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Zentralinstitut für Elektronenphysik der Deutschen Akademie der Wissenschaften zu Berlin, Abteilung Theoretische Physik

Theory of Bloch Electrons in a Magnetic Field

By

H. J. Fischbeck

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1. Introduction

The relevance of investigations of solid state properties under the influence of a homogeneous magnetic field needs no special justification. From such phenomena as galvanomagnetic, thermomagnetic, magnetoacoustic, and magnetooptical effects, microwave absorption in a magnetic field, and de Haas-van Alphen effect, etc., one can derive important informations of the electronic structure of solids. It is of special significance that the magnetic field creates periodicities of the motion of electrons giving rise to various oscillatory and resonance effects. Periods and resonances are easy to measure and often related to important parameters of the electronic structure.

The knowledge of the behaviour of Bloch electrons in a magnetic field is fundamental to the interpretation of such phenomena. Since the beginning of solid state physics conceptions based on the equations

$$\hbar\,\dot{\boldsymbol{k}} = \left(\frac{e}{c}\right)(\boldsymbol{v}\times\boldsymbol{B})\,, \qquad \dot{\boldsymbol{r}} = \boldsymbol{v} = \frac{1}{\hbar}\,\nabla_{\boldsymbol{k}} E_\nu(\boldsymbol{k})$$

have proved to be very useful. Here $\boldsymbol{k}$ and $\boldsymbol{v}$ are the wave vector and the velocity of a Bloch electron with the energy $E_\nu(\boldsymbol{k})$ in a magnetic field $\boldsymbol{B} = \operatorname{rot}\boldsymbol{A}$. These equations are essentially classical for they can be derived as equations of motion from the effective Hamiltonian [1]

$$H_{\text{eff}} = E_\nu\left(\boldsymbol{k} - \frac{e}{\hbar\,c}\boldsymbol{A}(\boldsymbol{r})\right).$$

But they already contain the quantum-mechanical energy band function $E_\nu(\boldsymbol{k})$. Because of this hybrid character their exact proof is difficult. According to these equations the $\boldsymbol{k}$-vector runs through intersection curves of constant energy surfaces with planes perpendicular to the magnetic field. The so determined classical electron orbits can be subjected to the Bohr-Sommerfeld quantization rule. In this way even typical quantum effects become accessible to this simple theory [2].

This semiclassical theory was very successful. Almost all relevant effects except, e.g., magnetic breakdown [3] can be understood in terms of it. Quite apart from its usefulness the semiclassical description can only be looked upon as a preliminary form of a real quantum-mechanical theory.

The first approaches to the quantum theory of the problem were due to Landau [4] and Peierls [5]. They influenced the further development decisively. Landau solved the problem of free electrons in a magnetic field and calculated their steady diamagnetic susceptibility. Using the tight-binding approximation, Peierls showed the Hamiltonian of the Bloch electron in a magnetic field to be approximately equivalent to

$$H_{\text{eff}} = E_\nu\left(\boldsymbol{k} - \frac{e}{\hbar\,c}\boldsymbol{A}(i\nabla_{\boldsymbol{k}})\right)$$

which is the quantum-mechanical analogy to the semiclassical Hamiltonian. This result is called the Peierls theorem. Therewith Peierls was able to evaluate the steady diamagnetic susceptibility of strongly bound electrons without knowing their energy spectrum.

A more general substantiation of the Peierls theorem was given by Luttinger [11]. Then it was tried to take into account interband coupling terms neglected in Peierls' theorem by diagonalizing transformations [6 to 8]. This development culminated in the papers of Kohn [9], Blount [10], Wannier and Fredkin [11], and Roth [12] in which the Hamiltonian of the Bloch electron in a magnetic field is transformed into effective one-band Hamiltonians by different and partly very complicated methods. The Peierls theorem is included as lowest-order approximation.

The eigenvalue problem given by a one-band Hamiltonian was at first treated in the effective-mass approximation of the energy band function leading to a simple generalization of Landau's result. The adequate solution of the general eigenvalue problem was achieved by Zilberman [13] by application of the WKB method. A close connection to the electron orbits of the semiclassical theory was found, and Onsager's quantization rule [2] was confirmed. Therewith the problem of crystal electrons in a magnetic field is, in principle, reduced to Bloch energies and wave functions, that is to say to the zero-field case. This indicates the close relation between the problems with and without field. Accordingly, the most experiments in magnetic fields are made to get informations about electronic structures in absence of field. On the other hand, this relation is lost little by little with increasing field, because it is established by nonconvergent (i.e. asymptotic) expansions in powers of field strength.

Because of this, the Bloch electron in a magnetic field should be considered as an independent problem, too. This way of questioning and the first approach to a solution were due to Harper [14], who therewith initiated the elucidation of the basic symmetry properties by Brown [15], Zak [16], and the present author [17 to 19]. The most important results were statements about general properties of eigenvalues and eigenfunctions of the Hamiltonian, which by this time can have been classified in a "magnetic" energy band scheme [19].

Moreover, new starting points for the solution of the Schrödinger equation were found [14, 18, 20 to 22]. Up to now these results are of principal rather than practical interest. But the more the field strength increases the more important the real magnetic band structure becomes. When the Landau radius becomes comparable with the lattice constant in extremely high magnetic fields of $10^6 \ldots 10^8$ G, the basic electronic structure of a solid will strongly depend on field strength [23]. In special cases first indications of this are already seen at fields available at present [24].

The present report attempts to give a survey of the present state of affairs. It is of importance to formulate the theory on the basis of the translational symmetry of the problem throughout the work. That corresponds to the composition of the paper. Section 2 deals with the magnetic translation group, its irreducible representations, and their consequences for the structure of energies and wave functions. On these principles Section 3 is concerned with the construction of an effective one-band Hamiltonian in accordance with Roth's work [12]. First a many-band Hamiltonian is deduced, which is diagonalized to a one-band Hamiltonian by a further transformation. Section 4 deals with concrete methods for the solution of the Schrödinger equation, which are mainly applications of the WKB method.

For the sake of clearness and conciseness of the exposition, restrictions of the subject were necessary. In particular applications of the theory are completely left out in order not to go beyond the scope of this article.

2. Symmetry Properties

2.1 Hamiltonian

The theory of the Bloch electron in a magnetic field is based on the Hamiltonian

$$H\left(\frac{1}{h}\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right), \boldsymbol{r}\right) \quad \frac{1}{2m}\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)^2 - V(\boldsymbol{r}) \quad \frac{e\hbar}{2mc}(\boldsymbol{\sigma}, \boldsymbol{B}) \; :$$

$$\cdot \quad + \frac{\hbar}{4m^2c^2}\left(\boldsymbol{\sigma}, \nabla_{\boldsymbol{r}} V \times \left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)\right), \tag{2.1}$$

where $\boldsymbol{p}$ and $\boldsymbol{r}$ are the momentum and position operator respectively. $\boldsymbol{\sigma}$ is the Pauli spin vector, $V(\boldsymbol{r}) = V(\boldsymbol{r} + \boldsymbol{R})$ the periodic potential with $\boldsymbol{R}$ a lattice vector, and $\boldsymbol{A}(\boldsymbol{r})$ the vector potential of the homogeneous magnetic field $\boldsymbol{B} = \nabla \times \boldsymbol{A}$ which gives

$$\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right) \times \left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right) = i\frac{e\hbar}{c}\boldsymbol{B}\,. \tag{2.2}$$

In addition to $\boldsymbol{A}(\boldsymbol{r})$ we define the conjugate vector potential

$$\overline{\boldsymbol{A}}(\boldsymbol{r}) = \int_0^{\boldsymbol{r}} \nabla\,(\boldsymbol{A}(\boldsymbol{r}')\,, \mathrm{d}\boldsymbol{r}') = \boldsymbol{A}(\boldsymbol{r}) + \boldsymbol{r} \times \boldsymbol{B}^{1}) \tag{2.3}$$

with the properties $\overline{\overline{\boldsymbol{A}}} = \boldsymbol{A}$, $\nabla \times \overline{\boldsymbol{A}} = -\boldsymbol{B}$,

$$\left(\boldsymbol{p} - \frac{e}{c}\overline{\boldsymbol{A}}\right) \times \left(\boldsymbol{p} - \frac{e}{c}\overline{\boldsymbol{A}}\right) = -i\frac{e\hbar}{c}\boldsymbol{B}\,, \tag{2.4}$$

and

$$\left[\boldsymbol{p} - \frac{e}{c}\boldsymbol{A},\ \boldsymbol{p} - \frac{e}{c}\overline{\boldsymbol{A}}\right] = 0\,. \tag{2.5}$$

As indicated by (2.2), (2.4), and (2.5), the Cartesian components of both the canonical momentum $\boldsymbol{p} - (e/c)\,\boldsymbol{A}$ and the conjugate momentum $\boldsymbol{p} - (e/c)\,\overline{\boldsymbol{A}}$ in the plane perpendicular to the magnetic field do not commute whereas all the components of $\boldsymbol{p} - (e/c)\,\boldsymbol{A}$ commute with those of $\boldsymbol{p} - (e/e)\,\overline{\boldsymbol{A}}$. Therefore, the most natural and besides gauge-independent formulation is achieved if we use the components of $\boldsymbol{p} - (e/c)\,\boldsymbol{A}$ and $\boldsymbol{p} - (e/c)\,\overline{\boldsymbol{A}}$ as canonically conjugated variables instead of momentum and position [17, 18].

Thus, the components of the three vector operators [19]

$$\left.\begin{aligned} \boldsymbol{w} &= \frac{1}{\hbar}\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right) = (u_{(1)}, v_{(1)}, v_{(3)})\,, \\ \boldsymbol{t} &= \frac{1}{\hbar}\left(\boldsymbol{p} - \frac{e}{c}\overline{\boldsymbol{A}}\right) = (v_{(2)}, u_{(2)}, v_{(3)})\,, \\ \boldsymbol{s} &= \boldsymbol{r} + \boldsymbol{w} \times \boldsymbol{\lambda} = \lambda(u_{(2)}, -v_{(2)}, u_{(3)}) \end{aligned}\right\} \tag{2.6}$$

[1]) Here the trivial assumption $\boldsymbol{A}(0) = 0$ is made.

in a Cartesian coordinate system $\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3$[2]) with $\boldsymbol{e}_3 \parallel \boldsymbol{B}$ fulfil the canonical commutation relations

$$[u_{(i)}, u_{(k)}] = \frac{1}{i\lambda}\,\delta_{ik}{}^{3)}\,, \tag{2.7}$$

where $\lambda = \hbar c / e B$, $B = |\boldsymbol{B}|$, and $\boldsymbol{\lambda} = \lambda\,\boldsymbol{e}_3$.

Furthermore, we have

$$[\boldsymbol{w}, \boldsymbol{t}] = 0 \quad \text{and} \quad [t_i, s_k] = \frac{1}{i}\,\delta_{ik}\,. \tag{2.8}$$

In terms of (2.6) the Hamiltonian (2.1) reads

$$H(\boldsymbol{w}, \boldsymbol{s} - \boldsymbol{w}\times\boldsymbol{\lambda}) = \frac{\hbar^2\,\boldsymbol{w}^2}{2\,m} + V(\boldsymbol{s} - \boldsymbol{w}\times\boldsymbol{\lambda}) - \frac{\hbar^2}{2\,m}(\boldsymbol{\sigma}, \boldsymbol{b}) - \\ - \frac{\hbar^2}{4\,m^2\,c^2}(\boldsymbol{\sigma}, \nabla_{\boldsymbol{s}} V\times\boldsymbol{w})\,, \tag{2.9}$$

where $\boldsymbol{b} = e\,\boldsymbol{B}/\hbar\,c = \lambda^{-1}\,\boldsymbol{e}_3$. Because of (2.8) it commutes with the so-called magnetic translation operators [14 to 17]

$$A_{\boldsymbol{R}} = \mathrm{e}^{i(\boldsymbol{t}, \boldsymbol{R})}\,. \tag{2.10}$$

The actual advantage of the quantities (2.6) is a partial separation of the problem as the kinetic energy does not contain $u_{(2)}$ or $v_{(2)}$ whereas the symmetry operators (2.10) are independent of $u_{(1)}$ or $v_{(1)}$. Therefore, it is useful to set up the Hilbert space $\mathfrak{H}$ of the problem as a product space $\mathfrak{H} = \mathfrak{H}'\times\mathfrak{H}''$, where $u_{(1)}$, $v_{(1)}$, and $\boldsymbol{\sigma}$ act only in $\mathfrak{H}'$ whereas $u_{(2)}$, $v_{(2)}$, $u_{(3)}$, $v_{(3)}$, and with them also $A_{\boldsymbol{R}}$ operate only in $\mathfrak{H}''$.

2.2 Magnetic translation group

The algebraic properties of the magnetic translation operators (2.10) are given by the product formula

$$A_{\boldsymbol{R}'}\,A_{\boldsymbol{R}} = \mathrm{e}^{(i/2)(\boldsymbol{R}'\times\boldsymbol{R}, \boldsymbol{b})}\,A_{\boldsymbol{R}'+\boldsymbol{R}} \tag{2.11}$$

following from (2.7) and (A1). The set of magnetic translation operators is not a group in the proper sense but only a group up to a factor. As is shown by Zak [16], it can be completed to a group by adding suitable phase factors. For convenience, we previously introduce periodic boundary conditions by the definition

$$A_{N\boldsymbol{R}}\,\psi = \psi \quad \text{for all} \quad \psi \in \mathfrak{H}'' \tag{2.12}$$

of the Hilbert space $\mathfrak{H}''$, where N is a (large) integer and $\boldsymbol{R}$ an arbitrary lattice vector. This definition implies a condition for the magnetic field. That is, $\mathfrak{H}''$ can only serve as a representation space for $A_{\boldsymbol{R}'}$ if both ψ and $A_{\boldsymbol{R}'}\,\psi$ are elements of $\mathfrak{H}''$ for any $\boldsymbol{R}'$. Since according to (2.11) and (2.12) $A_{N\boldsymbol{R}}\,A_{\boldsymbol{R}'}\,\psi = \mathrm{e}^{iN(\boldsymbol{R}\times\boldsymbol{R}', \boldsymbol{b})}\,A_{\boldsymbol{R}'}\,A_{N\boldsymbol{R}}\,\psi = \mathrm{e}^{iN(\boldsymbol{R}\times\boldsymbol{R}', \boldsymbol{b})}\,A_{\boldsymbol{R}'}\,\psi$, we must suppose $\mathrm{e}^{iN(\boldsymbol{R}\times\boldsymbol{R}', \boldsymbol{b})} = 1$ for any $\boldsymbol{R}$ and $\boldsymbol{R}'$. This is equivalent to the so-called rationality condition [15 to 17]

$$\boldsymbol{b} = \frac{e\,\boldsymbol{B}}{\hbar\,c} = \frac{2\,\pi}{\Omega_0}\,\frac{q}{p}\,\boldsymbol{R}_3 = \frac{1}{2\,\pi}\,\frac{q}{p}\,(\boldsymbol{K}_1\times\boldsymbol{K}_2) \tag{2.13}$$

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[2]) With respect to this coordinate system we write vectors as $\boldsymbol{a} = a_1\,\boldsymbol{e}_1 + a_2\,\boldsymbol{e}_2 + a_3\,\boldsymbol{e}_3 = (a_1, a_2, a_3)$.

[3]) Indices enclosed in brackets do not refer to vector components.

which we assume to be fulfilled in what follows. Ω_0 is the volume of the elementary cell of the lattice, q and p are relatively prime integers, p is a divisor of N, and $\boldsymbol{R}_3$ is the shortest lattice vector in any fixed direction. Obviously, (2.13) is no real restriction of generality.

We are now going to define the magnetic translation group. In addition to $\boldsymbol{R}_3$ we can always find two further lattice vectors $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$ so that $\boldsymbol{R}_1, \boldsymbol{R}_2, \boldsymbol{R}_3$ form a basis of the lattice and

$$\Omega_0 = (\boldsymbol{R}_1 \times \boldsymbol{R}_2, \boldsymbol{R}_3) . \tag{2.14}$$

The corresponding basis $\boldsymbol{K}_1, \boldsymbol{K}_2, \boldsymbol{K}_3$ of the reciprocal lattice is defined by $(\boldsymbol{R}_i, \boldsymbol{K}_j) = 2\pi\delta_{ij}$. The relation $\boldsymbol{R}_3 = (\Omega_0/4\pi^2)(\boldsymbol{K}_1 \times \boldsymbol{K}_2)$ is already used in (2.13). With respect to the basis $\boldsymbol{R}_1, \boldsymbol{R}_2, \boldsymbol{R}_3$ the arbitrary lattice vector $\boldsymbol{R}$ may be written as $\boldsymbol{R} = j\boldsymbol{R}_1 - k\boldsymbol{R}_2 - l\boldsymbol{R}_3$ (j, k, l integers). Instead of $A_{\boldsymbol{R}}$ we now define the new operators

$$A_0(\boldsymbol{R}) = \mathrm{e}^{-i\pi jkq/p} A_{\boldsymbol{R}} ; \quad \boldsymbol{R} = j\boldsymbol{R}_1 + k\boldsymbol{R}_2 + l\boldsymbol{R}_3 ; \quad j, k, l = 0, \ldots, N-1 . \tag{2.15}$$

Setting $\boldsymbol{R}' = j'\boldsymbol{R}_1 + k'\boldsymbol{R}_2 + l'\boldsymbol{R}_3$ and using (2.11), (2.13), and (2.14), we get the multiplication formula

$$A_0(\boldsymbol{R}')\, A_0(\boldsymbol{R}) = \mathrm{e}^{i2\pi j'kq/p} A_0(\boldsymbol{R} + \boldsymbol{R}') \tag{2.16}$$

which tells us that the product of two operators (2.15) is again such an operator multiplied by a p-th unit root. Because of this, the product of the set of the operators (2.15) and the cyclic group of the p-th unit roots is a group. That is to say, the operators

$$A_m(\boldsymbol{R}) = \mathrm{e}^{i2\pi mq/p} A_0(\boldsymbol{R}) ; \quad m = 0, \ldots, p-1 \tag{2.17}$$

form a group $\mathfrak{G}$ of pN^3 unitary transformations of the Hilbert space $\mathfrak{H}''$, the latter being defined by the periodic boundary condition (2.12) for rational magnetic fields (2.13) [18]. This group $\mathfrak{G}$ is called magnetic translation group. From (2.16) and (2.17) we have the multiplication rule

$$\begin{aligned} A_{m'}(\boldsymbol{R}')\, A_m(\boldsymbol{R}) &= A_{m+m'+j'k}(\boldsymbol{R} + \boldsymbol{R}') ; \quad \boldsymbol{R} = j\boldsymbol{R}_1 + k\boldsymbol{R}_2 + l\boldsymbol{R}_3 , \\ \boldsymbol{R}' &= j'\boldsymbol{R}_1 + k'\boldsymbol{R}_2 + l'\boldsymbol{R}_3 , \end{aligned} \tag{2.18}$$

where the indices of group elements are to be understood modulo p. The very simple structure of $\mathfrak{G}$ is reflected by the relations

$$\big(A_m(\boldsymbol{R})\big)^{-1} = A_{jk-m}(-\boldsymbol{R}) , \tag{2.19}$$

$$\big(A_m(\boldsymbol{R})\big)^{-1} A_{m'}(\boldsymbol{R}')\, A_m(\boldsymbol{R}) = A_{m'+j'k-k'j}(\boldsymbol{R}') , \tag{2.20}$$

$$\big(A_{m'}(\boldsymbol{R}')\big)^{-1} \big(A_m(\boldsymbol{R})\big)^{-1} A_{m'}(\boldsymbol{R}')\, A_m(\boldsymbol{R}) = A_{j'k-k'j}(\boldsymbol{O}) \tag{2.21}$$

which are simple consequences of (2.18). According to (2.21), the p elements $A_m(\boldsymbol{O})$ are the commutator subgroup $\mathfrak{G}_0$ of $\mathfrak{G}$ [25]. The Abelian factor group $\mathfrak{G}/\mathfrak{G}_0$ has the order N^3 and is isomorphic to the ordinary translation group of the crystal. Therefore, the magnetic translation group $\mathfrak{G}$ is a covering group of the ordinary translation group extended by $\mathfrak{G}_0$ [25]. From (2.18) and (2.20) we see that the operators belonging to each one-, two-, or three-dimensional "sublattice" form normal subgroups of $\mathfrak{G}$. Especially, the operators $A_m(\tilde{\boldsymbol{R}})$ with $\tilde{\boldsymbol{R}} = j j_0 \boldsymbol{R}_1 + k k_0 \boldsymbol{R}_2 + l\boldsymbol{R}_3$ and $j_0 k_0 = p$ form an Abelian normal subgroup $\mathfrak{F}$ of order N^3 and index p. $\mathfrak{F}$ contains the Abelian subgroup of the opera-

tors $A_0(\widetilde{\boldsymbol{R}})$. In the following we always choose $j_0 = 1$ and $k_0 = p$ so that

$$\widetilde{\boldsymbol{R}} = j\,\boldsymbol{R}_1 + k\,p\,\boldsymbol{R}_2 + l\,\boldsymbol{R}_3\,. \tag{2.22}$$

Then, the arrangement of $\mathfrak{G}$ in cosets of $\widetilde{\mathfrak{T}}$ [16] is given by

$$\mathfrak{G} = \widetilde{\mathfrak{T}} + A_0(\boldsymbol{R}_2)\,\widetilde{\mathfrak{T}} + A_0(2\,\boldsymbol{R}_2)\,\widetilde{\mathfrak{T}} + \cdots + A_0\left((p-1)\,\boldsymbol{R}_2\right)\widetilde{\mathfrak{T}}\,. \tag{2.23}$$

2.3 Irreducible representations

Using the concept of little groups [25, 26], the irreducible standard representations of $\mathfrak{G}$ [15, 16, 18] can easily be constructed from the N^3 one-dimensional representations of $\widetilde{\mathfrak{T}}$, which are immediately given by

$$\left.\begin{aligned} &\Delta^{\boldsymbol{k},r}\left(A_m(\widetilde{\boldsymbol{R}})\right) = \mathrm{e}^{i\,2\pi\,m\,r\,q/p}\,\mathrm{e}^{i(\boldsymbol{k},\widetilde{\boldsymbol{R}})}\,;\\ &\boldsymbol{k} = \frac{1}{N}\left(n_1\,\boldsymbol{K}_1 + n_2\,\boldsymbol{K}_2 + n_3\,\boldsymbol{K}_3\right)\,; \quad n_1, n_3 = 0, \ldots, N-1\,;\\ &n_2 = 0, \ldots, \frac{N}{p} - 1\,; \quad r = 0, \ldots, p-1\,. \end{aligned}\right\} \tag{2.24}$$

