wave. The factors p and q are the probability amplitudes (with definite phase) for transmission and reflection. The transmission coefficient is $|p|^2$ and conservation of probability requires that $|p|^2+|q|^2=1$. From (5.9) and (5.10), we have

$$p=C^{-1}e^{(1/4)a\pi}, \quad (5.14)$$

and

$$q=-iC^{-1}e^{-(1/4)a\pi}. \quad (5.15)$$

We can evaluate $|C|^2$ by imposing the conservation of probability,

$$|C|^2=2\cosh\tfrac{1}{2}a\pi. \quad (5.16)$$

From (5.14) and (5.16) we obtain for the transmission coefficient

$$|p|^2=1/(1+e^{-a\pi}). \quad (5.17)$$

In the limit of large, negative a, (5.17) agrees with the usual WKB tunneling probability.

If now we consider $A_2=0$, we can, with the help of (5.9) and (5.10) and the complex conjugates of (5.9) and (5.10), show that

$$A_1=pB_2, \quad (5.18)$$

and

$$B_1=qB_2. \quad (5.19)$$

Equations (5.18) and (5.19) are to be expected since the barrier appears the same from either side.

[20] A. B. Pippard, Proc. Roy. Soc. (London) **A1**, 270 (1962).

Let us write $C=|C|e^{i\alpha}$, where from (5.11),

$$\alpha=\tfrac{1}{2}a[1-\ln(\tfrac{1}{2}|a|)]+\arg\Gamma(\tfrac{1}{2}+\tfrac{1}{2}ia), \quad (5.20)$$

and from (5.16),

$$|C|=(2\cosh\tfrac{1}{2}a\pi)^{1/2}. \quad (5.21)$$

For $a=0, \alpha=0$, and from asymptotic expansion of $\Gamma(\frac{1}{2}+\frac{1}{2}ia)$ for large a (positive or negative)

$$=\alpha\underset{4}{a}-\ln\left(\frac{1+a^2}{a^2}\right)-\frac{1}{6a}+\cdots \quad (5.22)$$

which goes to zero as $1/12a$ for large a.

We now write (5.14) and (5.15) as

$$p=e^{-i\alpha}(1+e^{-a\pi})^{-1/2}, \quad (5.23)$$

$$q=-ie^{-i\alpha}(1+e^{a\pi})^{-1/2}. \quad (5.24)$$

To connect the solutions in adjacent valleys, then, we merely employ p and q as in (5.12), (5.13), (5.18), and (5.19). We find

$$A_1=qA_2+pB_2,$$

and

$$B_1=pA_2+qB_2. \quad (5.25)$$

At the origin, the WKB solutions also behave as if a barrier is present (see T_2 in Fig. 1 for example). We must, therefore, derive connection formulas appropriate for the saddle points such as P_4 and P_5.

For y near $y=0$ and $k(y)$ near $\frac{1}{2}K_2$, $E(-by, k(y))$ reaches a maximum W_2, and we can expand

$$E(-by, k(y))=W_2+\frac{\hbar^2b^2y^2}{2m_1^*}-\frac{\hbar^2}{2m_2}(k(y)-\tfrac{1}{2}K_2)^2+\cdots.$$

Hence, we have, for y near the origin and $k(y)$ near $\frac{1}{2}K_2$,

$$\frac{-\hbar^2}{2m_2}[k(y)-\tfrac{1}{2}K_2]^2+W_2+\frac{\hbar^2b^2y^2}{2m_1^*}=E. \quad (5.26)$$

Replacing $k(y)$ by $-i(d/dy)$ and operating on $\phi(y)$, we obtain after multiplication by -1,

$$\frac{-\hbar^2}{2m_2}\left(\frac{d}{dy}-\frac{i}{2}K_2\right)^2\phi-\frac{\hbar^2b^2y^2}{2m_1^*}\phi=(W_2-E)\phi. \quad (5.27)$$

If we let

$$\phi(y)=e^{(i/2)K_2y}\eta(y), \quad S'=\left(\frac{m_2}{m_1^*}b^2\right)^{1/4}y,$$

and

$$a'=2\frac{(m_1^*m_2)^{1/2}}{m}\left(\frac{W_2-E}{\hbar\omega_c}\right),$$

then $\eta(y)$ obeys an equation analogous to (5.4),

$$\frac{d^2\eta}{dS'^2}+(a'+S'^2)\eta=0, \quad (5.28)$$

for which there are two solutions η_1 and η_2.