We determine the little groups of the representations (2.24) by sorting out all the elements $A_{m'}(\boldsymbol{R}')$ with $\boldsymbol{R}' = j'\,\boldsymbol{R}_1 + k'\,\boldsymbol{R}_2 + l'\,\boldsymbol{R}_3$ for which the conjugate representations (see (2.20) and (2.22))

$$\begin{aligned} \Delta^{\boldsymbol{k},r}\left[\left(A_{m'}(\boldsymbol{R}')\right)^{-1} A_m(\widetilde{\boldsymbol{R}})\,A_{m'}(\boldsymbol{R}')\right] &= \Delta^{\boldsymbol{k},r}\left(A_{m+jk'}(\widetilde{\boldsymbol{R}})\right) = \mathrm{e}^{i\,2\pi\,(m+jk')\,r\,q/p}\,\mathrm{e}^{i(\boldsymbol{k},\widetilde{\boldsymbol{R}})} = \\ &= \mathrm{e}^{i\,2\pi\,m\,r\,q/p}\,\mathrm{e}^{i\,(\boldsymbol{k}+k'\,r(q/p)\,\boldsymbol{K}_1,\,\widetilde{\boldsymbol{R}})} = \Delta^{\boldsymbol{k}+k'\,r(q/p)\,\boldsymbol{K}_1,\,r}\left(A_m(\widetilde{\boldsymbol{R}})\right) \end{aligned} \tag{2.25}$$

are equal to the original ones (2.24). That is obviously the case only then if $k'\,r$ is a multiple of p. We distinguish three cases:

a) If $r = 0$, k' can be arbitrary, i.e. the little group of $\Delta^{\boldsymbol{k},0}\left(A_m(\widetilde{\boldsymbol{R}})\right)$ is $\mathfrak{G}$ itself. The corresponding allowable representations of $\mathfrak{G}$ [25, 26] are the N^3 one-dimensional representations $\mathrm{e}^{i(\boldsymbol{k},\boldsymbol{R})}$ that are given by the homomorphism of the ordinary translation group to $\mathfrak{G}$.

b) If r and p have a common divisor d, k' must be a multiple of p/d, i.e. the corresponding little groups are smaller than $\mathfrak{G}$ and larger than $\widetilde{\mathfrak{T}}$. They form a composition series from $\widetilde{\mathfrak{T}}$ to $\mathfrak{G}$ according to the prime factorization of p. The irreducible representations deriving from these little groups could be constructed step by step. But fortunately, they are physically meaningless as we shall indirectly show further below.

c) If r is prime to p, k' must be a multiple of p, i.e. the corresponding little group is $\widetilde{\mathfrak{T}}$ itself (cf. (2.22)). Its allowable representations (2.24) induce the irreducible representations we need. As we learn from (2.25), the orbits of $\widetilde{\mathfrak{T}}$ relative to $\mathfrak{G}$ [25, 26] consist of the p representations $\Delta^{\boldsymbol{k}+k\,r\,(q/p)\,\boldsymbol{K}_1,\,r}$, where $k = 0, \ldots, p-1$. Since in (2.25) the p vectors $\boldsymbol{k} + k\,r\,(q/p)\,\boldsymbol{K}_1$ are equivalent (mod $\boldsymbol{K}_1$) to $\boldsymbol{q} + (k''/p)\,\boldsymbol{K}_1$ ($k'' = 0, \ldots, p-1$), the different orbits may be characterized by the vector

$$\begin{aligned} \boldsymbol{q} = \frac{1}{N}\left(n_1\,\boldsymbol{K}_1 + n_2\,\boldsymbol{K}_2 + n_3\,\boldsymbol{K}_3\right)\,; \quad n_1, n_2 = 0, \ldots, \frac{N}{p} - 1\,;\\ n_3 = 0, \ldots, N-1\,. \end{aligned} \tag{2.26}$$

In difference to k, q is reduced to a zone $\mathfrak{Z}$ defined by the vectors $(1-p)\,\boldsymbol{K}_1$, $(1-p)\,\boldsymbol{K}_2$, $\boldsymbol{K}_3$, which we call magnetic Brillouin zone.[4]) We now put $\boldsymbol{R} = \widetilde{\boldsymbol{R}} + n\,\boldsymbol{R}_2$ $(n = 0, \ldots, p-1)$, select the representation $\mathfrak{D}^{q,r}$ from each orbit, and determine the p-dimensional induced representations of $\mathfrak{G}$ [25, 26] by using (2.18), (2.19), and (2.23). The result is

$$D^{q,r}_{s,t}\big(A_m(\widetilde{\boldsymbol{R}} + n\,\boldsymbol{R}_2)\big) = \mathrm{e}^{i\,2\pi\,m\,r\,q/p}\,\mathrm{e}^{i(\boldsymbol{q}+s(q/p)\boldsymbol{K}_2)\widetilde{\boldsymbol{R}}}\,\delta_{s,(t+n)_p}\,; \quad s,t,n = 0,\ldots,p-1\,, \tag{2.27}$$

where $\boldsymbol{q}$ and $\widetilde{\boldsymbol{R}}$ are given by (2.26) and (2.22) respectively, and r is prime to p. $(t+n)_p$ means: reduce $t+n$ modulo p so that $0 \leqq (t+n)_p \leqq p-1$.

If p is a prime number, case b) disappears. Then, the representations (2.27) combined with the one-dimensional representations (case a)) form the whole system of irreducible representations of $\mathfrak{G}$. We now want to show that among all the irreducible representations of $\mathfrak{G}$ only (2.27) with $r = 1$ gives rise to non-vanishing projection operators [26]. From (2.27) and (2.17) we find

$$P^{q,r}_{s} = \frac{p}{p\,N^3}\sum_{m=0}^{p-1}\sum_{\widetilde{\boldsymbol{R}}}\big[D^{q,r}_{s,s}\big(A_m(\widetilde{\boldsymbol{R}})\big)\big]^{*}\,A_m(\boldsymbol{R}) = \delta_{r,1}\,\frac{p}{N^3}\sum_{\widetilde{\boldsymbol{R}}}\mathrm{e}^{\;i(\boldsymbol{q}\,+\,s(q/p)\boldsymbol{K}_2)\widetilde{\boldsymbol{R}}}\,A_0(\widetilde{\boldsymbol{R}})\,, \tag{2.28}$$

i.e. $P^{q,r}_{s} = 0$ if $r \neq 1$. Since the decomposition of the identity

$$\sum_{s=0}^{p-1}\sum_{\boldsymbol{q}} P^{q,1}_{s} = A_0(\boldsymbol{O}) = 1$$

is given by the $P^{q,1}_{s}$ alone, the projection operators derived from the irreducible representations of the cases a) and b) must also be zero.

2.4 General structure of the wave functions

We are now in a position to construct partner functions belonging to the s-th row of (2.27) by application of the projection operators $P^{q,1}_{s}$ to an appropriate basis of the Hilbert space $\mathfrak{H}''$. By definition, the elements of $\mathfrak{H}''$ depend on two independent variables. We choose the 1- and 3-component $u_{(2)}$ and $u_{(3)}$ of $\boldsymbol{s}$ and denote the projections of $\boldsymbol{s}$ and $\boldsymbol{t}$ on the 1, 3 plane by

$$\bar{\boldsymbol{s}} = \lambda(u_{(2)}, 0, u_{(3)})\,, \qquad \bar{\boldsymbol{t}} = (v_{(2)}, 0, v_{(3)})\,. \tag{2.29}$$

The orientation of the 3-axis of the Cartesian coordinate system in the lattice is already fixed by (2.13). For convenience, we put the 2-axis parallel to $\boldsymbol{K}_2$

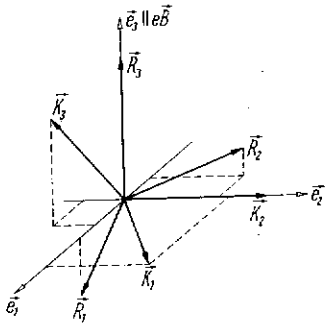

Fig. 1. Orientation of the Cartesian coordinate system relative to the bases $\boldsymbol{R}_1, \boldsymbol{R}_2, \boldsymbol{R}_3$ and $\boldsymbol{K}_1, \boldsymbol{K}_2, \boldsymbol{K}_3$ of the direct and the reciprocal lattice

[4]) It is quite instructive to visualize the geometrical shape of magnetic Brillouin zones. Because of (2.13), typically $p/q \approx (10^8 \ldots 10^9)/(B/G)$. Assuming $\boldsymbol{B}$ parallel to the c-axis of a hexagonal metal, $B = 10^5$ G, and $q = 1$, $\mathfrak{Z}$ looks like a very long pencil aligned with $\boldsymbol{B}$ which is about 10^3 or 10^4 times longer than thick.

so that, as shown in Fig. 1, the 1, 3 plane coincides with the $\boldsymbol{R}_1, \boldsymbol{R}_3$ plane of the lattice. This geometry is also reflected by the useful relations

$$\boldsymbol{K}_1 = \frac{2\pi}{\Omega_0}(\boldsymbol{R}_2 \times \boldsymbol{R}_3) = \frac{1}{\lambda}\frac{p}{q}(R_{22}\boldsymbol{e}_1 - R_{21}\boldsymbol{e}_2), \quad \boldsymbol{K}_2 = \frac{2\pi}{\Omega_0}(\boldsymbol{R}_3 \times \boldsymbol{R}_1) = \frac{1}{\lambda}\frac{p}{q}R_{11}\boldsymbol{e}_2 \tag{2.30}$$

resulting from (2.13). In the following we mark all the vectors that are defined in the 1, 3 plane by an upper cross bar, e.g. the lattice vectors $\bar{\boldsymbol{R}} = j\boldsymbol{R}_1 + l\boldsymbol{R}_3$ and the projections $\bar{\boldsymbol{K}}$ of reciprocal lattice vectors $\boldsymbol{K}$ on the 1, 3 plane, where $(\bar{\boldsymbol{R}}, \bar{\boldsymbol{K}}) = 2\pi l$. Now, the operators $A_0(\tilde{\boldsymbol{R}}) = A_0(\boldsymbol{R} + k\,p\,\boldsymbol{R}_2)$ defined by (2.15), (2.22), (2.10) may be rewritten as

$$A_0(\tilde{\boldsymbol{R}}) = \mathrm{e}^{(i/2)k^2(\boldsymbol{K}_0,\boldsymbol{R}_0)}\,\mathrm{e}^{ik(\bar{\boldsymbol{K}}_0,\boldsymbol{s})}\,\mathrm{e}^{i(\boldsymbol{t},\boldsymbol{R}+k\boldsymbol{R}_0)},$$

where $\boldsymbol{R}_0 = p\boldsymbol{R}_2$, $\boldsymbol{K}_0 = q\boldsymbol{K}_1$, and (A 1), (2.7), (2.29), and (2.30) are used. Before inserting them into (2.28), we pass over to the limit $N \to \infty$ of an infinite normalization volume. Then, the vector $\boldsymbol{q}$ varies continuously in the magnetic Brillouin zone $\mathscr{Z}$ and the normalization factor N^{-3} in front of (2.28) is to be replaced by $\Omega_0/(2\pi)^3$. Thus,

$$P_s^{\boldsymbol{q},1} = \frac{p\,\Omega_0}{(2\pi)^3}\sum_{k=-\infty}^{+\infty}\sum_{\bar{\boldsymbol{R}}}\mathrm{e}^{-i(\boldsymbol{q}+(s/p)\boldsymbol{K}_0,\bar{\boldsymbol{R}}+k\boldsymbol{R}_0)}\,\mathrm{e}^{(i/2)k^2(\bar{\boldsymbol{K}}_0,\boldsymbol{R}_0)}\,\mathrm{e}^{ik(\bar{\boldsymbol{K}}_0,\bar{\boldsymbol{s}})}\,\mathrm{e}^{i(\bar{\boldsymbol{t}},\bar{\boldsymbol{R}}+k\boldsymbol{R}_0)}. \tag{2.31}$$

After having performed the limit process $N \to \infty$, we can span the Hilbert space $\mathfrak{H}''$ by the complete system of plane waves

$$\frac{1}{2\pi}\mathrm{e}^{i(\boldsymbol{q}+s(q/p)\bar{\boldsymbol{K}}_3+\bar{\boldsymbol{K}},\bar{\boldsymbol{s}})}; \qquad s = 0, \ldots, p-1. \tag{2.32}$$

Operating with (2.31) on these basis vectors of $\mathfrak{H}''$, we obtain a set of functions that partly depend linearly on each other. It is not difficult, however, to sort out a complete set of orthonormal partner functions if in (2.32) $\boldsymbol{K} = \boldsymbol{K}_\mathrm{r} + \boldsymbol{K}_\mathrm{c}$ is split into the reduced part $\boldsymbol{K}_\mathrm{r} = j\boldsymbol{K}_1 + m\boldsymbol{K}_3$ $(j = 0, \ldots, q-1)$ and the complementary part $\boldsymbol{K}_\mathrm{c} = k\,q\,\boldsymbol{K}_1 + l\boldsymbol{K}_2$. This is outlined in [18]. Including a convenient phase factor, which makes further results a little more shapely, we obtain the partner functions [19]

$$\varphi_{\boldsymbol{q}s}(\boldsymbol{K}_\mathrm{r};\bar{\boldsymbol{s}}) = \mathrm{e}^{-i(\lambda/2)(q_1q_2+2K_{\mathrm{r}1}q_2+K_{\mathrm{r}1}K_{\mathrm{r}2})} \times$$
$$\times\left(\frac{p}{K_{22}}\right)^{1/2}\sum_{k=-\infty}^{-\infty}\mathrm{e}^{-(i/2)(k+s/p)^2R_{02}K_{02}}\,\mathrm{e}^{-i(k+s/p)(q_2+K_{\mathrm{r}2})R_{02}}\frac{1}{2\pi}\mathrm{e}^{i(\bar{\boldsymbol{q}}+\bar{\boldsymbol{K}}_\mathrm{r}+(k+s/p)\bar{\boldsymbol{K}}_0,\bar{\boldsymbol{s}})}. \tag{2.33}$$

The indices 1, 2 denote Cartesian components of the corresponding vectors, and $\bar{\boldsymbol{q}}, \bar{\boldsymbol{K}}_\mathrm{r}, \bar{\boldsymbol{K}}_0$ are the projections of $\boldsymbol{q}, \boldsymbol{K}_\mathrm{r}, \boldsymbol{K}_0$ on the 1, 3 plane. By construction, these functions have the properties

$$(\varphi_{\boldsymbol{q}'s'}(\boldsymbol{K}'_\mathrm{r};\bar{\boldsymbol{s}})\,|\varphi_{\boldsymbol{q}s}(\boldsymbol{K}_\mathrm{r};\bar{\boldsymbol{s}})) = \delta(\boldsymbol{q}'-\boldsymbol{q})\,\delta_{s's}\,\delta_{\boldsymbol{K}'_\mathrm{r}\boldsymbol{K}_\mathrm{r}} \tag{2.34}$$

and

$$A_0(\tilde{\boldsymbol{R}})\,\varphi_{\boldsymbol{q}s} = \mathrm{e}^{i(\boldsymbol{q}+(s/p)\boldsymbol{K}_0,\tilde{\boldsymbol{R}})}\,\varphi_{\boldsymbol{q}s}. \tag{2.35}$$

The p functions $\varphi_{\boldsymbol{q}s}(\boldsymbol{K}_\mathrm{r};\bar{\boldsymbol{s}})$ $(s = 0, \ldots, p-1)$ span the p-dimensional irreducible subspaces of $\mathfrak{H}''$. In each of these invariant subspaces they generate one of the irreducible representations (2.27) which do not depend on $\boldsymbol{K}_\mathrm{r}$. Therefore, the eigenfunctions of the Hamiltonian (2.9) can be written as linear combinations

of the functions $q_{\boldsymbol{q}s}(\boldsymbol{K}_\mathrm{r}; \boldsymbol{s})$ with respect to $\boldsymbol{K}_\mathrm{r}$, the (spinor) coefficients of which depend on the variable $u_{(1)}$, and a related quantum number $\varkappa$ according to the product formation $\tilde{\mathfrak{H}} = \tilde{\mathfrak{H}}' \otimes \tilde{\mathfrak{H}}''$ of the Hilbert space. With regard to further considerations we put them without loss of generality in a specified form and write [18, 19]

$$\psi_{\varkappa \boldsymbol{q} s}(u_{(1)}, \boldsymbol{s}) = \sum_{\boldsymbol{K}_\mathrm{r}} \mathrm{e}^{i(\boldsymbol{w} - \boldsymbol{q}, \boldsymbol{K}_\mathrm{r} - \lambda)} C_{\varkappa \boldsymbol{q}}(\boldsymbol{K}_\mathrm{r}; u_{(1)})\, q_{\boldsymbol{q}s}(\boldsymbol{K}_\mathrm{r}; \boldsymbol{s}) . \tag{2.36}$$

This relation expresses the translational symmetry of the Bloch electron in a magnetic field. We can look upon it as an analogy to Bloch's theorem all the more since, as a result of (2.35),

$$A_0(\tilde{\boldsymbol{R}})\, \psi_{\varkappa \boldsymbol{q} s} = \mathrm{e}^{i(\boldsymbol{q} + (s/p)\boldsymbol{K}_0, \tilde{\boldsymbol{R}})}\, \psi_{\varkappa \boldsymbol{q} s} . \tag{2.37}$$

It is fundamental to all further considerations.

2.5 Schrödinger equation

The unknown (spinor) functions $C_{\varkappa \boldsymbol{q}}(\boldsymbol{K}_\mathrm{r}; u_{(1)})$ are determined by the Schrödinger equation

$$H\, \psi_{\varkappa \boldsymbol{q} s} = \mathscr{E}_\varkappa(\boldsymbol{q})\, \psi_{\varkappa \boldsymbol{q} s} \tag{2.38}$$

with the Hamiltonian (2.9) and the normalization condition

$$\sum_{\boldsymbol{K}_\mathrm{r}} \int_{-\infty}^{+\infty} C^*_{\varkappa' \boldsymbol{q}}(\boldsymbol{K}_\mathrm{r}; u_{(1)})\, C_{\varkappa \boldsymbol{q}}(\boldsymbol{K}_\mathrm{r}; u_{(1)})\, \mathrm{d}u_{(1)} \equiv \langle C_{\varkappa' \boldsymbol{q}} \mid C_{\varkappa \boldsymbol{q}} \rangle = \delta_{\varkappa' \varkappa} . \tag{2.39}$$

Since the Hilbert space $\tilde{\mathfrak{H}}$ divides into p-dimensional invariant subspaces the energy values $\mathscr{E}_\varkappa(\boldsymbol{q})$ are p-fold degenerate, i.e. they are independent of the quantum number s. (2.38) is equivalent to the Schrödinger equation

$$\sum_{\boldsymbol{K}_\mathrm{r}} H_{\boldsymbol{q}}(\boldsymbol{K}'_\mathrm{r}, \boldsymbol{K}_\mathrm{r})\, C_{\varkappa \boldsymbol{q}}(\boldsymbol{K}_\mathrm{r}; u_{(1)}) = \mathscr{E}_\varkappa(\boldsymbol{q})\, C_{\varkappa \boldsymbol{q}}(\boldsymbol{K}'_\mathrm{r}; u_{(1)}) \tag{2.40}$$

for $C_{\varkappa \boldsymbol{q}}(\boldsymbol{K}_\mathrm{r}; u_{(1)})$, where

$$H_{\boldsymbol{q}}(\boldsymbol{K}'_\mathrm{r}; \boldsymbol{K}_\mathrm{r}) = \frac{\hbar^2}{2m} [(\tilde{\boldsymbol{w}} + \boldsymbol{K}'_\mathrm{r})^2 - (\boldsymbol{\sigma}, \boldsymbol{b})]\, \delta_{\boldsymbol{K}'_\mathrm{r} \boldsymbol{K}_\mathrm{r}} +$$

$$+ \left[1 + \frac{i\hbar^2}{4 m^2 c^2} (\tilde{\boldsymbol{w}} + \boldsymbol{K}'_\mathrm{r}, \boldsymbol{\sigma} \times (\boldsymbol{K}'_\mathrm{r} - \boldsymbol{K}_\mathrm{r} - i \nabla_{\boldsymbol{q}} \times \boldsymbol{b}))\right] V_{\boldsymbol{q}}(\boldsymbol{K}'_\mathrm{r}, \boldsymbol{K}_\mathrm{r}) , \tag{2.41}$$

$$V_{\boldsymbol{q}}(\boldsymbol{K}'_\mathrm{r}, \boldsymbol{K}_\mathrm{r}) = \sum_{\boldsymbol{K}_\mathrm{c}} V_{\boldsymbol{K}'_\mathrm{r} - \boldsymbol{K}_\mathrm{r} - \boldsymbol{K}_\mathrm{c}}\, \mathrm{e}^{i(\boldsymbol{q}, \boldsymbol{K}_\mathrm{c} \times \lambda)}\, B_0^+(\boldsymbol{K}_\mathrm{c}) , \tag{2.42}$$

and $\tilde{\boldsymbol{w}} = (u_{(1)}, v_{(1)}, q_3)$. $\boldsymbol{K}_\mathrm{r} = j \boldsymbol{K}_1 + m \boldsymbol{K}_3$ $(j = 0, \ldots, q-1)$ and $\boldsymbol{K}_\mathrm{c} = k \boldsymbol{K}_0 + l \boldsymbol{K}_2$ $(\boldsymbol{K}_0 = q \boldsymbol{K}_1)$ are the reduced and the complementary part of $\boldsymbol{K}$. For details of the derivation the reader may be referred to [19]. As a consequence of (A 4) and (2.13) the unitary operators

$$B_0(\boldsymbol{K}_\mathrm{c}) = \mathrm{e}^{i\pi klp}\, \mathrm{e}^{i(\boldsymbol{w}, \boldsymbol{K}_\mathrm{c} \times \lambda)} \tag{2.43}$$

form an Abelian group:

$$B_0(\boldsymbol{K}'_\mathrm{c})\, B_0(\boldsymbol{K}_\mathrm{c}) = B_0(\boldsymbol{K}'_\mathrm{c} + \boldsymbol{K}_\mathrm{c}) . \tag{2.44}$$

It should be noted that the vectors $\boldsymbol{K}_\mathrm{c} \times \boldsymbol{\lambda}$ form a "sublattice" of the orbit lattice Pippard has introduced in [27]. It is set up by the operators $B_0(\boldsymbol{K}_\mathrm{c})$ just as the crystal lattice by ordinary translations. In a plane perpendicular to the field (defined by $q_3 + K_{\mathrm{r}3}$) there are q parallel-shifted orbit sublattices that are distinguished by $\boldsymbol{K}_{\mathrm{r}1}$. Altogether they form Pippard's orbit lattice. The elec-

tronic motion over an orbit sublattice is described by $C_{\alpha q}(\boldsymbol{K}_r; u_{(1)})$. The coupling between different orbit sublattices is due to the non-diagonal elements of $\Gamma_q(\boldsymbol{K}_r', \boldsymbol{K}_r)$.

The Schrödinger equation (2.40) is an infinite system of ordinary differential-difference equations. We now want to show it to be equivalent to a system of ordinary differential equations with subsidiary conditions. To this end we multiply (2.40) from the left by $e^{i(\boldsymbol{q}, \boldsymbol{K}_c \times \lambda)} B_c^-(\boldsymbol{K}_c')$, apply (2.44) and (A 2), define

$$C_{\alpha q}^{\boldsymbol{K}}(u_{(1)}) = e^{i(\boldsymbol{q}, \boldsymbol{K}_c \times \lambda)} B_0^+(\boldsymbol{K}_c)\, C_{\alpha q}(\boldsymbol{K}_r; u_{(1)}), \tag{2.45}$$

and obtain

$$\left[\frac{\hbar^2}{2m}(\tilde{\boldsymbol{w}} - \boldsymbol{K}')^2 - \frac{\hbar^2}{2m}(\boldsymbol{\sigma}, \boldsymbol{b}) - \mathscr{E}_\alpha(\boldsymbol{q})\right] C_{\alpha q}^{\boldsymbol{K}'} +$$

$$+ \sum_{\boldsymbol{K}} V_{\boldsymbol{K}'-\boldsymbol{K}}\left[1 + i\frac{\hbar^2}{4m^2e^2}(\tilde{\boldsymbol{w}} + \boldsymbol{K}', \boldsymbol{\sigma} \times (\boldsymbol{K}' - \boldsymbol{K}))\right] C_{\alpha q}^{\boldsymbol{K}} = 0. \tag{2.46}$$

We interpret the definition (2.45) in the shape of

$$B_0(\boldsymbol{K}_c)\, C_{\alpha q}^{\boldsymbol{K}_r + \boldsymbol{K}_c} = e^{i(\boldsymbol{q}, \boldsymbol{K}_c \times \lambda)} C_{\alpha q}^{\boldsymbol{K}_r} \tag{2.47}$$

as subsidiary condition of (2.46). That is to say, those solutions of (2.46) that fulfil (2.47) are just the solutions $C_{\alpha q}(\boldsymbol{K}_r; u_{(1)}) \equiv C_{\alpha q}^{\boldsymbol{K}_r}(u_{(1)})$ of (2.40). Since (2.46) is in fact independent of $\boldsymbol{q}$, the dependence of the solutions we are looking for exclusively arises from (2.47). Equation (2.46) displays a close formal analogy to the Schrödinger equation for the Fourier components of Bloch functions. The latter changes into (2.46) when the c-number $\boldsymbol{k}$-vector is replaced by the operator $\tilde{\boldsymbol{w}} = (u_{(1)}, v_{(1)}, q_3)$. Therefore, (2.46) is the starting-point of deriving effective Hamiltonians in the third Section.

2.6 Magnetic energy bands

The p-fold degenerate energy eigenvalues $\mathscr{E}_\alpha(\boldsymbol{q})$ can be arranged in a magnetic energy band scheme. Some of its main characteristics shall now be derived. By means of (2.13) we realize the periodicity

$$H_{\boldsymbol{q}}(\boldsymbol{K}_r', \boldsymbol{K}_r) = H_{\boldsymbol{q} + (1/p)\boldsymbol{K}_c}(\boldsymbol{K}_r', \boldsymbol{K}_r) \tag{2.48}$$

of the Hamiltonian (2.41). As a result we have

$$\mathscr{E}_\alpha(\boldsymbol{q}) = \mathscr{E}_\alpha\left(\boldsymbol{q} + \frac{1}{p}\boldsymbol{K}_c\right). \tag{2.49}$$

In particular $\mathscr{E}_\alpha(\boldsymbol{q}) = \mathscr{E}_\alpha(\boldsymbol{q} + (q/p)\boldsymbol{K}_1)$, that is, one period extends over q magnetic Brillouin zones $\mathscr{Z}$ in the direction of $\boldsymbol{K}_1$. The reduction of a given energy function to one zone $\mathscr{Z}$ yields q different branches within $\mathscr{Z}$. This reduction may be performed by displacing branches of the extended energy function by appropriate multiples of $(1/p)\boldsymbol{K}_1$. More convenient is, however, the following way of reduction (Fig. 2): The full range of values of the extended energy function can be represented by $\mathscr{E}_\alpha(\boldsymbol{q} + n\boldsymbol{K}_1)$ where $\boldsymbol{q}$ is restricted to $\mathscr{Z}$ and $n = 0, \ldots, q-1$. We now label the magnetic energy values by $\alpha \equiv \mu, n$ like this:

$$\mathscr{E}_\alpha(\boldsymbol{q}) \equiv \mathscr{E}_{\mu n}(\boldsymbol{q}); \quad \mathscr{E}_{\mu n}(\boldsymbol{q}) = \mathscr{E}_{\mu 0}(\boldsymbol{q} + n\boldsymbol{K}_1), \tag{2.50}$$

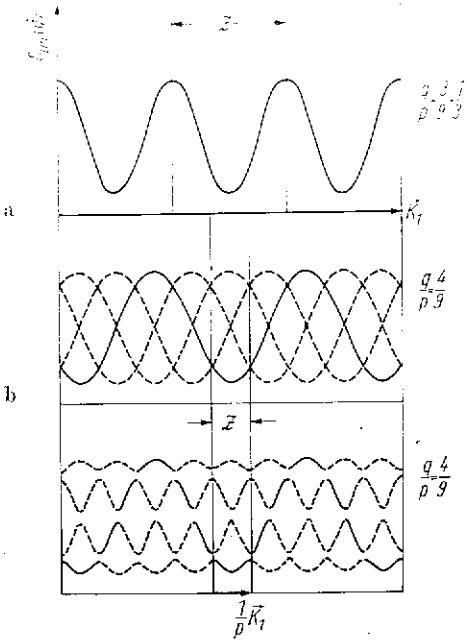

Fig. 2. Splitting of a magnetic energy band into q subbands. a) Single energy band for $q = 1$. b) In case of uncoupled orbit sublattices the reduction (2.50) of the continuous extended energy function (full line) to the magnetic Brillouin zone $\mathcal{E}$ gives overlapping subbands (dashed lines) within $\mathcal{E}$. c) Coupling of the q orbit sublattices makes the extended energy function (full line) discontinuous so as to separate the q reduced subbands by gaps

where μ is the magnetic band index, which corresponds to the Landau quantum number in case of free electrons. Thus, a magnetic energy band μ (in simple cases a broadened Onsager level) consists of q subbands $\mathcal{E}_{\mu n}(\boldsymbol{q})$ ($n = 0, \ldots, q-1$). We now discuss the curious dependence of the energy spectrum on the integers q and p, which spasmodically change with their ratio q/p (i.e. the field strength) varying continuously. In the simple case $q = 1$ we have only one orbit lattice in a plane perpendicular to the field. One of the corresponding energy bands may be given by Fig. 2a. Supposing we have q ($q > 1$) uncoupled orbit sublattices. Then, the extended energy function is continuous and resembles the one with $q = 1$. The reduction (2.50) gives q overlapping subbands, each of them belonging to one of the orbit sublattices (Fig. 2b). When the coupling between the orbit sublattices is turned on, gaps arise at the boundaries of magnetic Brillouin zones, and the extended energy function becomes discontinuous (Fig. 2c). The reduction (2.50) provides the q subbands with gaps at the crossings of Fig. 2b. It would be well to label the subbands by a new index according to increasing energy instead of using n which refers to the extended scheme. Nevertheless, we continue to use n because this is the only possibility of producing the subband splitting analytically. Thus, the level structure sensitively depends on q. The subbands of a magnetic energy band become narrower with increasing q, where the central ones appear to be broader than the outer ones. The main effect of the splitting of a magnetic energy band into q subbands is probably a lowering of the mean electron velocity (2.57), which is largest in case of $q = 1$. This suggests the appearance of "zone" oscillations [28] in the B^{-1} dependence of galvanomagnetic effects since, according to (2.13), $q = 1$ occurs with the period $\Delta\lambda = 2\pi/|\boldsymbol{K}_1 \times \boldsymbol{K}_2|$.

A (zero-field) Bloch band splits into $[p/q]$ magnetic energy bands, where $[p/q]$ is the largest integer smaller than p/q. This may be seen as follows. On periodic boundary conditions a Bloch band (i.e. a Brillouin zone) comprises N^3 states. A magnetic Brillouin zone contains N^3/p^2 p-fold degenerating states, i.e. N^3/p different states. Hence, within the energy range of a Bloch band we have p subbands, which are clustered in $[p/q]$ magnetic energy bands. This can be shown also by taking the absolute value of (2.13): $2\pi(p/q)\,|e|B/\hbar\,c = |\boldsymbol{K}_1 \times \boldsymbol{K}_2|$ is the cross-sectional area of the Brillouin zone perpendicular to $\boldsymbol{B}$. If all the orbits of the Bloch band in question are closed, Onsager's quantization rule tells

us that $|p\,q|$ is the total number of discrete energy levels within this band. This assertion is not quite strict. It fails, of course, if interband coupling (magnetic breakdown) plays a role. These general conclusions are confirmed by model calculations of magnetic energy bands [29 to 32].

Just as the subbands of a magnetic energy band, the corresponding wave functions are also related to each other. From (2.33) we derive the relation

$$\varphi_{\boldsymbol{q}+n\boldsymbol{K}_1,s}(\boldsymbol{K}_\mathrm{r};\bar{\boldsymbol{s}}) = \mathrm{e}^{-(i/2)(\boldsymbol{q}\times n\boldsymbol{K}_1,\lambda)}\,\mathrm{e}^{-(i/2)(\boldsymbol{K}_\mathrm{r}'+(k_0-n/q)\boldsymbol{K}_0,\lambda)}\,\varphi_{\boldsymbol{q}s}(\boldsymbol{K}_\mathrm{r}';\bar{\boldsymbol{s}})\,, \tag{2.51}$$

where $\boldsymbol{K}_\mathrm{r}' = (\boldsymbol{K}_\mathrm{r} + n\,\boldsymbol{K}_1)_\mathrm{r} = \boldsymbol{K}_\mathrm{r} + n\,\boldsymbol{K}_1 - k_0\,\boldsymbol{K}_0$, i.e. the integer k_0 is so determined as to make $\boldsymbol{K}_\mathrm{r}'$ a reduced reciprocal lattice vector. Combining (2.51) and (2.36) and using (A 4), we get

$$\psi_{\mu,0,\boldsymbol{q}+n\boldsymbol{K}_1,s}(u_{(1)},\bar{\boldsymbol{s}}) = \mathrm{e}^{-(i/2)(\boldsymbol{q}\times n\boldsymbol{K}_1,\lambda)}\sum_{\boldsymbol{K}_\mathrm{r}'}\mathrm{e}^{i(n\boldsymbol{c}-\boldsymbol{q},\boldsymbol{K}_\mathrm{r}'\times\lambda)}\,\mathrm{e}^{i(n\boldsymbol{c}-\boldsymbol{q},(k_0-n/q)\boldsymbol{K}_0\times\lambda)}\times$$
$$\times\, C_{\mu,0,\boldsymbol{q}+n\boldsymbol{K}_1}(\boldsymbol{K}_\mathrm{r}' - n\,\boldsymbol{K}_1 + k_0\,\boldsymbol{K}_0;u_{(1)})\;\varphi_{\boldsymbol{q}s}(\boldsymbol{K}_\mathrm{r}';\bar{\boldsymbol{s}})\,.$$

We interpret this result by setting up the relations

$$\psi_{\mu,0,\boldsymbol{q}+n\boldsymbol{K}_1,s}(u_{(1)},\bar{\boldsymbol{s}}) = \mathrm{e}^{-(i/2)(\boldsymbol{q}\times n\boldsymbol{K}_1,\lambda)}\;\psi_{\mu n\boldsymbol{q}s}(u_{(1)};\bar{\boldsymbol{s}})\,, \tag{2.52}$$

$$C_{\mu n\boldsymbol{q}}(\boldsymbol{K}_\mathrm{r};u_{(1)}) = \mathrm{e}^{i(n\boldsymbol{c}-\boldsymbol{q},(k_0-n/q)\boldsymbol{K}_0\times\lambda)}\,C_{\mu,0,\boldsymbol{q}+n\boldsymbol{K}_1}(\boldsymbol{K}_\mathrm{r} - n\,\boldsymbol{K}_1 + k_0\,\boldsymbol{K}_0;u_{(1)})\,. \tag{2.53}$$

To confirm the consistency of these relations we prove (2.50) by taking the expectation value of (2.41) in the state (2.53):

$$\mathscr{E}_{\mu n}(\boldsymbol{q}) = \sum_{\boldsymbol{K}_\mathrm{r}'\boldsymbol{K}_\mathrm{r}}(C_{\mu,0,\boldsymbol{q}+n\boldsymbol{K}_1}(\boldsymbol{K}_\mathrm{r}' - n\,\boldsymbol{K}_1 + k_0\,\boldsymbol{K}_0;u_{(1)})\times$$
$$\times\,|B_0^+\big((k_0\,q-n)\,\boldsymbol{K}_1\big)\,H_{\boldsymbol{q}}(\boldsymbol{K}_\mathrm{r}',\boldsymbol{K}_\mathrm{r})\,B_0\big((k_0\,q-n)\,\boldsymbol{K}_1\big)|\times$$
$$\times\,C_{\mu,0,\boldsymbol{q}+n\boldsymbol{K}_1}(\boldsymbol{K}_\mathrm{r} - n\,\boldsymbol{K}_1 + k_0\,\boldsymbol{K}_0;u_{(1)})\big)\,.$$

With (2.41), (A 2), and (A 4) it is easy to check that

$$B_0^+\big((k_0\,q-n)\,\boldsymbol{K}_1\big)\,H_{\boldsymbol{q}}(\boldsymbol{K}_\mathrm{r}',\boldsymbol{K}_\mathrm{r})\,B_0\big((k_0\,q-n)\,\boldsymbol{K}_1\big) =$$
$$= H_{\boldsymbol{q}+n\boldsymbol{K}_1}(\boldsymbol{K}_\mathrm{r}' - n\,\boldsymbol{K}_1 + k_0\,\boldsymbol{K}_0\,,\,\boldsymbol{K}_\mathrm{r} - n\,\boldsymbol{K}_1 + k_0\,\boldsymbol{K}_0)$$

which establishes (2.50). Finally, from (2.48) we conclude $C_{\mu,n,\boldsymbol{q}+(1/p)\boldsymbol{K}_1}$ to differ from $C_{\mu n\boldsymbol{q}}$ only by a phase factor.

So far we have only considered the translational symmetry of the Bloch electron in a magnetic field. The only possible operations of magnetic point groups [33] are the inversion and rotations about one of the symmetry axes of the crystal if $\boldsymbol{B}$ is aligned with it. Such symmetries result in

$$\mathscr{E}_{\mu n}(\boldsymbol{q}) = \mathscr{E}_{\mu n'}(\boldsymbol{\alpha}\,\boldsymbol{q})$$

with $\boldsymbol{\alpha}$ a rotation matrix or $\boldsymbol{\alpha} = -\mathbf{1}$. Magnetic space groups and their irreducible representations are studied in detail by Overhof and Rössler [33] and recently by Tam and Opechowski [34].

2.7 Matrix elements and expectation values

In this section we collect a lot of standard relations [19] which are important to applications of the theory. They indicate the essential analogy to the ordinary Bloch electron that rests upon the mutual translational symmetry.

If possible we return to the notation $\alpha \equiv n, \nu$ and neglect spin terms. The starting point is relation (2.36) and the resulting Schrödinger equation (2.40).

1. The first step is an expression for the matrix elements of the canonical momentum $\hbar\, \boldsymbol{w}$ with the states (2.36). Using (2.33), (2.34), and (A 2), we get

$$\langle \psi_{\alpha' \boldsymbol{q}' s'} \,|\, \boldsymbol{w} \,|\, \psi_{\alpha \boldsymbol{q} s} \rangle = \boldsymbol{w}_{\alpha' \alpha, \boldsymbol{q}}\, \delta(\boldsymbol{q}' - \boldsymbol{q})\, \delta_{s' s}\,;$$

$$\boldsymbol{w}_{\alpha' \alpha, \boldsymbol{q}} = \sum_{\boldsymbol{K}_\mathrm{r}} \int_{-\infty}^{\infty} C^*_{\alpha' \boldsymbol{q}}(\boldsymbol{K}_\mathrm{r}; u_{(1)})\, (\widetilde{\boldsymbol{w}} + \boldsymbol{K}_\mathrm{r})\, C_{\alpha \boldsymbol{q}}(\boldsymbol{K}_\mathrm{r}; u_{(1)})\, \mathrm{d}u_{(1)} \equiv \langle C_{\alpha' \boldsymbol{q}} \,|\, \widetilde{\boldsymbol{w}} + \boldsymbol{K}_\mathrm{r} \,|\, C_{\alpha \boldsymbol{q}} \rangle\,; \tag{2.54}$$

where the symbol $\langle | \rangle$ involves integration with respect to $u_{(1)}$ and summation over $\boldsymbol{K}_\mathrm{r}$.

2. The important relation

$$\begin{aligned} (\mathscr{E}_{\alpha'}(\boldsymbol{q}) - \mathscr{E}_{\alpha}(\boldsymbol{q}))\, (i \langle C_{\alpha' \boldsymbol{q}} \,|\, \boldsymbol{w} \times \boldsymbol{\lambda}, C_{\alpha \boldsymbol{q}} \rangle + \langle C_{\alpha' \boldsymbol{q}} \,|\, \nabla_{\boldsymbol{q}}\, C_{\alpha \boldsymbol{q}} \rangle) = \\ = \nabla_{\boldsymbol{q}}\, \mathscr{E}_{\alpha}(\boldsymbol{q})\, \delta_{\alpha' \alpha} - \frac{\hbar^2}{m}\, \boldsymbol{w}_{\alpha' \alpha, \boldsymbol{q}} \end{aligned} \tag{2.55}$$

is obtained by deriving the Schrödinger equation (2.40) with respect to $\boldsymbol{q}$ and using

$$\nabla_{\boldsymbol{q}}\, H_{\boldsymbol{q}}(\boldsymbol{K}'_\mathrm{r}, \boldsymbol{K}_\mathrm{r}) = i\, [H_{\boldsymbol{q}}(\boldsymbol{K}'_\mathrm{r}, \boldsymbol{K}_\mathrm{r}), \boldsymbol{w} \times \boldsymbol{\lambda}] + \frac{\hbar^2}{m}\, (\widetilde{\boldsymbol{w}} + \boldsymbol{K}_\mathrm{r})\, \delta_{\boldsymbol{K}'_\mathrm{r} \boldsymbol{K}_\mathrm{r}} \tag{2.56}$$

which is a consequence of (2.41), (2.42), and (A 3). The diagonal part of (2.55) gives the expectation value

$$\boldsymbol{v}_{\alpha \boldsymbol{q}} = \frac{\hbar}{m}\, \boldsymbol{w}_{\alpha \alpha, \boldsymbol{q}} = \frac{1}{\hbar}\, \nabla_{\boldsymbol{q}}\, \mathscr{E}_{\alpha}(\boldsymbol{q}) \tag{2.57}$$

of the velocity in the state $\psi_{\alpha \boldsymbol{q} s}$.

3. The off-diagonal part of (2.55) leads us to the f-sum rule if we express the first and the second factor of the oscillator strength tensor

$$\mathfrak{f}_{\alpha' \alpha, \boldsymbol{q}} = \frac{\hbar^2}{m}\, \frac{\boldsymbol{w}_{\alpha' \alpha, \boldsymbol{q}}\, \boldsymbol{w}_{\alpha \alpha', \boldsymbol{q}} + \boldsymbol{w}_{\alpha \alpha', \boldsymbol{q}}\, \boldsymbol{w}_{\alpha' \alpha, \boldsymbol{q}}}{\mathscr{E}_{\alpha'}(\boldsymbol{q}) - \mathscr{E}_{\alpha}(\boldsymbol{q})} \tag{2.58}$$

by (2.54) and (2.55) respectively. This gives

$$\begin{aligned} \sum_{\alpha' \neq \alpha} \mathfrak{f}_{\alpha' \alpha, \boldsymbol{q}} = i \langle C_{\alpha \boldsymbol{q}} \,|\, [\boldsymbol{w} \times \boldsymbol{\lambda}, \widetilde{\boldsymbol{w}}] \,|\, C_{\alpha \boldsymbol{q}} \rangle - \langle \nabla_{\boldsymbol{q}}\, C_{\alpha \boldsymbol{q}} \,|\, \widetilde{\boldsymbol{w}} + \boldsymbol{K}_\mathrm{r} \,|\, C_{\alpha \boldsymbol{q}} \rangle - \\ - \langle C_{\alpha \boldsymbol{q}} \,|\, \widetilde{\boldsymbol{w}} + \boldsymbol{K}_\mathrm{r} \,|\, \nabla_{\boldsymbol{q}}\, C_{\alpha \boldsymbol{q}} \rangle\,, \end{aligned} \tag{2.59}$$

where the completeness of the functions $C_{\alpha \boldsymbol{q}}$ and $\nabla_{\boldsymbol{q}} \langle C_{\alpha' \boldsymbol{q}} \,|\, C_{\alpha \boldsymbol{q}} \rangle = 0$ is used. Because of (2.7) and (2.39) the first term is equal to the 2×2 unit tensor in the plane perpendicular to $\boldsymbol{B}$. It can be completed to the whole 3×3 unit tensor by expressing the last two terms by $\nabla_{\boldsymbol{q}}\, \boldsymbol{w}_{\alpha \alpha, \boldsymbol{q}}$. Hence, from (2.57) we get

$$\sum_{\alpha' \neq \alpha} \mathfrak{f}_{\alpha' \alpha, \boldsymbol{q}} = \mathbf{1} - \frac{m}{\hbar^2}\, \nabla_{\boldsymbol{q}}\, \nabla_{\boldsymbol{q}}\, \mathscr{E}_{\alpha}(\boldsymbol{q}) = \mathbf{1} - \frac{m}{\mathfrak{m}^*_{\alpha}(\boldsymbol{q})}\,, \tag{2.60}$$

where the "magnetic" effective-mass tensor $\left(m^*_{\alpha}(\boldsymbol{q})\right)^{-1} = (1/\hbar^2)\, \nabla_{\boldsymbol{q}}\, \nabla_{\boldsymbol{q}}\, \mathscr{E}_{\alpha}(\boldsymbol{q})$ is introduced.