Let us define the turning points y_1' and y_2' analogously to y_1 and y_2 ($y_1'=y_2'=0$ when $E<W_2$) except shifted to the left by $\frac{1}{2}r_1$, and let $\kappa(y)=k(y)-\frac{1}{2}K_2$. Then the asymptotic expressions (5.9) and (5.10) can be taken over, for $y>0$

$$\eta_1 \rightarrow \frac{e^{(1/2)a'\pi}}{\sqrt{V}} \exp\left(i\int_{y_2'}^{y} \kappa dy\right), \tag{5.29}$$

and for $y<0$,

$$\eta_1 \rightarrow \frac{C'}{\sqrt{V}} e^{(1/4)a'\pi} \exp\left(-i\int_{y}^{y_1'} \kappa dy\right) - \frac{i}{\sqrt{V}} \exp\left(i\int_{y}^{y_1'} \kappa dy\right), \tag{5.30}$$

where

$$C'=\left(\frac{2}{\pi}\right)^{1/2}\left(\frac{|a'|}{2e}\right)^{-(1/2)ia'} \Gamma(\tfrac{1}{2}+\tfrac{1}{2}ia') \cosh\tfrac{1}{2}a'\pi.$$

The second solution η_2 gives the complex conjugate of (4.29) and of (4.30). Multiplying (4.29) and (4.30) by the factor $\exp(i/2)K_2y$ gives the form of $\phi(y)$ near the origin.

From (4.26), it is easy to see that the WKB solutions approach

$$\phi(y)=\frac{1}{\sqrt{V}} \exp i\left(\tfrac{1}{2}K_2y \pm i\int^{y} \kappa dy\right), \tag{5.31}$$

for y near the origin, and join onto the solutions

$$e^{(i/2)K_2y}\eta_1 \quad \text{and} \quad e^{(i/2)K_2y}\eta_2.$$

Hence, the connection formulas are given by equations like (5.12), (5.13), (5.18), and (5.19) if we replace p and q by p' and q'. The primes denote replacing a by a' in α and in (5.23) and (5.24).

VI. EIGENVALUES AND EIGENFUNCTIONS

In a recent paper, Roth[21] has derived a quantization condition for what could be called one-dimensional coupling. The term "one-dimensional" arises because the solutions couple only at points like P_1, P_2, P_3 in the electron orbits and at P_4 and P_5 in the hole orbits (in Fig. 1). As a consequence, the energy levels can be shown to depend upon a one-dimensional wave number Q. In this section, we consider two-dimensional coupling, which reduces to the one-dimensional case when W_2 exceeds W_1 by a few $\hbar\omega_c$ or more.

If W_2 is nearly equal to W_1 so that only a narrow region of open orbits exists, coupling occurs at

$$y=\pm\tfrac{1}{2}r_1, \quad \pm\tfrac{2}{3}r_1\cdots, \tag{6.1}$$

and at

$$y=0, \quad \pm r_1, \quad \pm 2r_1\cdots. \tag{6.2}$$

The intermediate open orbit (T_4 in Fig. 1) is an example of such two-dimensional coupling when W_2 is nearly equal to W_1. The term two-dimensional arises because $\phi(y)$ can be labeled with a two-dimensional wave vector (Q_1,Q_2).

The WKB solutions are accurate except near the points (6.1) and (6.2), where the solutions are to be connected with the p-q formulas. In Fig. 1 it is clear that the pairs of solutions coupled at (6.1) are not the same pairs coupled at (5.2). Hence, we must couple all possible solutions of the type $k(y)+mK_2$ where m is an integer. The WKB solution now becomes an infinite sum over m. We write for $y<y_1'$

$$\phi(y)=\sum_m \frac{A_m}{\sqrt{V}} \exp i\left(mK_2y+\int_{y}^{y_1'} kdy\right) + \sum_m \frac{B_m}{\sqrt{V}} \exp i\left(mK_2y-\int_{y}^{y_1'} kdy\right), \tag{6.3}$$

and for $y_2'<y$,

$$\phi(y)=\sum_m \frac{C_m}{\sqrt{V}} \exp i\left(mK_2y+\int_{y_2'}^{y} kdy\right) + \sum_m \frac{D_m}{\sqrt{V}} \exp i\left(mK_2y-\int_{y_2'}^{y} kdy\right), \tag{6.4}$$

where $k(y)$ is the branch depicted by T_4 or the closed-orbit branches nearest T_4. That (6.3) and (6.4) are solutions to (2.7) can be verified by direct substitution.