4. The interaction of Bloch electrons in a magnetic field with a periodic perturbation $e^{i(\boldsymbol{\varkappa}, \boldsymbol{r})}$ $e^{i(\boldsymbol{\varkappa}, \boldsymbol{s})}$ $e^{-i(\boldsymbol{\varkappa}, \boldsymbol{w} \times \boldsymbol{\lambda})}$ is determined by the expression

$$\sum_{s, s'}^{p-1}{}_0 (\psi_{\mu' n' \boldsymbol{q}' s'} e^{i(\boldsymbol{\varkappa}, \boldsymbol{r})} \psi_{\mu n \boldsymbol{q} s})^2 = p \sum_{\boldsymbol{K}_c} \sum_{n''=0}^{q-1} \delta\left(\boldsymbol{q} - \boldsymbol{q}' + \boldsymbol{\varkappa} + n'' \boldsymbol{K}_1 + \frac{1}{p} \boldsymbol{K}_c\right) \times$$

$$\times \left| \langle C_{\mu', (n'+n'')_q, \boldsymbol{q}+\boldsymbol{\varkappa}} | e^{-i(\boldsymbol{\varkappa}, \boldsymbol{w} \times \boldsymbol{\lambda})} C_{\mu n \boldsymbol{q}} \rangle \right|^2, \tag{2.61}$$

where $(n' + n'')_q$ means reduction of $n' + n''$ modulo q. The rather complicated proof is sketched in Appendix II. It makes use of the assumption $|\boldsymbol{\varkappa}| \ll |\boldsymbol{K}|$ of long waves. The same arguments give

$$\sum_{s, s'}^{p-1}{}_0 (\psi_{\mu n \boldsymbol{q} s} | \{e^{-i(\boldsymbol{\varkappa}, \boldsymbol{r})}, \boldsymbol{w}\} \psi_{\mu' n' \boldsymbol{q}' s'}) (\psi_{\mu' n' \boldsymbol{q}' s'} | \{e^{i(\boldsymbol{\varkappa}, \boldsymbol{r})}, \boldsymbol{w}\} \psi_{\mu n \boldsymbol{q} s}) =$$

$$= p \sum_{\boldsymbol{K}_c} \sum_{n''=0}^{q-1} \delta\left(\boldsymbol{q} - \boldsymbol{q}' + \boldsymbol{\varkappa} + n'' \boldsymbol{K}_1 + \frac{1}{p} \boldsymbol{K}_c\right) \langle C_{\mu n \boldsymbol{q}} | \{e^{i(\boldsymbol{\varkappa}, \boldsymbol{w} \times \boldsymbol{\lambda})}, \widetilde{\boldsymbol{w}} + \boldsymbol{K}_r\} \times$$

$$\times C_{\mu', (n'+n'')_q, \boldsymbol{q}+\boldsymbol{\varkappa}} \rangle \langle C_{\mu', (n'+n'')_q, \boldsymbol{q}+\boldsymbol{\varkappa}} | \{e^{-i(\boldsymbol{\varkappa}, \boldsymbol{w} \times \boldsymbol{\lambda})}, \widetilde{\boldsymbol{w}} + \boldsymbol{K}_r\} C_{\mu n \boldsymbol{q}} \rangle, \tag{2.62}$$

where $\{,\}$ is the anticommutator.

The last relation is significant for the interaction of "magnetic" Bloch electrons with electromagnetic waves and appears in the conductivity tensor. As an example we quote the RPA formulas derived by Mertsching [35]. Equation (2.61) is needed in the theory of ultrasonic attenuation. The δ-functions in (2.61) and (2.62) give the correct form of wave number selection rules of these interactions. The matrix elements (2.54) of the canonical momentum $\hbar \boldsymbol{w}$ are important to the theory of galvanomagnetic effects as they determine the dc conductivity [35]. The "magnetic" effective mass defined in (2.60) plays a similar role as in the ordinary Bloch case. It is easy to prove the time-dependent states

$$\psi(t) = e^{-(i/\hbar) H' t} \psi_{\alpha \boldsymbol{q} s}; \quad H' = H - e(\boldsymbol{E}, \boldsymbol{r}) \tag{2.63}$$

of the "magnetic" Bloch electron in an additional electric field $\boldsymbol{E}$ to be eigenfunctions of magnetic translations with wave numbers $\boldsymbol{q}(t) = \boldsymbol{q}_0 + (e/\hbar) \boldsymbol{E} t$ [19] so that the effective-mass theorem

$$\dot{\boldsymbol{v}}_{\alpha \boldsymbol{q}} = \frac{e}{\hbar^2} \nabla_{\boldsymbol{q}} \nabla_{\boldsymbol{q}} \mathscr{E}_\alpha(\boldsymbol{q}) \boldsymbol{E} = \left(\mathbf{m}^*_\alpha(\boldsymbol{q})\right)^{-1} e \boldsymbol{E} \tag{2.64}$$

should hold. This question is answered by the expectation value of the acceleration [19]

$$\left(\psi'(t) \left| \frac{\hbar}{m} \dot{\boldsymbol{w}} \right| \psi(t)\right) =$$

$$= \left[\left(\mathbf{m}^*_\alpha(\boldsymbol{q})\right)^{-1} + \frac{\hbar}{m^2} \sum_{\alpha' \neq \alpha} \frac{1}{\omega_{\alpha' \alpha}} (\boldsymbol{w}_{\alpha' \alpha, \boldsymbol{q}_0} \boldsymbol{w}_{\alpha \alpha', \boldsymbol{q}_0} e^{i \omega_{\alpha' \alpha} t} + \boldsymbol{w}_{\alpha \alpha', \boldsymbol{q}_0} \boldsymbol{w}_{\alpha' \alpha, \boldsymbol{q}_0} e^{-i \omega_{\alpha' \alpha} t})\right] \times$$

$$\times e \boldsymbol{E} \delta(\boldsymbol{q}'_0 - \boldsymbol{q}_0) \tag{2.65}$$

in the state (2.63), which is calculated linearly with respect to $\boldsymbol{E}$. Here $\hbar \omega_{\alpha' \alpha} = \mathscr{E}_{\alpha'}(\boldsymbol{q}_0) - \mathscr{E}_\alpha(\boldsymbol{q}_0)$ and $\psi'(t) = e^{-(i/\hbar) H' t} \psi_{\alpha \boldsymbol{q}'_0 s}$.[5])

[5]) The initial wave vectors of ψ and ψ' are distinguished only for formal reasons (normalization to δ-functions).

Starting from the initial value $(e\ m)\ \boldsymbol{E}$ at $t = 0$, the expectation value (2.65) oscillates about the mean value (2.64) with interband frequencies. Provided the banding of magnetic energy levels is not negligible (i.e. $\mathfrak{m}^*$ is not too large), this mean value becomes predominant if the relaxation time τ is long compared to interband periods of order $1/\omega_c$. Then, the interband contributions of (2.65) to the total current (which is obtained by integrating (2.65) together with $e^{t/\tau\varepsilon(\boldsymbol{q}_0)}$ with respect to time and summing over all occupied states) cancel each other to some extent. The Hall effect, however, is due to the interband terms of (2.65) as is already pointed out by Pippard [27].

3. Effective Hamiltonians

3.1 Roth's many-band Hamiltonian

So far we have developed the theory of Bloch electrons in a magnetic field without reference to the field-free case. We now want to establish this relation in order to take advantage of the knowledge of Bloch energies and wave functions. We start from the formal analogy of (2.46) to the Schrödinger equation of the Fourier components $c_\nu(\boldsymbol{k}+\boldsymbol{K})$ of the Bloch factors

$$u_\nu(\boldsymbol{k},\boldsymbol{x}) = \sum_{\boldsymbol{K}} c_\nu(\boldsymbol{k}+\boldsymbol{K})\, \mathrm{e}^{i(\boldsymbol{K},\boldsymbol{x})} = \sqrt{\Omega_0} \sum_{\boldsymbol{R}_i} a_\nu(\boldsymbol{x}+\boldsymbol{R})\, \mathrm{e}^{-i(\boldsymbol{k},\boldsymbol{x}+\boldsymbol{R})} \qquad (3.1)$$

(a_ν Wannier functions, ν Band index). Since (2.46) changes into the corresponding zero-field Schrödinger equation by replacing $\tilde{\boldsymbol{w}}$ by $\boldsymbol{k}$, we express the solutions

$$C^{\boldsymbol{K}}_{\alpha\boldsymbol{q}}(u_{(1)}) = \sum_{\nu} c_\nu(\tilde{\boldsymbol{w}}+\boldsymbol{K})\, b_{\alpha\boldsymbol{q}}(\nu; u_{(1)}) \qquad (3.2)$$

of (2.46) by $c_\nu(\tilde{\boldsymbol{w}}+\boldsymbol{K})$, where $\boldsymbol{k}$ is reversely replaced by $\tilde{\boldsymbol{w}}$. $c_\nu(\tilde{\boldsymbol{w}}+\boldsymbol{K})$ is an operator that acts on the element $b_{\alpha\boldsymbol{q}}$ of $\mathfrak{H}'$ and likewise an expansion coefficient for the $\boldsymbol{K}$-dependence of $C^{\boldsymbol{K}}_{\alpha\boldsymbol{q}}$. Inserting (3.2) into (2.46), multiplying from the left by $c^+_{\nu'}(\tilde{\boldsymbol{w}}+\boldsymbol{K}')$, and summing over $\boldsymbol{K}'$, we obtain Roth's many-band Schrödinger equation [12]

$$\sum_{\nu} \left[H_{\nu'\nu}(\tilde{\boldsymbol{w}}) - \mathscr{E}_\alpha(\boldsymbol{q})\, N_{\nu'\nu}(\tilde{\boldsymbol{w}})\right] b_{\alpha\boldsymbol{q}}(\nu; u_{(1)}) = 0\ ; \qquad (3.3)$$

$$H_{\nu'\nu}(\tilde{\boldsymbol{w}}) = \sum_{\boldsymbol{K}'} c^+_{\nu'}(\tilde{\boldsymbol{w}}+\boldsymbol{K}') \left\{\left[\frac{\hbar^2}{2m}(\tilde{\boldsymbol{w}}+\boldsymbol{K}')^2 - \frac{\hbar^2}{2m}(\boldsymbol{\sigma},\boldsymbol{b})\right] c_\nu(\tilde{\boldsymbol{w}}+\boldsymbol{K}') + \right.$$
$$\left. + \sum_{\boldsymbol{K}} V_{\boldsymbol{K}}\left[1 + \frac{i\hbar^2}{4m^2c^2}(\tilde{\boldsymbol{w}}+\boldsymbol{K}', \boldsymbol{\sigma}\times\boldsymbol{K})\right] c_\nu(\tilde{\boldsymbol{w}}+\boldsymbol{K}'-\boldsymbol{K})\right\}, \qquad (3.4)$$

$$N_{\nu'\nu}(\tilde{\boldsymbol{w}}) = \sum_{\boldsymbol{K}'} c^+_{\nu'}(\tilde{\boldsymbol{w}}+\boldsymbol{K}')\, c_\nu(\tilde{\boldsymbol{w}}+\boldsymbol{K}')\ . \qquad (3.5)$$

As functions of non-commuting vector components the operators $c_\nu(\tilde{\boldsymbol{w}}+\boldsymbol{K})$ are not unambiguously defined. Therefore we require that the components of $\tilde{\boldsymbol{w}}$ should occur symmetrically. That is the case if $c_\nu(\boldsymbol{k}+\boldsymbol{K})$ is expressed by the Wannier function $a_\nu(\boldsymbol{x})$:

$$c_\nu(\boldsymbol{k}+\boldsymbol{K}) = \Omega_0^{-1/2} \int \mathrm{e}^{-i(\boldsymbol{k}+\boldsymbol{K},\boldsymbol{x})}\, a_\nu(\boldsymbol{x})\, \mathrm{d}^3\boldsymbol{x}\ , \qquad (3.6)$$

and $\boldsymbol{k}$ is replaced by $\tilde{\boldsymbol{w}}$. This procedure provides $H_{\nu'\nu}(\tilde{\boldsymbol{w}})$ and $N_{\nu'\nu}(\tilde{\boldsymbol{w}})$ as symmetric operators with respect to $\tilde{\boldsymbol{w}}$. The $\boldsymbol{K}$-sum gives the potential $V(\boldsymbol{x})$. The $\boldsymbol{K}'$-sum results in a series of δ-functions that enable one of the $\boldsymbol{x}$-integrations

to be performed. By means of (A 6) and (A 7) the remaining integral takes the form [12]

$$\left.\begin{aligned} H_{\nu'\nu}(\tilde{\boldsymbol{w}}) &= \sum_{\boldsymbol{R}} H_{\nu'\nu}(\boldsymbol{R})\, \mathrm{e}^{i(\tilde{\boldsymbol{w}},\boldsymbol{R})}\,, \\ H_{\nu'\nu}(\boldsymbol{R}) &= \int a^*_{\nu'}(\boldsymbol{x}-\boldsymbol{R})\, \mathrm{e}^{(i/2)(\boldsymbol{x}-\boldsymbol{b},\boldsymbol{R})}\, H\left(\frac{1}{i}\nabla_{\boldsymbol{x}} - \frac{1}{2}\boldsymbol{x}\times\boldsymbol{b};\boldsymbol{x}\right) a_\nu(\boldsymbol{x})\, \mathrm{d}^3\boldsymbol{x}\,; \end{aligned}\right\} \tag{3.7}$$

$$N_{\nu'\nu}(\tilde{\boldsymbol{w}}) = \sum_{\boldsymbol{R}} N_{\nu'\nu}(\boldsymbol{R})\, \mathrm{e}^{i(\tilde{\boldsymbol{w}},\boldsymbol{R})}\,, \qquad N_{\nu'\nu}(\boldsymbol{R}) = \int a^*_{\nu'}(\boldsymbol{x}-\boldsymbol{R})\, \mathrm{e}^{(i/2)(\boldsymbol{x}-\boldsymbol{b},\boldsymbol{R})}\, a_\nu(\boldsymbol{x})\, \mathrm{d}^3\boldsymbol{x}\,. \tag{3.8}$$

$H\,(-i\nabla_{\boldsymbol{x}} + \boldsymbol{x}\times\boldsymbol{b}/2;\boldsymbol{x})$ is the original Hamiltonian (2.1), which must be taken here with the symmetric gauge $\boldsymbol{A}(\boldsymbol{x}) = (1/2)\,(\boldsymbol{B}\times\boldsymbol{x})$. (3.2) reads in terms of Wannier functions

$$C^{\boldsymbol{K}}_{\lambda\boldsymbol{q}}(u_{(1)}) = \Omega_0^{-1/2} \sum_\nu \int \mathrm{d}^3\boldsymbol{x}\, \mathrm{e}^{-i(\tilde{\boldsymbol{w}}-\boldsymbol{K},\boldsymbol{x})}\, a_\nu(\boldsymbol{x})\, b_{\lambda\boldsymbol{q}}(\nu;u_{(1)})\,. \tag{3.9}$$

Because of (A 2) and (3.2) the subsidiary condition (2.47) is equivalent to requiring

$$B_{\boldsymbol{0}}(\boldsymbol{K}_c)\, b_{\mu n\boldsymbol{q}}(\nu;u_{(1)}) = \mathrm{e}^{i\,(\boldsymbol{q}+\hat{n}\boldsymbol{K}_1,\boldsymbol{K}_c\times\lambda)}\, b_{\mu n\boldsymbol{q}}(\nu;u_{(1)})\,, \tag{3.10}$$

the solutions $b_{\mu n\boldsymbol{q}}$ to be eigenfunctions of the unitary operators $B_{\boldsymbol{0}}(\boldsymbol{K}_c)$. With regard to Section 2.6 this is written in the reduced form in which $\boldsymbol{q}$ is kept within the first magnetic Brillouin zone.

Roth's many-band Schrödinger equation is a complicated system of difference equations the general form of which is by no means simpler than the original Schrödinger equation (2.46) (or (2.40)). The main difficulty is the non-diagonality with respect to the band index ν (interband coupling). The actual relevance of (3.3) lies in the fact that it becomes accessible to practical solution methods by power expansions of $H_{\nu'\nu}(\boldsymbol{k})$ and $N_{\nu'\nu}(\boldsymbol{k})$ with respect to field strength. These expansions may be derived from (3.7) and (3.8). But also the alternate expressions [12]

$$H_{\nu'\nu}(\boldsymbol{k}) = \mathrm{e}^{(i/2)(\nabla_{\boldsymbol{k}'}\times\nabla_{\boldsymbol{k}'},\boldsymbol{b})}\, \frac{1}{\Omega_0} \int_{\Omega_0} u^*_{\nu'}(\boldsymbol{k}';\boldsymbol{x})\, H\left(\frac{1}{i}\nabla_{\boldsymbol{x}} + \boldsymbol{k} + \frac{i}{2}\nabla_{\boldsymbol{k}}\times\boldsymbol{b};\boldsymbol{x}\right)\times$$

$$\times\, u_\nu(\boldsymbol{k};\boldsymbol{x})\, \mathrm{d}^3\boldsymbol{x}\big|_{\boldsymbol{k}'=\boldsymbol{k}}\,; \tag{3.11}$$

$$N_{\nu'\nu}(\boldsymbol{k}) = \mathrm{e}^{(i/2)(\nabla_{\boldsymbol{k}'}\times\nabla_{\boldsymbol{k}'},\boldsymbol{b})}\, \frac{1}{\Omega_0} \int_{\Omega_0} u^*_{\nu'}(\boldsymbol{k}';\boldsymbol{x})\, u_\nu(\boldsymbol{k};\boldsymbol{x})\, \mathrm{d}^3\boldsymbol{x}\,|_{\boldsymbol{k}'=\boldsymbol{k}} \tag{3.12}$$

may be used. They are obtained by introducing Bloch factors into (3.4) and (3.5) and applying Roth's multiplication formula (A 9). In order to judge of the convergence of these power series, we modify (3.7) and (3.8) by expressing the $\boldsymbol{R}$-sums by Bloch functions $\psi_\nu(\boldsymbol{k};\boldsymbol{x}) = (2\pi)^{-3/2}\,\Omega_0^{1/2} \sum_{\boldsymbol{R}} a_\nu\,(\boldsymbol{x}+\boldsymbol{R})\, \mathrm{e}^{-i(\boldsymbol{k},\boldsymbol{R})}$:

$$H_{\nu'\nu}(\boldsymbol{k}) = \frac{(2\pi)^{3/2}}{\sqrt{\Omega_0}} \int \psi^*_{\nu'}\left(\boldsymbol{k}+\frac{1}{2}\boldsymbol{x}\times\boldsymbol{b};\boldsymbol{x}\right) H\left(\frac{1}{i}\nabla_{\boldsymbol{x}} + \frac{1}{2}\boldsymbol{x}\times\boldsymbol{b};\boldsymbol{x}\right) a_\nu(\boldsymbol{x})\, \mathrm{d}^3\boldsymbol{x}\,,$$

$$N_{\nu'\nu}(\boldsymbol{k}) = \frac{(2\pi)}{\sqrt{\Omega_0}} \int \psi^*_{\nu'}\left(\boldsymbol{k}+\frac{1}{2}\boldsymbol{x}\times\boldsymbol{b};\boldsymbol{x}\right) a_\nu(\boldsymbol{x})\, \mathrm{d}^3\boldsymbol{x}\,.$$

The desired expansions of $H_{\nu'\nu}(\boldsymbol{k})$ and $N_{\nu'\nu}(\boldsymbol{k})$ in powers of $|\boldsymbol{b}| = \lambda^{-1}$ are obtained by expanding $\psi^*_{\nu'}\,(\boldsymbol{k} + \boldsymbol{x}\times\boldsymbol{b}/2;\boldsymbol{x})$ at real $\boldsymbol{k}$-values with respect to $\boldsymbol{x}\times\boldsymbol{b}/2$

below the $\boldsymbol{x}$-integral. This is possible as Bloch functions are holomorphic at real $\boldsymbol{k}$-values unless band-touching is present. The $\boldsymbol{k}$-dependence of $\psi_\nu^*(\boldsymbol{k};\boldsymbol{x})$, however, exhibits algebraic singularities at certain finite points of the complex $\boldsymbol{k}$-space [36 to 38]. Hence, this expansion possesses a finite radius of convergence. It is not only a development in powers of $\boldsymbol{b}_\lambda = \lambda^{-1}$ but also a partial power expansion of the $\boldsymbol{x}$-dependence of the integrand. It must be integrated term by term over the whole space although the range of convergence is restricted. The resulting series cannot be convergent. They are asymptotic expansions for large λ, the "quality" of which is mainly determined by both the localization of $a_\nu(\boldsymbol{x})$ and the convergence radius of the expansion of $\psi_\nu^*(\boldsymbol{k} + \boldsymbol{x}\times\boldsymbol{b}/2;\boldsymbol{x})$. The latter is, by itself, closely related to the localization of the corresponding Wannier function $a_\nu^*(\boldsymbol{x})$ [36, 38] so that we may state: The more $a_{\nu'}$ and a_ν are localized the better are the asymptotic expansions. The dominating zeroth-order terms

$$H_{0\nu'\nu}(\boldsymbol{k}) = E_\nu(\boldsymbol{k})\,\delta_{\nu'\nu}\,, \qquad N_{0\nu'\nu}(\boldsymbol{k}) = \delta_{\nu'\nu} \tag{3.13}$$

may be inferred from (3.11) and (3.12), where $E_\nu(\boldsymbol{k})$ is the Bloch energy. They are diagonal with respect to band indices. By experience, asymptotic expansions are useful only if the dominating term is already a good approximation describing the most important features of the problem whereas the following terms only contribute small corrections. The approximation (3.13) reduces Roth's many-band Schrödinger equation (3.3) to

$$E_{\nu'}(\widetilde{\boldsymbol{w}})\,b_{\alpha_\nu\boldsymbol{q}}(\nu';u_{(1)}) = \mathscr{E}_{\alpha_\nu}(\boldsymbol{q})\,b_{\alpha_\nu\boldsymbol{q}}(\nu';u_{(1)})\;; \qquad b_{\alpha_\nu\boldsymbol{q}}(\nu';u_{(1)}) \equiv \delta_{\nu'\nu}\,b_{\alpha_\nu\boldsymbol{q}}(u)\,, \tag{3.14}$$

where α_ν denotes the quantum numbers α belonging to the Bloch band ν. This result is the so-called Peierls theorem. Up to now there are only very crude estimates [39] of the range of field strengths in which the asymptotic power series and Peierls' theorem are significant for the analytic structure of Bloch energies and wave functions and the related properties of Wannier functions are not sufficiently investigated.

3.2 Diagonalization of the many-band Hamiltonian

For many problems Peierls' theorem is a completely sufficient approach. The higher-order contributions to the many-band Hamiltonian give rise to corrections of Onsager's quantization rule [40] and the Zeeman splitting [40]. They are not diagonal with respect to band indices. On certain conditions they can be successively diagonalized by Roth's transformation [12] as described in what follows.

We seek a symmetric[6]) nonunitary operator $S(\widetilde{\boldsymbol{w}}) \equiv S_{\nu'\nu}(\widetilde{\boldsymbol{w}})$ that transforms the many-band Hamiltonian $H(\widetilde{\boldsymbol{w}}) \equiv H_{\nu'\nu}(\widetilde{\boldsymbol{w}})$ into the one-band Hamiltonian $\overline{H}(\widetilde{\boldsymbol{w}}) \equiv \overline{H}_\nu(\widetilde{\boldsymbol{w}})\,\delta_{\nu'\nu}$ and, at the same time, $N(\widetilde{\boldsymbol{w}}) \equiv N_{\nu'\nu}(\widetilde{\boldsymbol{w}})$ into $1 \equiv \delta_{\nu'\nu}$ according to

$$\overline{H}(\widetilde{\boldsymbol{w}}) = S^+(\widetilde{\boldsymbol{w}})\,H(\widetilde{\boldsymbol{w}})\,S(\widetilde{\boldsymbol{w}}) \quad \text{and} \quad 1 = S^+(\widetilde{\boldsymbol{w}})\,N(\widetilde{\boldsymbol{w}})\,S(\widetilde{\boldsymbol{w}})\,, \tag{3.15}$$

where matrix multiplication is to be understood. We substitute the asymptotic power expansions

$$H(\boldsymbol{k}) = H_0(\boldsymbol{k}) + \lambda^{-1}H_1(\boldsymbol{k}) + \lambda^{-2}H_2(\boldsymbol{k}) + \ldots\,, \tag{3.16}$$

$$N(\boldsymbol{k}) = 1 + \lambda^{-1}N_1(\boldsymbol{k}) + \lambda^{-2}N_2(\boldsymbol{k}) + \ldots\,, \tag{3.17}$$

$$S(\boldsymbol{k}) = 1 + \lambda^{-1}S_1(\boldsymbol{k}) + \lambda^{-2}S_2(\boldsymbol{k}) + \ldots \tag{3.18}$$

[6]) In the sense of p. 26.

in (3.15), apply the multiplication formula (A 9), which is also to be developed in powers of λ^{-1}, arrange the terms according to powers of λ^{-1}, and obtain

$$\begin{aligned}\overline{H}(\boldsymbol{k}) &= H_0(\boldsymbol{k}) + \lambda^{-1} H_1(\boldsymbol{k}) + \lambda^{-2} H_2(\boldsymbol{k}) + \dots \\ &= H_0 + \lambda^{-1}(H_1 + S_1^+ H_0 + H_0 S_1) + \lambda^{-2}\Big[H_2 + S_2^+ H_0 + H_0 S_2 + S_1^+ H_1 + H_1 S_1 + \\ &\quad + S_1^+ H_0 S_1 + \frac{i}{2}(\nabla_{\boldsymbol{k}} \times \nabla_{\boldsymbol{k}'}, \boldsymbol{e}_3)\,(S_1^+(\boldsymbol{k})\, H_0(\boldsymbol{k}') - H_0(\boldsymbol{k})\, S_1(\boldsymbol{k}'))_{\boldsymbol{k}'=\boldsymbol{k}}\Big] + \dots,\end{aligned} \tag{3.19}$$

$$1 = 1 + \lambda^{-1}(N_1 + S_1^+ + S_1) + \\ + \lambda^{-2}(N_2 + S_2^+ + S_2 + S_1^+ N_1 - N_1 S_1 + S_1^+ S_1) + \dots . \tag{3.20}$$

Now we are going to ascertain $S_1, S_2, \dots$ recursively so that a) the higher-order terms of (3.20) vanish and b) (3.19) is diagonal in each order. Condition a) gives the Hermitian part $(S_j - S_j^+)/2$ of S_j $(j = 1, 2, \dots)$. From b) we find the nondiagonal elements of the anti-Hermitian part $(S_j - S_j^+)/2$. The diagonal elements of $(S_j - S_j^+)/2$ are arbitrary. For simplicity we put $(S_j - S_j^+)_{\nu\nu} = 0$. In first order we have $S_1 + S_1^+ = -N_1$ and $H_{1\nu'\nu} + E_\nu S_{1\nu'\nu}^+ + E_{\nu'} S_{1\nu'\nu} = 0$ $(\nu' \neq \nu)$ giving

$$S_{1\nu'\nu} = \frac{E_\nu N_{1\nu'\nu} - H_{1\nu'\nu}}{E_{\nu'} - E_\nu} \quad (\nu \neq \nu') \quad \text{and} \quad S_{1\nu\nu} = -\frac{N_{1\nu\nu}}{2}. \tag{3.21}$$

Then, the first-order term of (3.19) becomes

$$\overline{H}_1(\boldsymbol{k}) = [H_{1\nu\nu}(\boldsymbol{k}) - E_\nu(\boldsymbol{k})\, N_{1\nu\nu}(\boldsymbol{k})]\,\delta_{\nu'\nu}. \tag{3.22}$$

In second order we get $S_2 + S_2^+ = -N_2 - S_1^+ N_1 - N_1 S_1 - S_1^+ S_1$, which is sufficient to calculate the diagonal part of the second-order term of (3.19):

$$\overline{H}_{2\nu\nu} = H_{2\nu\nu} - E_\nu [N_{2\nu\nu} + (S_1^+ N_1)_{\nu\nu} + (N_1 S_1)_{\nu\nu} + (S_1^+ S_1)_{\nu\nu}] + (S_1^+ H_1)_{\nu\nu} + \\ + (H_1 S_1)_{\nu\nu} + (S_1^+ H_0 S_1)_{\nu\nu} + \frac{i}{2}(\nabla_{\boldsymbol{k}} E_\nu \times \nabla_{\boldsymbol{k}} (S_1 - S_1^+)_{\nu\nu}, \boldsymbol{e}_3). \tag{3.23}$$

The last term vanishes as we have chosen $(S_1 - S_1^+)_{\nu\nu} = 0$. Using (3.21), we see that

$$(S_1^+ H_0 S_1)_{\nu\nu} - E_\nu (S_1^+ S_1)_{\nu\nu} = E_\nu (S_1^+ N_1)_{\nu\nu} - (S_1^+ H_1)_{\nu\nu} - S_{1\nu\nu}^+ (E_\nu N_{1\nu\nu} - H_{1\nu\nu})$$

and obtain

$$\overline{H}_2(\boldsymbol{k}) = \Big[H_{2\nu\nu} - E_\nu N_{2\nu\nu} - N_{1\nu\nu}(H_{1\nu\nu} - E_\nu N_{1\nu\nu}) + \\ + \sum_{\nu'' \neq \nu} \frac{(H_{1\nu\nu''} - E_\nu N_{1\nu\nu''})(H_{1\nu''\nu} - E_\nu N_{1\nu''\nu})}{E_{\nu''} - E_\nu}\Big]\delta_{\nu'\nu}, \tag{3.24}$$

where (3.21) is used once more. The off-diagonal elements of H_2 vanish by the appropriate choice of $(S_2 - S_2^+)_{\nu'\nu}$ $(\nu' \neq \nu)$.

With (3.22) and (3.24) we have derived the diagonalized Hamiltonian

$$\overline{H}_\nu(\tilde{\boldsymbol{w}}) = E_\nu(\tilde{\boldsymbol{w}}) + \lambda^{-1}\overline{H}_{1\nu}(\tilde{\boldsymbol{w}}) + \lambda^{-2}\overline{H}_{2\nu}(\tilde{\boldsymbol{w}}) + \dots \tag{3.25}$$

to second order of field strength. For two reasons it is not unique. The first one concerns the freedom of phase choice of $c_\nu(\boldsymbol{k} + \boldsymbol{K})$ so that the definition

(3.4) of $H(\tilde{\boldsymbol{\pi}}\tilde{\boldsymbol{r}})$ is already ambiguous. However, an additional phase factor $e^{i\Phi_\nu(k)}$ merely induces a unitary transformation

$$e^{-i\Phi_{\nu'}(\tilde{\boldsymbol{\pi}})}\, H_{\nu'\nu}(\tilde{\boldsymbol{\pi}}\tilde{\boldsymbol{r}})\, e^{i\Phi_\nu(\tilde{\boldsymbol{\pi}})}$$

leaving the energy spectrum unaffected. The second reason is the arbitrariness of $(S_j - S_{j'})_{\nu\nu}$. By using (A 9) a definite choice of $(S_1 - S_1^-)_{\nu\nu}$ in (3.23) is shown to be also equivalent to a unitary transformation.

The solutions $\bar{b}_{\alpha_\nu \boldsymbol{q}}(\nu'; u_{(1)}) \equiv \bar{b}_{\alpha_\nu \boldsymbol{q}}(u_{(1)})\, \delta_{\nu'\nu}$ of the decoupled Schrödinger equation

$$H_\nu(\tilde{\boldsymbol{\pi}}\tilde{\boldsymbol{r}})\, \bar{b}_{\alpha_\nu \boldsymbol{q}}(u_{(1)}) = \varepsilon_{\alpha_\nu}(\boldsymbol{q})\, \bar{b}_{\alpha_\nu \boldsymbol{q}}(u_{(1)}) \tag{3.26}$$

are connected with the solutions $b_{\alpha \boldsymbol{q}}(\nu'; u_{(1)})$ of the original many-band equation (3.3) according to

$$b_{\alpha_\nu \boldsymbol{q}}(\nu'; u_{(1)}) = \sum_{\nu''} S_{\nu'\nu''}(\tilde{\boldsymbol{\pi}}\tilde{\boldsymbol{r}})\, \bar{b}_{\alpha_\nu \boldsymbol{q}}(\nu''; u_{(1)}) = S_{\nu'\nu}(\tilde{\boldsymbol{\pi}}\tilde{\boldsymbol{r}})\, \bar{b}_{\alpha_\nu \boldsymbol{q}}(u_{(1)})\,, \tag{3.27}$$

where α_ν stands for the quantum numbers α that belong to the Bloch band ν.

In case of inversion symmetry and neglected spins it can be shown [12] that $H_{1\nu\nu}(\boldsymbol{k})$ and $N_{1\nu\nu}(\boldsymbol{k})$ and, consequently, $\bar{H}_{1\nu}(\boldsymbol{k})$ vanish. Because of the asymptotic character of the initial expansions (3.16) and (3.17), Roth's decoupling procedure is also asymptotic only. Additionally, the appearance of energy denominators in (3.24) indicates that the diagonalization does not work if the band gaps $E_\nu(\boldsymbol{k}) - E_{\nu'}(\boldsymbol{k})$ become too small. That is to say, Bloch bands that are nearing each other very much cannot be decoupled. In general, Bloch bands are twofold degenerate with respect to spin. This is inconsiderable for neglected spin–orbit interaction as the Bloch factors are equal for both spin directions. In case of inversion symmetry the double spin degeneracy is not lifted by spin–orbit coupling. But now the Bloch factors are different in the two spin states, so that the decoupling formalism needs a slight modification. Band indices are only to be referred to energetically different bands. Then, the elements of the matrix $H_{\nu'\nu}(\boldsymbol{k})$ are 2×2 matrices by itself so that $\bar{H}_\nu(\boldsymbol{k})$ is also a 2×2 matrix [40, 41].

In principle Roth's procedure yields the successive terms of the asymptotic series (3.18). We could have some doubt that this nonconvergent series defines a function $S(\boldsymbol{k})$, i.e. that, strictly speaking, the diagonalizing transformation (3.15) exists at all. Wannier and Fredkin [11] have shown the Hamiltonian (2.1) (without spin[7]) to be exactly equivalent to a one-band Hamiltonian if the equation

$$H\, B_\nu(\boldsymbol{k}; \boldsymbol{r}) = \sum_{\boldsymbol{R}} \bar{H}_\nu(\boldsymbol{R})\, e^{i(\boldsymbol{k},\boldsymbol{R})}\, B_\nu\left(\boldsymbol{k} + \frac{1}{2}\,\boldsymbol{b}\times\boldsymbol{R}; \boldsymbol{r}\right) \tag{3.28}$$

[7]) The handling of spin–orbit interaction within this formalism is demonstrated by Appel [41].

is solvable by energy coefficients $H_\nu(\boldsymbol{R})$ and basis functions $B_\nu(\boldsymbol{k};\boldsymbol{r})$ which represent the eigenfunctions of H according to

$$\psi(\boldsymbol{r}) \quad \int b(\boldsymbol{k})\, B_\nu(\boldsymbol{k};\boldsymbol{r})\, \mathrm{d}^3k\,.$$

Indeed, with (3.28) we have

$$H\,\psi(\boldsymbol{r}) \quad \sum_{\boldsymbol{R}} H_\nu(\boldsymbol{R}) \int \mathrm{d}^3k\, \mathrm{e}^{i(\boldsymbol{k},\boldsymbol{R})}\, b\left(\boldsymbol{k} \quad \frac{1}{2}\,\boldsymbol{b}\times\boldsymbol{R}\right) B_\nu(\boldsymbol{k};\boldsymbol{r})$$

$$= \int \mathrm{d}^3k \sum_{\boldsymbol{R}} H_\nu(\boldsymbol{R})\, B_\nu(\boldsymbol{k};\boldsymbol{r})\, \mathrm{e}^{i\left(\boldsymbol{k}-\frac{i}{2}\,\boldsymbol{b}\times\nabla_{\boldsymbol{k}},\boldsymbol{R}\right)} \bar{b}(\boldsymbol{k}) = \mathscr{E}\,\psi(\boldsymbol{r})\,.$$

Equating the coefficients of $B_\nu(\boldsymbol{k};\boldsymbol{r})$, we find

$$H_\nu\left(\boldsymbol{k} - \frac{i}{2}\,\boldsymbol{b}\times\nabla_{\boldsymbol{k}}\right) b(\boldsymbol{k}) \quad \mathscr{E}\,\bar{b}(\boldsymbol{k})\,.$$

The basis functions $B_\nu(\boldsymbol{k};\boldsymbol{r}) \equiv \beta_\nu(\boldsymbol{k} \quad \boldsymbol{b}\times\boldsymbol{r}/2;\boldsymbol{r})$ [14] may be derived from Bloch-like functions $\beta_\nu(\boldsymbol{k};\boldsymbol{x}) = \mathrm{e}^{-i(\boldsymbol{k},\boldsymbol{R})}\,\beta_\nu(\boldsymbol{k};\boldsymbol{x} \quad \boldsymbol{R})$ defined by

$$\left[\frac{1}{2m}\left(\frac{\hbar}{i}\,\nabla_{\boldsymbol{x}} - \frac{1}{2}\,\boldsymbol{b}\times(\boldsymbol{x} + i\,\nabla_{\boldsymbol{k}})\right)^2 + V(\boldsymbol{x})\right]\beta_\nu(\boldsymbol{k};\boldsymbol{x}) =$$

$$= \sum_{\boldsymbol{R}} \bar{H}_\nu(\boldsymbol{R})\, \mathrm{e}^{i\left(\boldsymbol{k}+\frac{1}{2}\,\boldsymbol{b}\times\boldsymbol{x},\boldsymbol{R}\right)} \beta_\nu\left(\boldsymbol{k}+\frac{1}{2}\,\boldsymbol{b}\times\boldsymbol{R};\boldsymbol{x}\right). \tag{3.29}$$

The left-hand side of this equation is just Zak's $\boldsymbol{k},\boldsymbol{x}$ representation [42] of the Hamiltonian (2.1) with the symmetrically gauged vector potential (without spin). The relation to Bloch bands consists in the fact that (3.28) turns into Bloch's Schrödinger equation for $B \to 0$ whereas $B_\nu(\boldsymbol{k};\boldsymbol{r})$ and $\bar{H}_\nu(\boldsymbol{R})$ merge into $\psi_\nu(\boldsymbol{k};\boldsymbol{r})$ and the Fourier coefficients of $E_\nu(\boldsymbol{k})$ respectively. This consideration can be looked upon as an argument for the existence of a one-band operator, the conclusiveness of which, however, is not quite out of question. This problem has been attacked from another point of view by Brown [15, 43]. His existence proof is based on the supposition that there are any partner functions of irreducible representations of the magnetic translation group that span the subspace of the energy band ν. Then it is possible to define generalized Wannier functions that derive from each other by virtue of magnetic translations. The matrix elements of the Hamiltonian (2.1) with such "magnetic" Wannier functions are the Fourier components of an effective one-band operator. This is, however, no way of calculating one-band Hamiltonians explicitly. But also Wannier's equations (3.28) and (3.29) are not very constructive for practical use because they are by no means simpler than the original Schrödinger equation $H\psi = \mathscr{E}\psi$. To calculate $\bar{H}_\nu(\boldsymbol{R})$ and $B_\nu(\boldsymbol{k};\boldsymbol{r})$ practically, we should make an expansion of all terms in (3.28) (or (3.29)) in powers of B, and after that carry out a successive method of solution. But now one may raise the question: Why not apply this procedure directly to the actual Schrödinger equation? We shall really do it in the next chapter. Against this, Roth's method is more constructive as it relatively simply yields concrete expressions involving Bloch factors and energies only. More or less modified versions of Roth's theory are given by W. G. Chambers [44], Eilenberger [39], Schnakenberg [45], and Zak [46].

Although we can consider the existence of a one-band Hamiltonian to be established for arbitrarily high fields, its practical application is restricted to field strengths for which the asymptotic expansions (3.16), (3.17), (3.18) and (3.25) are significant. Otherwise its determination is not simpler than the direct solution of the original Schrödinger equation. As mentioned above, this range of field strength depends on the minimal interband spacing $E_r(\boldsymbol{k}) - E_{r'}(\boldsymbol{k})$ and the localization of the Wannier function $a_r(\boldsymbol{x})$ [44]. Both are closely connected with the analytic structure of Bloch bands [36, 38]. There are no reliable estimates up to now [39, 44]. Weakly bound electrons have small band gaps so that the limits of a one-band description are often reached quickly (magnetic breakdown). In such cases a direct solution of the problem [22] is more adequate than a description by effective Hamiltonians. If small band gaps (e.g. small spin–orbit splitting) appear in case of stronger binding, nondiagonal Hamiltonians involving the bands concerned are not avoidable. One can use either a Roth Hamiltonian uncoupled from sufficiently distant bands [47, 48] or an effective Hamiltonian formed from a secular Hamiltonian [49, 50, 44] of a finite band model [38]. The latter seems to be more appropriate for describing magnetic breakdown effects.

3.3 Symmetry properties of effective Hamiltonians

Looking at (A 8), we immediately see that effective Hamiltonians

$$H(\tilde{\boldsymbol{w}}) = \sum_{\boldsymbol{R}} H(\boldsymbol{R})\, \mathrm{e}^{i(\tilde{\boldsymbol{w}}, \boldsymbol{R})}$$

are invariant under the transformations

$$B_0(\hat{\boldsymbol{K}}) = \mathrm{e}^{i\pi j l p/q}\, \mathrm{e}^{i(\boldsymbol{w}, \hat{\boldsymbol{K}} \times \boldsymbol{\lambda})},$$

where $\hat{\boldsymbol{K}} = j\,\boldsymbol{K}_1 + l\,\boldsymbol{K}_2$ is a reciprocal lattice vector in the plane perpendicular to the magnetic field. For $\boldsymbol{K} = \boldsymbol{K}_c$ we have defined these operators before (2.43) and found them to constitute an Abelian group. In the general case we get the multiplication formula

$$B_0(\hat{\boldsymbol{K}}')\, B_0(\hat{\boldsymbol{K}}) = \mathrm{e}^{-i2\pi j' l p/q}\, B_0(\hat{\boldsymbol{K}}' + \hat{\boldsymbol{K}})\ ; \quad \hat{\boldsymbol{K}} = j\,\boldsymbol{K}_1 + l\,\boldsymbol{K}_2\,, \quad \hat{\boldsymbol{K}}' = j'\,\boldsymbol{K}_1 + l'\,\boldsymbol{K}_2$$

from (A 4) and (2.13). Hence we infer that the operators can be completed to a group $\mathfrak{G}'$ by the q-th unit roots according to

$$B_r(\hat{\boldsymbol{K}}) = \mathrm{e}^{-i2\pi r p/q}\, B_0(\hat{\boldsymbol{K}})\ ; \qquad r = 0, \ldots, q-1\,.$$

In $\mathfrak{G}'$ we have the multiplication rule

$$B_{r'}(\hat{\boldsymbol{K}}')\, B_r(\hat{\boldsymbol{K}}) = B_{r+r'+j'l}\,(\hat{\boldsymbol{K}}' + \hat{\boldsymbol{K}})\,,$$

where indices of group elements are to be taken modulo q. The structure of $\mathfrak{G}'$ is completely analogous to that one of $\mathfrak{G}$. Especially, $\mathfrak{G}'$ contains the Abelian normal subgroup $\mathfrak{F}'$ of the elements $B_r(\boldsymbol{K}_c)$ with respect to with it is arranged in left cosets:

$$\mathfrak{G}' = \mathfrak{F}' + B_0(\boldsymbol{K}_1)\,\mathfrak{F}' + B_0(2\,\boldsymbol{K}_1)\,\mathfrak{F}' + \cdots + B_0\left((q-1)\,\boldsymbol{K}_1\right)\mathfrak{F}'\,.$$

Along the lines of Section 2.3 the irreducible representations of $\mathfrak{G}'$ are induced by the allowable representations of the little groups that belong to the one-

dimensional representations

$$D'^{k,\,t}\big(B_r(\boldsymbol{K}_c)\big) \qquad e^{-i2\pi rtp/q}\, e^{i(k,\,\boldsymbol{K}_c\times\lambda)}\,;$$

$$k = \frac{1}{N}\,(n_1\,\boldsymbol{K}_1 + n_2\,\boldsymbol{K}_2): \qquad n_1 = 0, \ldots, \frac{N}{p}\,q - 1\,; \qquad n_2 = 0, \ldots, \frac{N}{p} - 1\,;$$

$$t = 0, \ldots, q - 1$$

of the Abelian normal subgroup $\mathfrak{F}'$. The orbits of $\mathfrak{F}'$ relative to $\mathfrak{G}'$ can again be characterized by the vector $\boldsymbol{q}$ (cf. equation (2.26)). Also in this case only the q-dimensional irreducible representations

$$\left.\begin{aligned} D'^{\boldsymbol{q},\,1}_{m\,n}\big(B_r\,(\boldsymbol{K}_c + j\,\boldsymbol{K}_1)\big) &= e^{-i2\pi rp/q}\; e^{i\,(\boldsymbol{q}+n\,\boldsymbol{K}_1,\,\boldsymbol{K}_c\times\lambda)}\,\delta_{n,\,(m+j)_q}; \\ n, m, j &= 0, \ldots, q-1 \end{aligned}\right\} \tag{3.30}$$

belonging to $t = 1$ give rise to non-zero projectors

$$P'^{\boldsymbol{q},\,1}_{n} = \frac{p^2}{N^2\,q}\sum_{\boldsymbol{K}_c} e^{-i\,(\boldsymbol{q}+n\,\boldsymbol{K}_1,\,\boldsymbol{K}_c\times\lambda)}\,B_0(\boldsymbol{K}_c)\,. \tag{3.31}$$

In the limit $N \to \infty$ N^2 is to be replaced by $|\boldsymbol{K}_1\times\boldsymbol{K}_2|$.