Near $y=0$, we can see from (5.26) that

$$\int_{y_2'}^{y} kdy=\tfrac{1}{2}K_2(y-y_2')+\int_{y_2'}^{y} \kappa dy,$$

and (6.5)

$$\int_{y}^{y_1'} kdy=\tfrac{1}{2}K_2(y_1'-y)+\int_{y}^{y_1'} \kappa dy,$$

so for a given m, A_{m+1} and C_m represent outgoing waves while B_m and D_{m+1} represent incoming waves near $y=0$:

$$\overset{A_{m+1}}{\leftarrow} \quad \overset{C_m}{\rightarrow}$$

$$\overset{B_m}{\rightarrow} \quad \overset{D_{m+1}}{\leftarrow}.$$

The connection formulas give

$$C_m e^{-(i/2)K_2y_2'}=p'B_m e^{-(i/2)K_2y_1'}+q'D_{m+1}e^{(i/2)K_2y_2'},$$

and (6.6)

$$A_{m+1}e^{(i/2)K_2y_1'}=q'B_m e^{-(i/2)K_2y_1'}+p'D_{m+1}e^{(i/2)K_2y_2'}.$$

The appearance of $m+1$ terms in (6.6) reflects the two-dimensional character of the problem, because the coupling at $y=0$ is between m and $m+1$ solutions while the coupling at $\frac{1}{2}r_1$ involves only m solutions. At $\frac{1}{2}r_1$, the connection formulas give, after imposing the Bloch

[21] L. M. Roth, Phys. Rev. **145**, 434 (1966).

condition (2.9),

$$B_m e^{-i(\xi+Q_1 r_1)} = pC_m e^{i\xi} + qA_m e^{i(\xi+Q_1 r_1)},$$

and

$$D_m e^{-i\xi} = qC_m e^{i\xi} + pA_m e^{i(\xi+Q_1 r_1)}, \tag{6.7}$$

where

$$\xi = \int_{y_2'}^{y_1} k\,dy.$$

We can solve (6.6) and (6.7) if we assume that

$$A_{m+1} = e^{iQ_2 r_2} A_m,$$

and

$$D_{m+1} = e^{iQ_2 r_2} D_m, \tag{6.8}$$

where $r_2 = K_2/b$ and Q_2 is a wave number of range $2\pi/r_2$. Equations (6.6), (6.7), and (6.8) have a solution only if their secular determinant vanishes. The secular equation then gives the quantization condition after some manipulations:

$$\cos[2\xi + \tfrac{1}{2}K_2(y_2' - y_1') + \alpha + \alpha'] = \frac{\cos Q_1 r_1}{[(1+e^{-a\pi})(1+e^{-a'\pi})]^{1/2}} + \frac{\cos Q_2 r_2}{[(1+e^{a\pi})(1+e^{a'\pi})]^{1/2}}. \tag{6.9}$$

It can be shown that (6.9) gives the correct results for one-dimensional coupling when W_2 exceeds W_1 by a few $\hbar\omega_c$ or more.[21,22] Our results are also in agreement with the calculations of Brailsford,[23] who solved the equivalent Schrödinger equation for the tight-binding case by the finite-difference technique of Harper.[24]

It is clear that for all closed orbits, except those near open orbits, the energy levels are essentially discrete. In Fig. 3 we have shown how the energy levels appear near W_1 (for the one-dimensional case). For $W_2 = W_1$, the relative linewidth at $E = W_1 = W_2$ ($a = a' = 0$) is unity and significant broadening extends roughly twice as far into the discrete region of the spectrum as in the case of one-dimensional coupling. In both cases, the transition from discrete to continuous behavior occurs in an extremely narrow energy range (5–10 $\hbar\omega_c$). The dependence of the eigenvalues on a two-dimensional wave vector (Q_1, Q_2) is similar to the magnetic-breakdown case in hexagonal metals,[25,26] and reflects the symmetry between the x and y directions not apparent in our original choice of wave function (2.17).