To find partner functions belonging to the m-th row of (3.30) the latter are applied to the basis vectors

$$\frac{1}{\sqrt{2\pi}}\, e^{-i\lambda\left[q_1+\left(\frac{n}{q}+\frac{m}{p}+k\right)K_{02}\right]}v_{(1)}\;;\quad n = 0, \ldots, q-1\;;\quad m = 0, \ldots, p-1 \tag{3.32}$$

of the Hilbert space $\mathfrak{H}'$. This is done in Appendix III and the complete orthonormal set

$$\chi_{n\,\boldsymbol{q}}(m;\,v_{(1)}) = \left(\frac{\lambda\,p}{K_{22}}\right)^{1/2}\sum_{k=-\infty}^{+\infty} e^{i(\lambda/2)\left(k+\frac{n}{q}+\frac{m}{p}\right)^2 K_{01}\,K_{02}}\, e^{i\,\lambda\left(k+\frac{n}{q}+\frac{m}{p}\right)q_2\,K_{01}}\times$$

$$\times\,\frac{1}{\sqrt{2\,\pi}}\, e^{-i\lambda\left[q_1+\left(k+\frac{n}{q}+\frac{m}{p}\right)K_{01}\right]}v_{(1)} \tag{3.33}$$

with the properties

$$\left.\begin{aligned} &\text{and} \qquad (\chi_{n'\,\boldsymbol{q}'}(m';\,v_{(1)})\,|\chi_{n\,\boldsymbol{q}}(m;\,v_{(1)})) = \delta_{n'\,n}\,\delta_{m'\,m}\,\delta\,(\boldsymbol{q}'_\perp - \boldsymbol{q}_\perp) \\ &\qquad\qquad B_0(\boldsymbol{K}_c)\,\chi_{n\,\boldsymbol{q}} = e^{i\,(\boldsymbol{q}+n\,\boldsymbol{K}_1,\,\boldsymbol{K}_c\times\lambda)}\,\chi_{n\,\boldsymbol{q}} \end{aligned}\right\} \tag{3.34}$$

is obtained. We now enter the effective one-band equation (3.26) with the expansion

$$\bar{b}_{\alpha_\nu\,\boldsymbol{q}}(v_{(1)}) = \sum_{m=0}^{p-1}\bar{b}_{\alpha_\nu\,\boldsymbol{q}}(m)\,\chi_{n\,\boldsymbol{q}}(m;\,v_{(1)})$$

which automatically satisfies the boundary condition (3.10), and obtain the algebraic eigenvalue equation

$$\sum_{m'=0}^{p-1} \bar{H}_{\nu\,\boldsymbol{q}}(m', m)\, \bar{b}_{\alpha_\nu \boldsymbol{q}}(m) = \mathscr{E}_{\alpha_\nu}(\boldsymbol{q})\, \bar{b}_{\alpha_\nu \boldsymbol{q}}(m') \,. \tag{3.35}$$

The $p \times p$ matrix

$$\left.\begin{aligned} \bar{H}_{\nu\,\boldsymbol{q}}(m', m) &= \sum_{\tilde{\boldsymbol{R}}} \bar{H}'_\nu(\tilde{\boldsymbol{R}} + (m - m')_p \boldsymbol{R}_2)\, \mathrm{e}^{i(\boldsymbol{q} - (m/p)\boldsymbol{K}_0)\tilde{\boldsymbol{R}} + (m - m')_p \boldsymbol{R}_2)} \,; \\ \bar{H}'_\nu(\boldsymbol{R}) &= \mathrm{e}^{-i\pi j (k p - k')\, q/p}\, \bar{H}_\nu(\boldsymbol{R}) \,; \quad \boldsymbol{R} = \tilde{\boldsymbol{R}} + k' \tilde{\boldsymbol{R}}_2 \,; \\ \tilde{\boldsymbol{R}} &= j \boldsymbol{R}_1 + k\, p \boldsymbol{R}_2 + l \boldsymbol{R}_3 \,; \quad k' = (m - m')_p = 0, \ldots, p-1 \end{aligned}\right\} \tag{3.36}$$

results from (A 11) and (A 12), where $(m - m')_p$ means $m - m'$ modulo p. These considerations analogously apply, of course, to nondiagonal effective Hamiltonians, too.

The q-dimensionality of the representations (3.30) does not mean that there is an additional q-fold degeneracy of the energy values $\mathscr{E}_{\alpha_\nu}(\boldsymbol{q})$. It simply reflects the periodicity $\mathscr{E}_{\alpha_\nu}(\boldsymbol{q}) = \mathscr{E}_{\alpha_\nu}(\boldsymbol{q} + n \boldsymbol{K}_1)$ which is obvious because of $\bar{H}_{\nu\,\boldsymbol{q}}(m', m) = \bar{H}_{\nu,\,\boldsymbol{q} + n \boldsymbol{K}_1}(m', m)$. This is not in contradiction to (2.50) but corresponds to another way of labelling the energy values. (2.50) was concluded from (2.49) and (2.48). Here we have

$$\bar{H}_{\nu,\,\boldsymbol{q} + (1/p)\boldsymbol{K}_0}(m', m) = \mathrm{e}^{i 2\pi (m - m')\, l/p}\, \bar{H}_{\nu\,\boldsymbol{q}}(m + j, m' + j) \,; \quad \boldsymbol{K}_0 = j \boldsymbol{K}_0 + l \boldsymbol{K}_2 \,,$$

i.e. the substitution $\boldsymbol{q} \to \boldsymbol{q} + (1/p)\boldsymbol{K}_0$ only involves a cyclic shift of the row and column indices and a trivial phase change of the solutions. This can be ascribed to a unitary transformation so that the eigenvalues of $\bar{H}_{\nu,\boldsymbol{q} + (1/p)\boldsymbol{K}_0}(m', m)$ agree with those of $\bar{H}_{\nu\,\boldsymbol{q}}(m', m)$ if they are correspondingly relabelled. In this way (2.49) and (2.50) can be recovered. The common measure of the two periods $\boldsymbol{K}_1$ and $(q/p)\,\boldsymbol{K}_1$ is $(1/p)\,\boldsymbol{K}_1$ which is the real period of magnetic subbands (cf. Fig. 2). In line with Section 2.6 we mention the well-known fact that the $p \times p$ Hermitian matrix (3.36) possesses p eigenvalues.

An algebraic Schrödinger equation similar to (3.35) has been solved for a simple model with several q/p values by Butler and Brown [31]. Besides they used a two-band model to include magnetic interband breakdown.

4. Solution Methods of the Schrödinger Equation

In Sections 2 and 3 various forms (cf. equations (2.40), (2.46), (3.3), (3.26), and (3.36)) of the Schrödinger equation $H \psi = \mathscr{E} \psi$ have been derived in utilizing the basic invariance properties of the problem. The equations (2.40) and (2.46) as well as Roth's many-band equation (3.3) are exact, whereas the one-band equations (3.26) and (3.36) are significant only in case of more or less strongly bound electrons as is pointed out in Section 3.2. Accordingly, we distinguish weak and strong binding in what follows. To give a general survey of the problem involved we first deal with the asymptotic approximation without restricting the potential. In case of strong binding we treat the one-band equation (3.26) confining ourselves to cases in which magnetic breakdown is unimportant. In case of weak binding we apply Schrödinger's perturbation theory and, besides, specialize the general asymptotic approximation (magnetic breakdown).

4.1 Asymptotic approximation

The asymptotic approximation we here develop is a generalization of the well-known WKB method to systems of ordinary differential equations [22]. It shall be applied to (2.46), which is such a system and an infinite one, too. First we make it a finite system by restricting ourselves to the r shortest reciprocal lattice vectors. This allows theorems of linear algebra to be used. After that we proceed again to the infinite case.

We write (2.46) in the $u_{(1)}$-representation

$$\frac{\hbar^2}{2m}\left[\left(\frac{1}{i\lambda}\frac{\mathrm{d}}{\mathrm{d}u}+K_2'\right)^2+(u+K_1')^2+(q_3+K_3')^2-\frac{2m\mathscr{E}}{\hbar^2}\right]C^{\boldsymbol{K}'}(u)+$$
$$+\sum_{\boldsymbol{K}''}V_{\boldsymbol{K}'-\boldsymbol{K}''}\,C^{\boldsymbol{K}''}(u)=0\,. \tag{4.1}$$

$\boldsymbol{K}'$ and $\boldsymbol{K}''$ take r different values. For simplicity and brevity we have dropped the spin terms and omitted the quantum numbers α, $\boldsymbol{q}$ as well as the index of $u_{(1)}$. The ansatz

$$C^{\boldsymbol{K}'}(u)=\mathrm{e}^{i\lambda\int\varphi(u)\,\mathrm{d}u}\sum_l\lambda^{-l}f_{\boldsymbol{K}',l}(u) \tag{4.2}$$

is an asymptotic expansion of $C^{\boldsymbol{K}'}$ in powers of λ^{-1}. We insert it in (4.1) and assume the arising equations

$$\sum_l\lambda^{-l}\left\{\frac{\hbar^2}{2m}\left[-i\lambda^{-1}\varphi'\,f_{\boldsymbol{K}',l}-2i\lambda^{-1}(\varphi+K_2')\,f_{\boldsymbol{K}',l}'-\lambda^{-2}f_{\boldsymbol{K}',l}''\right]+\right.$$
$$+\frac{\hbar^2}{2m}\left[(u+K_1')^2+(\varphi+K_2')^2+(q_3+K_3')^2-\frac{2m\mathscr{E}}{\hbar^2}\right]f_{\boldsymbol{K}',l}+$$
$$\left.+\sum_{\boldsymbol{K}''}V_{\boldsymbol{K}'-\boldsymbol{K}''}\,f_{\boldsymbol{K}'',l}\right\}=0 \tag{4.3}$$

to be separately fulfilled in each order. Primes denote derivatives with respect to u. In zeroth order we have the homogeneous system

$$\left.\begin{aligned}&\sum_{\boldsymbol{K}''}B_{\boldsymbol{K}'\boldsymbol{K}''}(u,\varphi,q_3;\mathscr{E})\,f_{\boldsymbol{K}'',0}(u)=0\,;\\ &B_{\boldsymbol{K}'\boldsymbol{K}''}(u,\varphi,q_3;\mathscr{E})=\\ &=\frac{\hbar^2}{2m}\left[(u+K_1')^2+(\varphi+K_2')^2+(q_3+K_3')^2-\frac{2m\mathscr{E}}{\hbar^2}\right]\delta_{\boldsymbol{K}'\boldsymbol{K}''}+V_{\boldsymbol{K}'-\boldsymbol{K}''}\end{aligned}\right\} \tag{4.4}$$

of algebraic equations, where $V_{\boldsymbol{0}}=0$ is assumed. Its solvability condition

$$\det B_{\boldsymbol{K}'\boldsymbol{K}''}(u,\varphi,q_3;\mathscr{E})=0 \tag{4.5}$$

implicitly defines the phase function $\varphi=\varphi(u)$ as a $2r$-valued algebraic function (Fig. 3). With the so determined $\varphi(u)$ and any fixed $\boldsymbol{K}$ equation (4.4) is satisfied by

$$f_{\boldsymbol{K}',0}=\frac{\mathscr{B}_{\boldsymbol{K}\boldsymbol{K}'}}{\mathscr{B}_{\boldsymbol{K}\boldsymbol{K}}}f_{\boldsymbol{K},0}\,, \tag{4.6}$$

where $\mathscr{B}_{\boldsymbol{K}\boldsymbol{K}'}$ is the algebraic complement of $B_{\boldsymbol{K}\boldsymbol{K}'}$. $f_{\boldsymbol{K},0}(u)$ is arbitrary for the time being. Apparently, we must suppose that $\mathscr{B}_{\boldsymbol{K}\boldsymbol{K}}$ and $\det B_{\boldsymbol{K}'\boldsymbol{K}}$ do not vanish

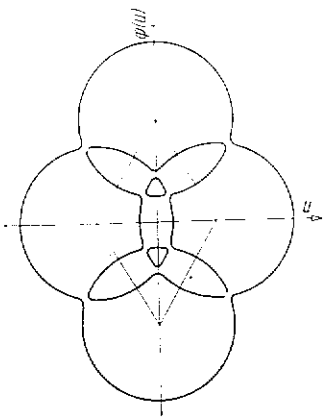

Fig. 3. Example of a 2 r-valued phase function for $r = 4$. The rhombus is a unit cell of the basal plane of a hexagonal lattice

at the same time. The first-order terms of (4.3) form the inhomogeneous system

$$\sum_{\boldsymbol{K}''} B_{\boldsymbol{K}'\boldsymbol{K}''} f_{\boldsymbol{K}'',1} = i \frac{\hbar^2}{2m} [\varphi' f_{\boldsymbol{K}',0} + 2(\varphi + K_2') f'_{\boldsymbol{K}',0}]$$

of equations whose determinant is equal to zero according to (4.5). It is solvable if and only if the inhomogeneity is orthogonal to the solutions (4.6) of the corresponding homogeneous system (4.4), that is if

$$\sum_{\boldsymbol{K}'} [\varphi' f_{\boldsymbol{K}',0} + 2(\varphi + K_2') f'_{\boldsymbol{K}',0}] \mathcal{B}^*_{\boldsymbol{K}\boldsymbol{K}'} = 0 .$$

Because of (4.6), this condition can be written as the ordinary first-order differential equation

$$2 f'_{\boldsymbol{K},0} \sum_{\boldsymbol{K}'} (\varphi + K_2') |\mathcal{B}_{\boldsymbol{K}\boldsymbol{K}'}|^2 + f_{\boldsymbol{K},0} \sum_{\boldsymbol{K}'} \left[\varphi' + 2(\varphi + K_2') \left(\frac{\mathcal{B}'_{\boldsymbol{K}\boldsymbol{K}'}}{\mathcal{B}_{\boldsymbol{K}\boldsymbol{K}'}} - \frac{\mathcal{B}'_{\boldsymbol{K}\boldsymbol{K}}}{\mathcal{B}_{\boldsymbol{K}\boldsymbol{K}}}\right)\right] |\mathcal{B}_{\boldsymbol{K}\boldsymbol{K}'}|^2 = 0$$

for the function $f_{\boldsymbol{K},0}(u)$, which was yet arbitary in (4.6). The solution

$$f_{\boldsymbol{K},0}(u) = \left[\sum_{\boldsymbol{K}'} (\varphi + K_2') |\mathcal{B}_{\boldsymbol{K}\boldsymbol{K}'}|^2\right]^{-1/2} \mathcal{B}_{\boldsymbol{K}\boldsymbol{K}}$$

can easily be verified. Because of $\mathcal{B}^*_{\boldsymbol{K}\boldsymbol{K}'} = \mathcal{B}_{\boldsymbol{K}'\boldsymbol{K}}$ the more expedient expression

$$f_{\boldsymbol{K},0}(u) = \left[\sum_{\boldsymbol{K}'} (\varphi + K_2') \mathcal{B}_{\boldsymbol{K}'\boldsymbol{K}'}\right]^{-1/2} \mathcal{B}^{1/2}_{\boldsymbol{K}\boldsymbol{K}}$$

is justified by the relation $\mathcal{B}_{\boldsymbol{K}'\boldsymbol{K}} \mathcal{B}_{\boldsymbol{K}''\boldsymbol{K}'} = \mathcal{B}_{\boldsymbol{K}''\boldsymbol{K}} \mathcal{B}_{\boldsymbol{K}'\boldsymbol{K}'}$ that exists between algebraic complements of the elements of a vanishing determinant. The other solutions (4.6) with $\boldsymbol{K}' \neq \boldsymbol{K}$ are now given by

$$f_{\boldsymbol{K}',0}(u) = \left[\sum_{\boldsymbol{K}''} (\varphi + K_2'') \mathcal{B}_{\boldsymbol{K}''\boldsymbol{K}''}\right]^{-1/2} \mathcal{B}_{\boldsymbol{K}\boldsymbol{K}'} \mathcal{B}^{-1/2}_{\boldsymbol{K}\boldsymbol{K}} . \tag{4.7}$$

Therewith, in the lowest-order asymptotic approximation, we have determined the $2r$ independent solution "vectors" with the r components

$$C^{\boldsymbol{K}'}(u) = f_{\boldsymbol{K}',0}(u) \, e^{i\lambda \int \varphi(u) \, du} \tag{4.8}$$

that belong to the $2r$ branches of the algebraic function $\varphi(u)$. We now ask for the meaning of these solutions if $\boldsymbol{K}'$ runs through all the points of the reciprocal lattice ($r \to \infty$). In comparing (4.4) with the plane-wave representation of

Bloch's Schrödinger equation,

$$\left[\frac{\hbar^2}{2m}(\boldsymbol{k}-\boldsymbol{K}')^2 - E_\nu(\boldsymbol{k})\right] c_\nu(\boldsymbol{k},\boldsymbol{K}') + \sum_{\boldsymbol{K}''} V_{\boldsymbol{K}'-\boldsymbol{K}''}\, c_\nu(\boldsymbol{k},\boldsymbol{K}'') \equiv$$

$$\equiv \sum_{\boldsymbol{K}''} B_{\boldsymbol{K}'\boldsymbol{K}''}\big(\boldsymbol{k}; E_\nu(\boldsymbol{k})\big)\, c_\nu(\boldsymbol{k},\boldsymbol{K}'') = 0\ , \tag{4.9}$$

we find (4.5) to be equivalent to the defining equation

$$E_\nu(u, \varphi(u), q_3) = \mathscr{E} \tag{4.10}$$

of the phase function $\varphi(u)$ for $r \to \infty$, where $E_\nu(\boldsymbol{k}) \equiv E_\nu(k_1, k_2, k_3)$ is the Bloch energy. Thus, $\varphi(u)$ just describes the cyclotron orbits of the semiclassical theory. On the other hand, $\det B_{\boldsymbol{K}'\boldsymbol{K}''}\big(\boldsymbol{k}; E_\nu(\boldsymbol{k})\big) = 0$ is identically fulfilled for any $\boldsymbol{k}$ so that

$$\frac{\partial}{\partial k_2} \det B_{\boldsymbol{K}'\boldsymbol{K}''}\big(\boldsymbol{k}; E_\nu(\boldsymbol{k})\big) = \sum_{\boldsymbol{K}'} \mathscr{B}_{\boldsymbol{K}'\boldsymbol{K}'} \left[\frac{\hbar^2}{m}(k_2 - K_2') - \frac{\partial E_\nu}{\partial k_2}\right] = 0 \tag{4.11}$$

is also satisfied for any $\boldsymbol{k}$. Moreover, the solutions of (4.9) may be written as

$$c_\nu(\boldsymbol{k}, \boldsymbol{K}') = \left(\sum_{\boldsymbol{K}''} |\mathscr{B}_{\boldsymbol{K}\boldsymbol{K}''}|^2\right)^{-1/2} \mathscr{B}_{\boldsymbol{K}\boldsymbol{K}'} = \mathscr{B}_{\boldsymbol{K}\boldsymbol{K}}^{-1/2} \left(\sum_{\boldsymbol{K}''} \mathscr{B}_{\boldsymbol{K}''\boldsymbol{K}''}\right)^{-1/2} \mathscr{B}_{\boldsymbol{K}\boldsymbol{K}'}\ . \tag{4.12}$$

In (4.11) and (4.12) $\mathscr{B}_{\boldsymbol{K}'\boldsymbol{K}''}$ is imagined to be the algebraic complement of $B_{\boldsymbol{K}'\boldsymbol{K}''}\big(\boldsymbol{k}; E_\nu(\boldsymbol{k})\big)$. Combining (4.11) and (4.12) with (4.7) and making use of the well-known fact that the Fourier components of Bloch factors can be chosen so that $c_\nu(\boldsymbol{k}, \boldsymbol{K}') = c_\nu(\boldsymbol{k} + \boldsymbol{K}')$, we find

$$f_{\boldsymbol{K}',0}(u) = \left(\frac{\partial E_\nu}{\partial k_2}\right)^{-1/2}_{\boldsymbol{k}=\bar{\bar{\boldsymbol{w}}}} c_\nu(\bar{\bar{\boldsymbol{w}}} + \boldsymbol{K}')\ , \tag{4.13}$$

where the quasi-classical value $\bar{\bar{\boldsymbol{w}}} = (u, \varphi(u), q_3)$ of $\tilde{\boldsymbol{w}}$ is the radius vector of the cyclotron path. The general solution of (4.1) is a linear combination

$$C^{\boldsymbol{K}}(u) = \sum_{\nu,i} \sum_{l=-\infty}^{+\infty} \alpha_{\nu,i}^{(l)} \left(\frac{\partial E_\nu}{\partial k_2}\right)^{-1/2}_{\boldsymbol{k}=\bar{\bar{\boldsymbol{w}}}_{\nu,i}} c_\nu(\bar{\bar{\boldsymbol{w}}}_{\nu,i}^{(l)} + \boldsymbol{K})\, \mathrm{e}^{\mathrm{i}\int \varphi_{\nu,i}^{(l)} \mathrm{d}u}\ ; \quad \bar{\bar{\boldsymbol{w}}}_{\nu,i}^{(l)} = \big(u, \varphi_{\nu,i}^{(l)}(u), q_3\big) \tag{4.14}$$

of the independent solutions (4.8), (4.13) belonging to the different branches $\varphi_{\nu,i}^{(l)} = \varphi_{\nu,i}^{(0)} + l\, K_{22}$ of $\varphi(u)$, where ν denotes the Bloch bands that overlap at the energy $\mathscr{E}$, i labels the branches within the band ν, and l allows for the branches of φ in different Brillouin zones.

The asymptotic solutions (4.8), (4.13) of (4.1) fail in the vicinity of branch points of $\varphi(u)$. These are multiple zeros of (4.10), i.e. such (generally complex) points u_0, where at the same time (4.10) and $(\partial/\partial k_2)\, E_\nu(\boldsymbol{k})\big|_{\boldsymbol{k}=\bar{\bar{\boldsymbol{w}}}_0} = 0$ are fulfilled. There (4.13) tends to infinity. Since the asymptotic solutions are needed only on the real u-axis, merely the branch points near the real axis are important. There are two types of branch points which are generally two-sheeted [22]. The first one comprises the relatively isolated turning points, which are always real and two-sheeted. They join branches of $\varphi(u)$ that belong to one and the same Bloch band. The branch points of the other type lie in pairs close together near or on the real axis. We call them breakdown points because they are responsible for magnetic breakdown. We further distinguish between intra- and interband breakdown points. The former connect two branches of $\varphi(u)$ belonging

to the same Bloch band. They appear close to saddle points of $E_\nu(\boldsymbol{k})$ where the semiclassical orbits near each other very much so that a strong coupling happens between them. The latter occur at branch points of continuous Bloch bands $E_\nu(\boldsymbol{k})$, $E_{\nu'}(\boldsymbol{k})$ with very small interband energies $E_\nu(\boldsymbol{k}) - E_{\nu'}(\boldsymbol{k})$, i.e. the corresponding branches of $\varphi(u)$ change from one band to the other one. They appear in pairs near the real u-axis in the vicinity of those values u for which $E_\nu(\bar{\boldsymbol{k}}) - E_{\nu'}(\bar{\boldsymbol{k}})$ becomes minimum. In general only two bands are nearing each other at one point in $\boldsymbol{k}$-space. Therefore, also interband breakdown points are mostly two-sheeted [22, 38].

The asymptotic solutions (4.8) right and left of branch points of this kind are distinctively connected with each other. A solution, which on the left of a branch point u_0 contains only one branch φ_1 of φ, goes on the right over into a linear combination of solutions that belong to both branches φ_1 and φ_2 joining there (and vice versa):

$$C^{\boldsymbol{K}}(u) = \begin{cases} f^{(1)}_{\boldsymbol{K},0}(u)\, \mathrm{e}^{i\lambda \int \varphi_1 \mathrm{d}u} \,; & u < u_0 \,, \\ A_1\, f^{(1)}_{\boldsymbol{K},0}(u)\, \mathrm{e}^{i\lambda \int \varphi_1 \mathrm{d}u} + A_2\, f^{(2)}_{\boldsymbol{K},0}\, \mathrm{e}^{i\lambda \int \varphi_2 \mathrm{d}u} \,; & u > u_0 \,. \end{cases}$$

For turning points these so-called connecting relations are well-known from the WKB method [48]. For breakdown points they are just Pippard's compatibility relations at junctions of a network of semiclassical orbits [51]. These connecting relations determine the coherence between the coefficients of the linear combination (4.14) on both sides of a branch point so that the general asymptotic solution of (4.1) is given on the whole real u-axis. Finally, the asymptotic eigenfunctions of (2.40) are obtained by subjecting this general solution of (4.1) to the subsidiary condition (2.47). This makes adjacent coefficients of the linear combination obey a homogeneous system of equations the determinantal condition of which yields the energy eigenvalues in dependence on the magnetic wave vector $\boldsymbol{q}$.

Ascertaining connecting relations requires more elaborate investigations. We come back to this question in case of turning points (Section 4.2) and interband breakdown points (Section 4.3.3) and refer the reader to original papers in case of intraband breakdown.

The lowest-order asymptotic solution of the Schrödinger equation (2.46) has been obtained without using the effective-Hamiltonian theory. In principle, our procedure could be carried to higher orders thus making effective Hamiltonians needless at all. But this is easier said than done. Remembering that the difficulties in Section 3.2 just began with higher-order terms, we prefer to apply the theory we have already worked out.

4.2 Strong binding

This section is concerned with the solution of the effective one-band equation (3.26). As pointed out above the decoupling procedure leading to (3.26) is significant chiefly in case of (more or less) strong binding. It should be mentioned once more that a one-band approach is unsatisfactory if spin effects such as small spin–orbit band gaps or inversion asymmetry splitting [52] are important.

The adequate solution method of the one-band Schrödinger equation (3.26) is the asymptotic (or WKB) method since the one-band Hamiltonian is already given as the asymptotic expansion (3.19). The application of the WKB method

to effective Schrödinger equations originated in the papers of Zilberman [13, 53], Harper [54], and Brailsford [55].

We put the ansatz

$$b(u) = \mathrm{e}^{i\lambda \int \varphi(u)\,\mathrm{d}u} \sum_l \lambda^{-l} g_l(u) \tag{4.15}$$

into the one-band equation (3.26), write $\mathrm{e}^{i(\widetilde{\boldsymbol{w}}, \boldsymbol{R})} = \mathrm{e}^{i R_1 k_1 + 2i} \mathrm{e}^{i(u R_1 - q_3 R_3)} \mathrm{e}^{i R_2 \lambda} \,\mathrm{d}u$ as well as $H_\nu(\boldsymbol{R}) = H_0(\boldsymbol{R}) + \lambda^{-1} H_1(\boldsymbol{R}) + \lambda^{-2} H_2(\boldsymbol{R}) + \cdots$ and expand all the terms to second order in powers of λ^{-1}. Supposing the arising equation to be separately fulfilled in each order, we obtain the equations

$$\overline{H}_0(u, \varphi(u), q_3)\, g_0(u) = \mathscr{E}\, g_0(u)\,, \tag{4.16}$$

$$\overline{H}_0\, g_1 + \frac{1}{i}\frac{\partial \overline{H}_0}{\partial \varphi}\, g_0' + \left(\overline{H}_1 - \frac{i}{2}\varphi' \frac{\partial^2 \overline{H}_0}{\partial \varphi^2} - \frac{i}{2}\frac{\partial^2 \overline{H}_0}{\partial u\, \partial \varphi}\right) g_0 = \mathscr{E}\, g_1\,, \tag{4.17}$$

$$\begin{aligned}
&\overline{H}_0\, g_2 + \frac{1}{i}\frac{\partial \overline{H}_0}{\partial \varphi}\, g_1' + \left(\overline{H}_1 - \frac{i}{2}\varphi' \frac{\partial^2 \overline{H}_0}{\partial \varphi^2} - \frac{i}{2}\frac{\partial^2 \overline{H}_0}{\partial u\, \partial \varphi}\right) g_1 - \\
&\quad - \frac{1}{2}\frac{\partial^2 \overline{H}_0}{\partial \varphi^2}\, g_0'' - \left(\frac{1}{2}\varphi' \frac{\partial^3 \overline{H}_0}{\partial \varphi^3} + \frac{1}{2}\frac{\partial^3 \overline{H}_0}{\partial u\, \partial \varphi^2} - \frac{1}{i}\frac{\partial \overline{H}_1}{\partial \varphi}\right) g_0' + \\
&\quad + \left(-\frac{1}{6}\varphi'' \frac{\partial^3 \overline{H}_0}{\partial \varphi^3} - \frac{1}{8}\varphi'^2 \frac{\partial^4 \overline{H}_0}{\partial \varphi^4} - \frac{1}{4}\varphi' \frac{\partial^4 \overline{H}_0}{\partial u\, \partial \varphi^3} - \right. \\
&\quad \left. - \frac{1}{8}\frac{\partial^4 \overline{H}_0}{\partial u^2\, \partial \varphi^2} + \overline{H}_2 - \frac{i}{2}\varphi' \frac{\partial^2 \overline{H}_1}{\partial \varphi^2} - \frac{i}{2}\frac{\partial^2 \overline{H}_1}{\partial u\, \partial \varphi}\right) g_0 = \mathscr{E}\, g_2
\end{aligned} \tag{4.18}$$

in zeroth, first, and second order. Here $\overline{H}_0(\boldsymbol{k}) \equiv E(\boldsymbol{k})$ is the Bloch energy (with the band index omitted). $\overline{H}_0 \equiv E$, $\overline{H}_1$, and $\overline{H}_2$ are to be taken with the argument $\widetilde{\boldsymbol{w}} = (u, \varphi(u), q_3)$ which is the semiclassical value of $\widetilde{\boldsymbol{w}}$. A partial derivative with respect to φ means $\partial \overline{H}_0/\partial \varphi \equiv (\partial \overline{H}_0(\boldsymbol{k})/\partial k_2)_{\boldsymbol{k} = \widetilde{\boldsymbol{w}}}$ by way of example. Equation (4.16) is identical with (4.10). It defines the phase function $\varphi(u)$ that describes the cyclotron orbits in $\boldsymbol{k}$-space. By integrating (4.17) we find

$$g_0(u) = h(\widetilde{\boldsymbol{w}})\, \mathrm{e}^{i \int \Phi^{(1)}\,\mathrm{d}u}\,; \qquad h(\widetilde{\boldsymbol{w}}) = \left(\frac{\partial E}{\partial \varphi}\right)^{-1/2}, \qquad \Phi^{(1)}(\widetilde{\boldsymbol{w}}) = -\,\overline{H}_1\, h^2\,. \tag{4.19}$$

Taking this into account, we obtain

$$g_1(u) = g_0(u)\left[i \int \Phi^{(2)}\,\mathrm{d}u + \frac{1}{2}\frac{\partial \Phi^{(1)}}{\partial \varphi}\right];$$

$$\Phi^{(2)}(u) = \frac{h}{2}\left[\left(\frac{\partial^2 E}{\partial \varphi^2}\, h'\right)' + \frac{1}{4}\left(\frac{\partial^2 E}{\partial \varphi^2}\right)'' h + \frac{1}{12}\varphi''' \frac{\partial^3 E}{\partial \varphi^3}\, h\right] + h^2\left[\frac{1}{2}\frac{\partial}{\partial \varphi}(h^2\, \overline{H}_1^2) - \overline{H}_2\right] \tag{4.20}$$

from (4.18) by integration, where primes denote total derivatives with respect to u. We now combine (4.19) and (4.20) according to (4.15) and arrive at

$$\overline{b}(u) = h\left(1 + \frac{1}{2\lambda}\frac{\partial \Phi^{(1)}}{\partial \varphi}\right)\mathrm{e}^{i\lambda \int \Phi\,\mathrm{d}u}\,; \qquad \Phi = \varphi + \lambda^{-1}\, \Phi^{(1)} + \lambda^{-2}\, \Phi^{(2)}\,. \tag{4.21}$$

This result (inclusive of $\Phi^{(2)}$) has been first derived by Zilberman [53], however without having regard to corrections like $\bar{H}_1$ and H_2. From the lowest-order asymptotic solution $\bar{b}(u) = h(u) \exp i\lambda \int q \, du$ we can easily obtain the corresponding approximation of the independent solutions $C^{\boldsymbol{K}}(u)$ of (2.46). Writing $e^{-i(\widetilde{\boldsymbol{ic}}, x)} = e^{i x_1 x_2/2\lambda} \, e^{-i(u x_1 + \eta_3 x_3)} \, e^{-(x_2/\lambda) \mathrm{d}_1 \mathrm{d}u}$ we find

$$e^{-i(\widetilde{\boldsymbol{ic}}, x)} \, \bar{b}(u) = e^{-i(\overline{\widetilde{\boldsymbol{ic}}}, x)} \, \bar{b}(u)$$

in zeroth order of λ^{-1}. Inserting this with (3.27) ($S_{\nu'\nu} = \delta_{\nu'\nu}$) into (3.9) and using (3.6), we recover (4.8) and (4.13), i.e.

$$C^{\boldsymbol{K}}(u) = c_\nu(\overline{\widetilde{\boldsymbol{ic}}} + \boldsymbol{K}) \left(\frac{\partial E}{\partial \varphi}\right)^{-1/2} e^{i\lambda \int \varphi \, \mathrm{d}u} \,. \tag{4.22}$$

Here is a point of contact with the work of R. G. Chambers [56] on wave functions of Bloch electrons in a magnetic field. But it is difficult to make it explicit here.

Our next task is to derive quantum conditions from the subsidiary condition (3.10) and a eventual WKB boundary condition. The phase function $\varphi(u)$ can represent either a) closed or b) open orbits.

a) In case of closed orbits each branch of φ exhibits (at least) two real two-sheeted branch points (turning points). We take the branches $\varphi_1(u)$ and $\varphi_2(u)$ that ramify at u_1 and u_2 (Fig. 4) and apply the connecting relations between the corresponding asymptotic solutions (4.21) in the shape of the so-called WKB boundary condition [57]. This means that the linear combination of these solutions is to be chosen so as to represent an exponentially decreasing function beyond the turning points where φ gets purely imaginary. Near a turning point, say u_1, the effective Schrödinger equation $E(\widetilde{\boldsymbol{w}})\, \bar{b} = \mathcal{E}\, \bar{b}$ can be approximated by Airy's differential equation [57]. In doing so we easily check that the linear combination

$$\bar{b}_{\mathcal{E}}(u) = c \left[\left(\frac{\partial E}{\partial \varphi_2}\right)^{-1/2} e^{\,i\lambda \int_{u_1}^{u} \varphi_2 \, \mathrm{d}u'} \, e^{-i\frac{\pi}{4}} + \left(\frac{\partial E}{\partial \varphi_1}\right)^{-1/2} e^{\,i\lambda \int_{u_1}^{u} \varphi_1 \, \mathrm{d}u'} \, e^{\,i\frac{\pi}{4}} \right]; \qquad u_1 < u < u_2 \tag{4.23}$$

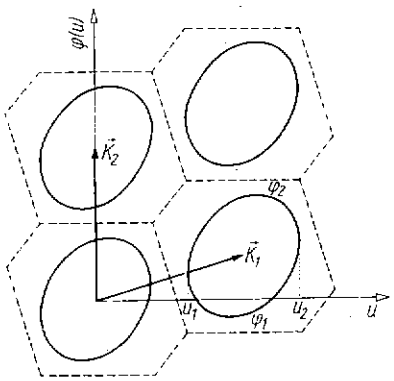

Fig. 4. Closed orbits

corresponds to that Airy function which has the desired property [57]. Here c is a normalization constant.[8]) Accordingly, at u_2 the WKB boundary condition requires

$$\bar{h}_\lambda(u) = c\left[\left(\frac{\partial E}{\partial \varphi_2}\right)^{-1/2} e^{i\lambda\int_{u_2}^{u}\varphi_2\,du'} e^{i\frac{\pi}{4}} + \left(\frac{\partial E}{\partial \varphi_1}\right)^{-1/2} e^{i\lambda\int_{u_2}^{u}\varphi_1\,du'} e^{-i\frac{\pi}{4}}\right]; \quad u_1 < u < u_2 \tag{4.24}$$

which must be equal to (4.23) up to a phase factor. That is the case if and only if the area $\mathcal{A}_{q_3}(\mathcal{E})$ of the closed orbit satisfies the Onsager condition

$$\mathcal{A}_{q_3}(\mathcal{E}) = \int_{u_1}^{u_2}(\varphi_2 - \varphi_1)\,du = \frac{2\pi}{\lambda}\left(\mu + \frac{1}{2}\right) \tag{4.25}$$

with integral μ. This fixes the energy levels

$$\mathcal{E}_\mu(q_3) = \mathcal{A}_{q_3}^{-1}\left(\frac{2\pi}{\lambda}\left(\mu + \frac{1}{2}\right)\right), \tag{4.26}$$

where $\mathcal{A}_{q_3}^{-1}$ is the reverse function of $\mathcal{A}_{q_3}$. The difference between two Onsager levels is well-known. Using $\partial\varphi/\partial\mathcal{E} = (\partial E/\partial\varphi)^{-1}$, from (4.25) we easily obtain

$$\mathcal{E}_{\mu+1}(q_3) - \mathcal{E}_\mu(q_3) = \frac{2\pi}{\lambda}\left(\frac{\partial\mathcal{A}_{q_3}}{\partial\mathcal{E}}\right)^{-1} = \hbar\,\omega_c\,, \tag{4.27}$$

where the cyclotron frequency ω_c is given by the path integral

$$\frac{2\pi}{\lambda\,\omega_c} = \hbar\frac{\partial\mathcal{A}}{\partial\mathcal{E}} = \hbar\int_{u_1}^{u_2}\left[\left(\frac{\partial E}{\partial\varphi_2}\right)^{-1} - \left(\frac{\partial E}{\partial\varphi_1}\right)^{-1}\right]du = \oint\frac{dk_s}{|\boldsymbol{v}_\perp|} \tag{4.28}$$

of the reciprocal velocity $\hbar\,|\boldsymbol{v}_\perp| = [(\partial E/\partial u)^2 + (\partial E/\partial\varphi)^2]^{1/2}$ over the cyclotron orbit. The inclusion of the higher-order terms (4.21) of the phase function leads to the following modification of Onsager's rule:

$$\mathcal{A}_{q_3}(\mathcal{E}) = \frac{2\pi}{\lambda}(\mu + \gamma)\;;$$

$$\gamma = \frac{1}{2} - \frac{1}{2\pi}\int_{u_1}^{u_2}(\Phi_2^{(1)} - \Phi_1^{(1)})\,du - \frac{\lambda^{-1}}{2\pi}\int_{u_1}^{u_2}(\Phi_2^{(2)} - \Phi_1^{(2)})\,du\,,$$

where $\Phi^{(1)}$ and $\Phi^{(2)}$ are given by (4.19) and (4.20). The subscripts of $\Phi^{(1)}$ and $\Phi^{(2)}$ indicate which of the branches of φ is to be inserted. This is in fact Roth's correction [40] of the Onsager condition (4.25). The terms arising from $\overline{H}_1$ and $\overline{H}_2$ are identical with the ones derived by Roth. However, the equivalence

[8]) The square modulus of c follows [57] from

$$|c|^2\int_{u_1}^{u_2}\left(\left|\frac{\partial E}{\partial\varphi_1}\right|^{-1} + \left|\frac{\partial E}{\partial\varphi_2}\right|^{-1}\right)du = \frac{|c|^2}{\hbar}\oint\frac{dk_s}{|\boldsymbol{v}_\perp|} = 1,\ \text{i.e. } |c|^2 = \hbar\,\omega_c\,\lambda/2\pi\ \text{(see (4.28))}.$$

of Zilberman's term [53] (the first square bracket of $\Phi^{(2)}$ in (4.20)) to the corresponding one of Roth has not been established up to now.

Applying the WKB boundary condition at turning points involves neglecting any coupling between the orbits so that the energies (4.26) do not depend on $\boldsymbol{q}_\perp$. The subsidiary condition (3.10) only plays a formal part in this approximation. It is satisfied by the functions

$$b^{(j)}_{\mu n \boldsymbol{q}}(u) = \frac{p}{(q\,|\boldsymbol{K}_1 \times \boldsymbol{K}_2|)^{1/2}} \sum_{\boldsymbol{K}_c} \mathrm{e}^{-i(\boldsymbol{q} - n\,\boldsymbol{K}_1,\, \boldsymbol{K}_c \times \boldsymbol{\lambda})}\, B_0\,(\boldsymbol{K}_c + j\,\boldsymbol{K}_1)\, b_{\mathcal{E}_\mu}(u)\,; \qquad j = 0, \ldots, q-1 \tag{4.29}$$

which we obtain by applying the projectors (3.31) to $B_0(j\,\boldsymbol{K}_1)\,\bar{b}_{\mathcal{E}_\mu}(u)$ with $\bar{b}_{\mathcal{E}_\mu}$ given by (4.23). This situation is similar to the one of tightly bound electrons with small overlap integrals and band splittings. Equation (4.29) is something like a "Bloch sum" of uncoupled orbital functions over one of the q orbit sublattices. To give an idea of the level-broadening due to intraband coupling we wish to translate Peierls' tight-binding approximation into the present case. To this end we think (4.23) to be the actual WKB solution of a Hamiltonian $\varepsilon(\tilde{\boldsymbol{w}})$ that in fact possesses localized eigenfunctions only. That is, $\varepsilon(\boldsymbol{k})$ is not periodic (e.g., $\varepsilon(\boldsymbol{k}) = \hbar^2\,\boldsymbol{k}^2/2\,m$) and in the corresponding Brillouin zone $\varepsilon(\boldsymbol{k}) \approx E(\boldsymbol{k})$ for the energy range in question. Then, the splitting into q subbands arises from the q-dimensional secular equation

$$\det\,[(\bar{b}^{(j')}|E(\tilde{\boldsymbol{w}})|\bar{b}^{(j)}) - \mathcal{E}(\bar{b}^{(j')}|\bar{b}^{(j)})] = 0\,,$$

where $\bar{b}^{(j)}$ is given by (4.29). In the simple case $q = 1$ we find

$$\mathcal{E}_\mu(\boldsymbol{q}) = \mathcal{E}_\mu + \frac{\sum_{\boldsymbol{K}_c} \mathrm{e}^{-i(\boldsymbol{q},\, \boldsymbol{K}_c \times \boldsymbol{\lambda})}\, (\bar{b}_{\mathcal{E}_\mu}\,|E(\tilde{\boldsymbol{w}}) - \varepsilon(\tilde{\boldsymbol{w}})|\, B_0(\boldsymbol{K}_c)\, \bar{b}_{\mathcal{E}_\mu})}{\sum_{\boldsymbol{K}_c} \mathrm{e}^{-i(\boldsymbol{q},\, \boldsymbol{K}_c \times \boldsymbol{\lambda})}\, (\bar{b}_{\mathcal{E}_\mu}|B_0(\boldsymbol{K}_c)\, \bar{b}_{\mathcal{E}_\mu})}$$

by using (2.44) and $\varepsilon(\tilde{\boldsymbol{w}})\,\bar{b}_{\mathcal{E}_\mu} = \mathcal{E}_\mu\,\bar{b}_{\mathcal{E}_\mu}$, where $\mathcal{E}_\mu$ and $\bar{b}_{\mathcal{E}_\mu}$ are given by (4.26) and (4.23) respectively.

b) Without restricting generality we assume the open orbits to be directed along $\boldsymbol{K}_2$ (Fig. 5). On the open orbit in question are (at least) two turning points u_1

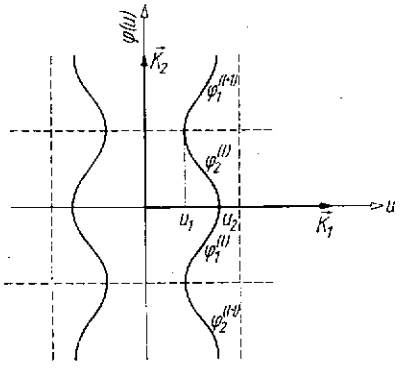

Fig. 5. Open orbits

and u_2, where the respective branches $q_2^{(l)}$, $q_1^{(l)}$ and $q_1^{(l-1)}$, $q_2^{(l)}$ join each other. The general open orbit wave function reads (cf. (4.14))

$$b_{\mathcal{E}}(u) = \sum_{i=1,2} \sum_{l=-\infty}^{+\infty} a_i^{(l)}\, h_i(u)\, \mathrm{e}^{i\lambda \int_{u_2}^{u} q_i^{(l)}\,\mathrm{d}u'} \;; \qquad q_i^{(l)} = q_i^{(0)} + l\, K_{22}\,,$$

where (4.21) is taken in the lowest-order approximation. The WKB boundary condition at u_1 and u_2 is satisfied if (cf. (4.23) and (4.24))

$$a_1^{(l-1)}\, \mathrm{e}^{i\lambda \int_{u_2}^{u_1} q_1^{(l+1)}\,\mathrm{d}u}\, \mathrm{e}^{i\frac{\pi}{4}} = a_2^{(l)}\, \mathrm{e}^{i\lambda \int_{u_2}^{u_1} q_2^{(l)}\,\mathrm{d}u}\, \mathrm{e}^{-i\frac{\pi}{4}} \;; \qquad a_2^{(l)}\, \mathrm{e}^{i\frac{\pi}{4}} = a_1^{(l)}\, \mathrm{e}^{i\frac{\pi}{4}}$$

from which $a_i^{(l-1)} = a_i^{(l)} \exp i\lambda \int_{u_2}^{u_2} (q_2^{(l)} - q_1^{(l-1)})\,\mathrm{d}u$ follows. This gives

$$\bar{b}_{\mathcal{E}}(u) = c \sum_{l=-\infty}^{+\infty} \mathrm{e}^{i\lambda l \int_{u_2}^{u_1} (q_2^{(l)} - q_1^{(l+1)})\,\mathrm{d}u} \left[h_1(u)\, \mathrm{e}^{i\lambda \int_{u_2}^{u} q_1^{(l)}\,\mathrm{d}u'}\, \mathrm{e}^{-i\frac{\pi}{4}} + h_2(u)\, \mathrm{e}^{i\lambda \int_{u_2}^{u} q_2^{(l)}\,\mathrm{d}u'}\, \mathrm{e}^{i\frac{\pi}{4}} \right]. \tag{4.30}$$

To obtain the functions that fulfil the subsidiary condition (3.10), we act with the projectors (3.31) on (4.30). Writing $B_0(\boldsymbol{K}_c) = B_0(k\,\boldsymbol{K}_0)\, B_0(l'\,\boldsymbol{K}_2)$ with $\boldsymbol{K}_c = k\,\boldsymbol{K}_0 + l'\,\boldsymbol{K}_2$ and utilizing (2.30) we perform the l'-summation which gives a sum of δ-functions. The result is proportional to

$$\left.\begin{aligned} \bar{b}_{\mu n \boldsymbol{q}}(u) &\sum_m \delta\left(q_1 + n\,K_{11} + \frac{m}{p}\,K_{01} \mp \frac{1}{2\,K_{22}}\,\mathcal{A}_{q_3}(\mathcal{E})\right); \\ \bar{b}_{\mu n \boldsymbol{q}}(u) &= \left(\frac{p}{K_{22}}\right)^{1/2} \sum_k \mathrm{e}^{-ik(\boldsymbol{q},\, \boldsymbol{K}_0 \times \boldsymbol{\lambda})}\, B_0(k\,\boldsymbol{K}_0)\, \bar{b}_{\mathcal{E}}(u)\,, \end{aligned}\right\} \tag{4.31}$$

where $\mathcal{A}_{q_3}(\mathcal{E})$ is the area enclosed by the open orbits within a Brillouin zone and the upper (lower) sign refers to the right (left) open orbit of Fig. 5. The δ-function gives the magnetic energy bands

$$\mathcal{E}_{\mu n}(q_1, q_3) = \mathcal{A}_{q_3}^{-1}\left(\pm\, 2\, K_{22}\left(q_1 + n\, K_{11} + \frac{\mu}{p}\, K_{01}\right)\right), \tag{4.32}$$

$\mathcal{A}_{q_3}^{-1}$ being the reverse function of $\mathcal{A}_{q_3}$. With these energies (4.30) appears in (4.31). Similarly to (4.27) the distance between two open orbit energy bands is found to be

$$\mathcal{E}_{\mu+1,\,n}(\boldsymbol{q}) - \mathcal{E}_{\mu n}(\boldsymbol{q}) = \frac{2\pi}{\lambda}\left(\frac{\partial \mathcal{A}}{\partial \mathcal{E}}\right)^{-1} = \hbar\,\omega_c; \qquad \frac{2\pi}{\lambda\,\omega_c} = \int \frac{\mathrm{d}k_s}{|\boldsymbol{v}_\perp|},$$

when (2.13) is taken into account. The path integral defining ω_c extends over one period of the open orbit. We do not enter into the details of the splitting of open orbit energy bands due to intraband coupling, which has been first discussed by W. G. Chambers [58]. It is graphically demonstrated in Fig. 6.