The two-dimensional coupling case is particularly important because the effective-Hamiltonian solution can be related to the actual solution of the exact

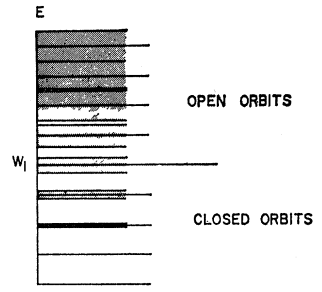

FIG. 3. Landau-level broadening in the transition region between open and closed orbits.

Hamiltonian (1.2) in an interesting manner. In Sec. II it was shown that the eigenvalues are independent of k_x, but from group theory[10] we know that there must indeed be some dependence upon the x component, as well as the y component, of some wave vector. As we shall demonstrate, the wave vector (Q_1, Q_2) serves this purpose and thus makes the effective-Hamiltonian analysis consistent with the requirements of group theory.

To relate the solutions $\psi(\mathbf{r})$ that we have found to the solutions $\Phi(\mathbf{r})$ of the exact Hamiltonian (1.2), we must transform from the effective-Hamiltonian representation to the Schrödinger representation. We take the form of the transformation to be that given by (2.12) (for a single band)

$$\Phi(\mathbf{r}) = \sum_j \psi(\mathbf{R}_j) u(\mathbf{r}, \mathbf{R}_j). \tag{6.10}$$

The general form of $\psi(\mathbf{r})$ for our model is from (2.17), (6.3), (6.4), and (6.8):

$$\psi(\mathbf{r}) = e^{ik_z + ik_x x - i(b/2)xy} \sum_m e^{i[mK_2(y - k_x/b) + mQ_2 r_2]} \times g\left(y - \frac{k_x}{b}\right), \tag{6.11}$$

where $g(y)$ is of the form (except near the turning points)

$$g(y) = \frac{A}{\sqrt{V}} \exp\left(i\int^y k\,dy\right) + \frac{B}{\sqrt{V}} \exp\left(-i\int^y k\,dy\right). \tag{6.12}$$

In (6.10), only the value of $\psi(\mathbf{r})$ at $\mathbf{R}_j$ is important. Since $K_2 Y_j$ equals an integral number of 2π and $br_2 = K_2$, it is easy to see that the infinite sum vanishes unless

$$k_x = Q_2 + \mu^2 \pi b / K_2, \tag{6.13}$$

where μ is an integer. Since the actual wave function vanishes unless (6.13) is satisfied, the degeneracy of the solutions in k_x is only a degeneracy in μ. Therefore, for each Q_2, k_x takes on only a discrete set of values. The wave function and the eigenvalues also depend upon Q_1 since $g(y)$ is of the form

$$g(y + r_1) = e^{iQ_1 r_1} g(y). \tag{6.14}$$

Since r_1 and r_2 are much larger than the lattice spac-

[22] I. M. Lifshitz and M. I. Kaganov, Usp. Fiz. Nauk **69**, 419 (1959) [English transl.: Soviet Phys.—Usp. **2**, 831 (1960)].
[23] A. D. Brailsford, Proc. Phys. Soc. (London) **A70**, 275 (1957).
[24] P. H. Harper, Proc. Phys. Soc. (London) **A68**, 874 (1955).
[25] A. B. Pippard, Phil. Trans. Roy. Soc. London **256**, 317 (1964).
[26] R. G. Chambers, Proc. Phys. Soc. (London) **88**, 701 (1966).

ings (typically 10^2 to 10^3 times larger), Q_1 and Q_2 span only a small fraction of the Brillouin zone. One can, in fact, show that the fraction spanned is the same as predicted by group theory. Following Brown,[10] we require that b satisfy[27]

$$b=2\pi/Na_1a_2, \tag{6.15}$$

where N is an integer, a_1 and a_2 are the lattice spacings in the x and y directions. A requirement such as (6.15) is necessary if periodic boundary conditions are to be imposed upon a finite volume.[10]

Since $br_1=K_1$ and $K_1=2\pi/a_1$, (6.15) implies that

$$r_1=Na_2. \tag{6.16}$$

Similarly, for r_2 we have

$$r_2=Na_1. \tag{6.17}$$

The range of Q_1 is $2\pi/r_1$, which is, from (6.16), $2\pi/Na_2$. Likewise, the range of Q_2 is $2\pi/Na_1$. The range of Q_1 and the range of Q_2 coincide with those described by Brown, so the proper fraction of the Brillouin zone is spanned.

One can also show that the effective-Hamiltonian formalism accounts for all the states and the appropriate degeneracies in accordance with group theory. In a unit area of the xy plane, there are $[1/(2\pi)^2](2\pi/Na_1)\times(2\pi/Na_2)$ states in the fraction of the Brillouin zone spanned by Q_1 and Q_2. Just as in the group-theory approach, the states are degenerate with respect to μ in (6.13). If we allow μ to take on N values, the range of k_x is $2\pi/a_1$, and the total number of states per unit area for a given k_z and n (Landau-level quantum number) is $1/Na_1a_2$, which agrees with Brown. It is also shown in the Appendix that the solution $\Phi(\mathbf{r})$ which we have obtained by solving the equivalent Schrödinger equation satisfies the magnetic-translational symmetries of the exact Schrödinger equation.

Since the eigenvalues and eigenfunctions found in the effective-Hamiltonian approach are of the form required from group-theoretical considerations of the exact Hamiltonian, it would seem that the analysis is correct, and that no source of level broadening due to the lattice potential has been omitted. Hence, the Landau levels in a perfect crystal are discrete even in the presence of the strong lattice potential of a real metal except when some type of infinite coupling of the orbits exists.

VII. DISCUSSION

A detailed analysis of a simplified model of the effective-Hamiltonian formalism has been given. The simplifications assumed were made primarily for convenience and clarity, and were not essential to the analysis. The conclusions drawn from the model are, in fact, correct beyond its range of validity. As a bridge between the model and the general problem, a brief description of the analysis of the general problem will be indicated.

Blount[5] has discussed the types of solutions to be expected when $\mathbf{H}$ (and k_z) are oriented at an arbitrary direction with respect to a symmetry axis. The repetitious pattern of the curves of constant energy for fixed k_z (such as Fig. 1) can be quite tortuous, but we should not expect the degeneracies among solutions in different zones to be lifted in the absence of any coupling.

As we have shown in Sec. II, the general problem can be reduced to an equation in a single variable y. But, this one-dimensional approach is not useful for complicated orbits such as a star-shaped orbit. The one-dimensional approach only works nicely if the coupling points are of the type of Fig. 2(a) or 2(b). That is, when $k(y)$ and y coincide with the principal axes of the saddle point. In the star-shaped orbit, for example, the $k(y)$-y coordinate system cannot be chosen so that all of the coupling points (assumed to be at the tips of the star) are of the two types in Fig. 2. The local equations near the coupling point mix $k(y)$ and y since there are cross terms in an expansion of $E(\mathbf{k})$ about the saddle point. The cross terms complicate the differential equations for $\phi(y)$ when $k(y)$ is replaced by $-i(d/dy)$.

Perhaps an even simpler approach to the general problem, than that of the model, is an equivalent semiclassical treatment such as Pippard's[20,25] analysis of magnetic breakdown. In the semiclassical approach, we suppose that the electron is a wave packet traveling about a trajectory in real space similar to the $k(y)$-y curves of Fig. 1. The phase change of the wave packet between two points is related to simple geometrical properties of the trajectory as in the Onsager rules. When a wave packet of unit amplitude encounters a coupling point, the amplitude of the transmitted portion is p and the amplitude of the reflected portion is q. Since we can verify the semiclassical approach for Pippard's one-dimensional network within the framework of the effective-Hamiltonian formalism, we expect the semiclassical approach to be quite useful for the complicated networks found in real metals, if we are not concerned with details such as $\pi/2$ in factors of $(n+\frac{1}{2})\pi$, which are omitted in Pippard's analysis.

Whether we treat the orbits in terms of wave functions or in terms of semiclassical wave packets, the conclusions must be the same as in the model. Significant broadening of the energy levels associated with closed orbits in a perfect crystal can only occur when there is either intraband coupling, or interband coupling, to other degenerate orbits and the conditions for such coupling to occur are extremely stringent. Broadening can also arise when impurities and dislocations are present.[28–30] Since we have been able to show that the

[27] Brown's expression corresponding to (6.15) also contains a multiplicative integer n on the right-hand side which we set equal to 1.

[28] R. B. Dingle, Proc. Roy. Soc. (London) **A500**, 211 (1952a)
[29] R. B. Dingle, Proc. Roy. Soc. (London) **A517**, 211 (1952b).
[30] A. B. Pippard, Proc. Roy. Soc. (London) **A165**, 287 (1965).

effective-Hamiltonian formalism is completely consistent with the requirements of a group-theoretical treatment of the exact Hamiltonian, it would appear that no source of level broadening in a perfect crystal has been omitted, and the analysis given in this investigation is essentially correct.

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APPENDIX

Zak[16] has shown that when[31]

$$b=4\pi/Na_1a_2, \tag{A1}$$

the symmetry-adapted wave function $\Phi(\mathbf{r})$ obeys

$$\tau(\mathbf{R}_N)\Phi(\mathbf{r})=e^{i\mathbf{k}\cdot\mathbf{R}_N}\Phi(\mathbf{r}). \tag{A2}$$

The magnetic translation operator $\tau(\mathbf{R})$ is defined as

$$\tau(\mathbf{R})=\exp[i(-iv-\tfrac{1}{2}\mathbf{b}\times\mathbf{r})\cdot\mathbf{R}], \tag{A3}$$

and $\mathbf{R}_N$ is given by

$$\mathbf{R}_N=(n_1a_1,n_2Na_2,n_3a_3), \tag{A4}$$

where n_1, n_2, and n_3 are integers. The wave vector $\mathbf{k}$ corresponds to

$$\mathbf{k}=(Q_2+\mu 2\pi b/K_2, Q_1,k_z). \tag{A5}$$

Now, if we write $\Phi(\mathbf{r})$ as in (6.10), the magnetic Wannier functions have the property[10]

$$u(\mathbf{r},\mathbf{R}_j)=\tau(-\mathbf{R}_j)u(\mathbf{r},0). \tag{A6}$$

Equations (6.10), (A2), and (A6) then imply that

$$\psi(\mathbf{R}_j+\mathbf{R}_N)=\exp[i(\mathbf{k}+\tfrac{1}{2}\mathbf{b}\times\mathbf{R}_j)\cdot\mathbf{R}_N]\psi(\mathbf{R}_j). \tag{A7}$$

From (6.11) and (6.14), it is easy to see that our solution for $\psi(\mathbf{R}_j)$ satisfies (A7), and therefore our solution for $\Phi(\mathbf{r})$ has the proper magnetic translational symmetry.

[31] Note that (A1) and (6.16) differ by a factor of 2 on the right-hand side. The analysis of Zak is good only for field values which satisfy (A1), whereas the analysis of Brown is good only when (6.15) holds.

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Friedel Phase-Shift Sum Rule for Semiconductors

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The Friedel sum rule relating the phase shifts for scattering by an ion to the charge of the ion is extended to apply to semiconductors by taking nondegenerate statistics and the presence of several types of carriers into account. When the first Born approximation is valid, the phase shifts for the customary screened Coulomb potential obey the sum rule.

I. THE PHASE-SHIFT SUM RULE

WHEN carriers with spherical energy surfaces are scattered by a spherically symmetric potential which goes to zero faster than r^{-1} at large r, the differential scattering cross section is given in terms of the phase shifts η_l for angular momentum l.[1] It was shown by Friedel[2] that the phase shifts also give the magnitude of the electronic charge attracted to, or repelled from, the neighborhood of the scattering center. The requirement that the center should appear neutral at large distances imposes a condition on the phase shifts, and thus on the potential.

Most applications of the Friedel sum rule have been to metals, which have degenerate statistics. In semiconductors, the relation must be extended to take account of Fermi statistics at $T\neq 0$ and the presence of carriers of more than one type. We confine ourselves here to spherical energy surfaces, although more general cases can be treated.[3,4]

We find, by obvious modification of the derivation[2,5,6] of the Friedel phase-shift sum rule, that its extended form for semiconductors can be written

$$\pi^{-1}\sum_{l,i}(2l+1)g_iq_i\int_{-\infty}^{\infty}\left(\frac{d\eta_{l,i}}{dE}\right)f_i(E)dE=-Ze. \tag{1}$$

Here the index i identifies the populated bands, each with degeneracy g_i; E is the energy of the scattered

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