In general the intraband coupling between open or closed orbits is very small. Only in the vicinity of saddle points of $E_\nu(\boldsymbol{k})$ ($k_3 = q_3$ fixed) we have a strong coupling of orbits that are nearing each other very much. This is accompanied with the change from open to closed orbits. The connecting relations at intra-

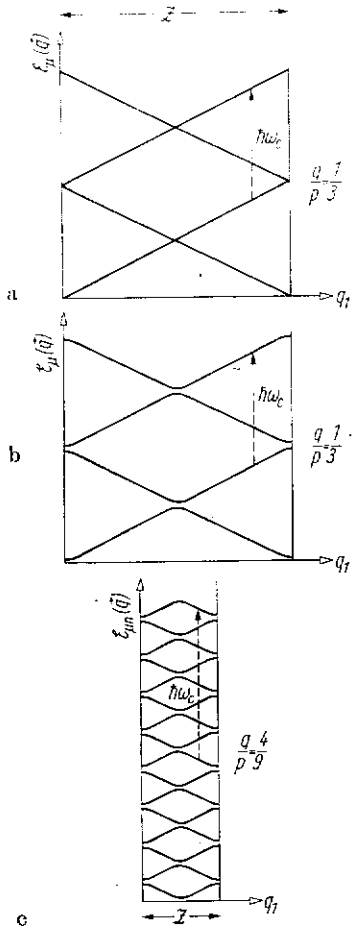

Fig. 6. Open-orbit energy bands. a) Energy bands (4.32) for $q = 1$. b) Splitting of the bands a) due to intraband coupling. c) The field strength is raised by the factor 4/3 so that each of the bands b) splits into 4 subbands

band breakdown points can be derived by expanding $E_\nu(\boldsymbol{k})$ about the corresponding saddle point and replacing $\boldsymbol{k}$ and $\widetilde{i\boldsymbol{c}}$. The arising differential equation is equivalent to the one of parabolic cylinder functions that asymptotically fit the WKB wave functions left and right of the pair of breakdown points. Thus, the asymptotic behaviour of the parabolic cylinder functions gives the desired connection formulas. We do not carry out this here because in a following section similar considerations are made in context of interband breakdown. We refer the reader to the papers of Azbel [59] and Davis and Liu [60]. Both are concerned with interband breakdown in rectangular orbit lattices. The former gives a general solution of the problem. The latter is more transparent but restricted to $q = 1$. A one-dimensional coupling in the transition region between open and closed orbits is discussed in Roth's paper [40]. In this context we also mention the case of self-intersecting "figure-eight" orbits which is first considered by Zilberman [61], generally solved by Azbel [62], and later discussed by Roth [40].

4.3 Weak binding

4.3.1 Empty lattice

Energies and wave functions of free electrons in a magnetic field are well-known since Landau's paper [4]. Nevertheless, we wish to give the corresponding expressions here in a symmetry-adapted fashion. For vanishing potential equation (2.41) is diagonal with respect to $\boldsymbol{K}_\mathrm{r}$, i.e. $\boldsymbol{K}_\mathrm{r}$ is to be considered a quantum number. Eigenfunctions and eigenvalues of the empty lattice are

$$C^{(0)}_{\mu \boldsymbol{K}_\mathrm{r} \boldsymbol{q}}(\boldsymbol{K}'_\mathrm{r};\, u_{(1)}) = \mathrm{e}^{-i(\boldsymbol{\kappa}_c,\, \boldsymbol{K}'_\mathrm{r} \times \boldsymbol{\lambda})} \left(\mu!\sqrt{\frac{\pi}{\lambda}}\right)^{-1/2} D_\mu(\sqrt{2\lambda}\, u_{(1)})\, \delta_{\boldsymbol{K}'_\mathrm{r}\, \boldsymbol{K}_\mathrm{r}}\,, \tag{4.33}$$

$$\mathscr{E}^{(0)}_{\mu \boldsymbol{K}_\mathrm{r}}(\boldsymbol{q}) = \hbar\, \omega_\mathrm{c}^{(0)} \left(\mu + \frac{1}{2}\right) + \frac{\hbar^2}{2\, m}\,(q_3 + K_{\mathrm{r}3})^2; \quad \mu = 0, 1, \ldots, \quad \omega_\mathrm{c}^{(0)} = \frac{|e|\, B}{m\, c}\,, \tag{4.34}$$

where D_μ denotes parabolic cylinder functions with the integral index μ. The

energies are degenerate with respect to $\boldsymbol{q}_\perp$ and the 1-component of $\boldsymbol{K}_\mathrm{r}$. The complete wave function (2.36) reads

$$\psi^{(0)}_{\mu \boldsymbol{K}_\mathrm{r} \boldsymbol{q} s}(u_{(1)}, s) = \left(\mu! \Big/ \frac{\pi}{\lambda}\right)^{1/2} \mathrm{e}^{-i(\boldsymbol{q}, \boldsymbol{K}_\mathrm{r} \times \lambda)} D_\mu(\sqrt{2\lambda}\, u_{(1)})\, q_{\boldsymbol{q} s}(\boldsymbol{K}_\mathrm{r}; s)\,. \quad (4.35)$$

4.3.2 Nearly-free approximation

We first calculate the matrix elements of the perturbation (2.42) with the unperturbed solutions (4.33) and obtain the expression

$$\begin{aligned}
(C_{\mu' \boldsymbol{K}'_\mathrm{r} \boldsymbol{q}} \,|\, V_{\boldsymbol{q}}(\boldsymbol{K}'_\mathrm{r}, \boldsymbol{K}_\mathrm{r})\,|\, C_{\mu \boldsymbol{K}_\mathrm{r} \boldsymbol{q}}) &\equiv V^{\mu' \boldsymbol{K}'_\mathrm{r}}_{\mu \boldsymbol{K}_\mathrm{r}}(\boldsymbol{q}) = \\
&= \sum_{\boldsymbol{K}_\mathrm{c}} V_{\boldsymbol{K}}\, \mathrm{e}^{-i\pi k l p}\, \mathrm{e}^{i\left(\boldsymbol{q} + \frac{1}{2}(\boldsymbol{K}'_\mathrm{r} + \boldsymbol{K}_\mathrm{r}),\, \boldsymbol{K}_\mathrm{c} \times \lambda\right)}\, \mathrm{e}^{\frac{i}{2}(\boldsymbol{K}'_\mathrm{r} \times \boldsymbol{K}_\mathrm{r},\, \lambda)} \times \\
&\times \sqrt{\frac{\lambda}{\pi}}\, (\mu!\, \mu'!)^{-1/2} \int_{-\infty}^{+\infty} D_{\mu'}(\sqrt{2\lambda}\, u_{(1)})\, \mathrm{e}^{i(\boldsymbol{u},\, \boldsymbol{K} \times \lambda)}\, D_\mu(\sqrt{2\lambda}\, u_{(1)})\, \mathrm{d}u_{(1)} = \\
&= \left(\frac{\mu!}{\mu'!}\right)^{1/2} \sum_{\boldsymbol{K}_\mathrm{c}} V_{\boldsymbol{K}}\, \mathrm{e}^{-i\pi k l p}\, \mathrm{e}^{i\left(\boldsymbol{q} + \frac{1}{2}(\boldsymbol{K}'_\mathrm{r} + \boldsymbol{K}_\mathrm{r}),\, \boldsymbol{K}_\mathrm{c} \times \lambda\right)}\, \mathrm{e}^{\frac{i}{2}(\boldsymbol{K}'_\mathrm{r} \times \boldsymbol{K}_\mathrm{r},\, \lambda)} \times \\
&\times \mathrm{e}^{-(\lambda/4)|\boldsymbol{K}_\perp|^2} \left(\sqrt{\frac{\lambda}{2}}\, |\boldsymbol{K}_\perp|\, \mathrm{e}^{-i\beta}\right)^{\mu' - \mu} L_\mu^{(\mu' - \mu)}\left(\frac{\lambda}{2}\, |\boldsymbol{K}_\perp|^2\right), \qquad (4.36)
\end{aligned}$$

where $\boldsymbol{K} = \boldsymbol{K}'_\mathrm{r} - \boldsymbol{K}_\mathrm{r} - \boldsymbol{K}_\mathrm{c}$, $\boldsymbol{K}_\mathrm{c} = k\,\boldsymbol{K}_0 + l\,\boldsymbol{K}_2$, $\boldsymbol{K}_\perp = (K_1, K_2, 0)$ is the projection of $\boldsymbol{K}$ on the plane perpendicular to the magnetic field, $\beta = \mathrm{arctg}\,(K_2/K_1)$, and $L_\mu^{(\mu' - \mu)}$ is a Laguerre polynomial. The unperturbed energies (4.34) are q-fold degenerate with respect to the 1-component of $\boldsymbol{K}_\mathrm{r}$. Since the matrix elements (4.36) are not diagonal in this regard, degenerate perturbation theory applies and a q-dimensional secular equation should be solved which yields the splitting of (4.34) into q subbands. To spare that we are contented with the special case $q = 1$. Then the perturbed energies and wave functions are with (4.34) and (4.35) given by

$$\mathscr{E}_{\mu \boldsymbol{K}_\mathrm{r}}(\boldsymbol{q}) = \mathscr{E}^{(0)}_{\mu \boldsymbol{K}_\mathrm{r}}(q_3) + V^{\mu \boldsymbol{K}_\mathrm{r}}_{\mu \boldsymbol{K}_\mathrm{r}}(\boldsymbol{q}) + \sum_{\mu' \boldsymbol{K}'_\mathrm{r}}{}' \frac{|V^{\mu' \boldsymbol{K}'_\mathrm{r}}_{\mu \boldsymbol{K}_\mathrm{r}}(\boldsymbol{q})|^2}{\mathscr{E}^{(0)}_{\mu \boldsymbol{K}_\mathrm{r}}(q_3) - \mathscr{E}^{(0)}_{\mu' \boldsymbol{K}'_\mathrm{r}}(q_3)}\,, \qquad (4.37)$$

$$\psi_{\mu \boldsymbol{K}_\mathrm{r} \boldsymbol{q} s} = \psi^{(0)}_{\mu \boldsymbol{K}_\mathrm{r} \boldsymbol{q} s} + \sum_{\mu' \boldsymbol{K}'_\mathrm{c}}{}' \frac{V^{\mu' \boldsymbol{K}'_\mathrm{r}}_{\mu \boldsymbol{K}_\mathrm{r}}(\boldsymbol{q})\, \psi^{(0)}_{\mu' \boldsymbol{K}'_\mathrm{r} \boldsymbol{q} s}}{\mathscr{E}^{(0)}_{\mu \boldsymbol{K}_\mathrm{r}}(q_3) - \mathscr{E}^{(0)}_{\mu' \boldsymbol{K}'_\mathrm{r}}(q_3)}\,, \qquad (4.38)$$

where $\boldsymbol{K}_\mathrm{r} = m\,\boldsymbol{K}_3$ because of $q = 1$. The primed summation sign means omitting the term μ', $\boldsymbol{K}'_\mathrm{r} = \mu$, $\boldsymbol{K}_\mathrm{r}$.

The perturbed energy spectrum (4.37) reflects the influence of the lattice potential in two respects. On the one hand it removes the degeneracy of the Landau spectrum (4.34) by producing a $\boldsymbol{q}_\perp$-dependence, which is in first order given by the diagonal element

$$V^{\mu \boldsymbol{K}_\mathrm{r}}_{\mu \boldsymbol{K}_\mathrm{r}}(\boldsymbol{q}) = \sum_{\boldsymbol{K}_\mathrm{c}} V_{-\boldsymbol{K}_\mathrm{c}}\, \mathrm{e}^{-i\pi k l p}\, \mathrm{e}^{i(\boldsymbol{q} + \boldsymbol{K}_\mathrm{r},\, \boldsymbol{K}_\mathrm{c} \times \lambda)}\, \mathrm{e}^{-(\lambda/4)|\boldsymbol{K}_\mathrm{c}|^2}\, L_\mu\left(\frac{\lambda}{2}\, |\boldsymbol{K}_\mathrm{c}|^2\right) \quad (4.39)$$

with $\boldsymbol{K}_\mathrm{c} = \widehat{\boldsymbol{K}} = j\,\boldsymbol{K}_1 + l\,\boldsymbol{K}_2$. On the other hand it generates numerous gaps in

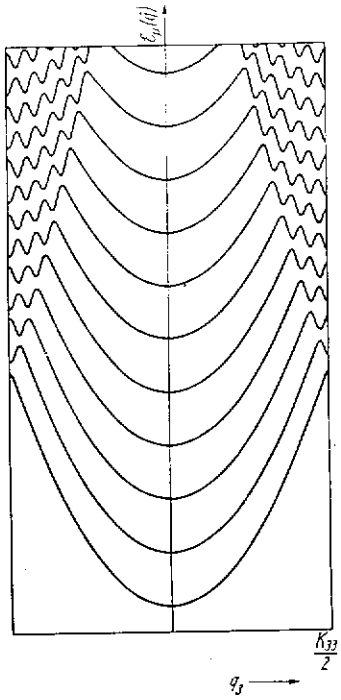

Fig. 7. q_3-dependence of the nearly-free energy spectrum

the q_3-dependence of the perturbed spectrum. These appear whenever $\mathcal{E}^{(0)}_{\mu \boldsymbol{K}_r}(q_3) = \mathcal{E}^{(0)}_{\mu' \boldsymbol{K}_r'}(q_3)$ is met. The expressions (4.37) and (4.38) fail near such values of q_3. There the pertubed energies and wave functions are to be calculated in a well-known way by adaptation of the two degenerating functions, which gives rise to a splitting by twice the absolute value of the corresponding matrix element (4.36). This is shown in Fig. 7.

The perturbation theory is only significant as long as the broadening (4.39) of the Landau levels is smaller than their distance $\hbar\,\omega_c^{(0)}$. It is mainly affected by the Fourier components $V_{\hat{\boldsymbol{K}}}$ and the behaviour of the Laguerre polynomials. Because $\mathrm{e}^{-x/2}\,L_\mu(x) \leqq 1$ for $x \geqq 0$ [63], the perturbation theory is applicable in any case if $\hbar\,\omega^{(0)} > |V_{\hat{\boldsymbol{K}}}|$, where $V_{\hat{\boldsymbol{K}}}$ is supposed to be the largest Fourier component for one of the shortest reciprocal lattice vectors $\hat{\boldsymbol{K}}$ in the plane perpendicular to the magnetic field. For large μ $\mathrm{e}^{-x/2}\,L_\mu(x)$ oscillates in the region $0 < x < M = 4\,\mu + 2$ as the asymptotic expression [63]

$$\mathrm{e}^{-x/2}\,L_\mu(x) \simeq 2\,(-1)^\mu\,(M\,\pi \sin 2\,\vartheta)^{-1/2} \sin\left[\frac{M}{4}\,(2\,\vartheta - \sin 2\,\vartheta) + \frac{\pi}{4}\right];$$

$$x = M\cos^2\vartheta\,, \qquad (4.40)$$

whereas it decreases exponentially for $x > M$. Because of this the level broadening is small if $x = \lambda\,|\hat{\boldsymbol{K}}|^2/2 > 4\,\mu + 2$ which is the same as

$$\mathcal{E}_\perp = \hbar\,\omega_c^{(0)}\left(\mu + \frac{1}{2}\right) < \mathcal{E}_0 = \frac{\hbar^2}{2\,m}\left(\frac{\hat{\boldsymbol{K}}}{2}\right)^2. \qquad (4.41)$$

According to (4.40) the functions $\mathrm{e}^{-x/2}\,L_\mu(x)$ become small also in the oscillatory region for large $M = 4\,\mu + 2$. Hence, from the inequality

$$\hbar\,\omega_c^{(0)} \gg |V_{\hat{\boldsymbol{K}}}|\,2\left[2\,\pi\,M\left(\frac{x}{M}\right)^{1/2}\left(1 - \frac{x}{M}\right)^{1/2}\right]^{-1/2}; \quad x = \frac{\lambda\,|\hat{\boldsymbol{K}}|^2}{2} = \frac{4\,\mathcal{E}_0}{\hbar\,\omega_c^{(0)}},$$

we get the further condition

$$\mathcal{E}_\perp \gg \mathcal{E}_0\left[1 + \frac{|V_{\hat{\boldsymbol{K}}}|^4}{(2\,\pi\,\hbar\,\omega_c^{(0)}\,\mathcal{E}_0)^2}\right] \qquad (4.42)$$

of the applicability of the perturbation theory. Fig. 8 illustrates the validity range of the perturbation theory according to (4.41) and (4.42). It shows the

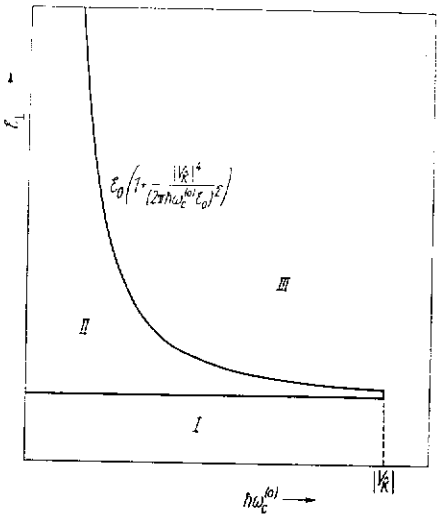

Fig. 8. Validity regions of the nearly-free approximation

regions of a weakly broadened Landau spectrum in an $\mathcal{E}_\perp$ vs. $\hbar\omega_c^{(0)}$ plot. $\mathcal{E}_\perp$ is the energy part of the motion in the plane perpendicular to the field. $\hbar\omega_c^{(0)}$ is a measure of field strength. In region I $\mathcal{E}_\perp$ is smaller than the smallest possible energy $\mathcal{E}_0$ of free electrons on the periphery of the first Brillouin zone. That is to say, unperturbed circular orbits that remain within the first Brillouin zone suffer only a weak perturbation. The electron orbits of region II, however, cross the boundaries of the first Brillouin zone so that Bragg reflexion becomes possible. Thus, the orbits are considerably altered also by a weak lattice potential. Their energy spectrum has nothing in common with a Landau spectrum so that the perturbation theory breaks down. Nevertheless, on reaching region III with increasing fields, electrons with $\mathcal{E}_\perp > \mathcal{E}_0$ again get a weakly perturbed Landau spectrum of broken down circular orbits. Accordingly, (4.42) is just Blount's breakdown criterion [10] in a slightly modified fashion.

A similar discussion was given by Reitz [64]. He considered the probability of transitions between unperturbed Landau states due to a Fourier component of the lattice potential and interpreted it in terms of magnetic breakdown. The first attempt to employ perturbation theory was made by Zilberman [65]. It was, however, inadequate because he did not use symmetrized zeroth-order wave functions. The level broadening (4.39) was first derived by Zak [66]. The complete perturbation-theoretical treatment given here is contained in [18]. Recently, Langbein [32] has made a detailed study of the subband splitting, among others, in the frame of the nearly-free approximation. The connection of the network model of magnetic breakdown with the nearly-free approximation has been elaborated in a recent work of Capel [67].

4.3.3 Asymptotic approximation for weak potentials (magnetic breakdown)

The region II, where the perturbation theory breaks down, is of special importance for the interpretation of magnetoresistance and de Haas-van Alphen effect of polyvalent metals. The adequate solution method of the Schrödinger equation in this range is the asymptotic approximation described in Section 4.1 if being specialized for weak potentials. It proves to be the mathematical justification of the Pippard network model.

The analytical structure of $\varphi(u)$ in the vicinity of (interband) breakdown points can be studied in detail by expanding (4.5) to second order in powers of the potential:

$$\prod_{\boldsymbol{K}''} B_{\boldsymbol{K}''\boldsymbol{K}''}(u,\varphi,q_3;\mathcal{E})\left[1-\frac{1}{2}\sum_{\boldsymbol{K}'\boldsymbol{K}}\frac{|V_{\boldsymbol{K}-\boldsymbol{K}'}|^2}{B_{\boldsymbol{K}\boldsymbol{K}}(u,\varphi,q_3;\mathcal{E})\,B_{\boldsymbol{K}'\boldsymbol{K}'}(u,\varphi,q_3;\mathcal{E})}\right]=0\,. \tag{4.43}$$

Apparently, for $V \to 0$ the (infinitely) multi-valued phase function $\varphi(u)$ falls into the two-valued functions $\varphi_{\boldsymbol{K}}^{(0)}(u)$ defined by $B_{\boldsymbol{K}\boldsymbol{K}}(u, \varphi_{\boldsymbol{K}}^{(0)}(u), q_3; \mathscr{E}) = 0$. Since q_3 is given as a quantum number, these equations describe the circular free-electron orbits in the u, φ, q_3 space with the centres $(-K_1, -K_2, q_3)$ and the radii $K_{\mathscr{E}\perp} = \sqrt{(2m\mathscr{E}/\hbar^2) - (q_3 + K_3)^2}$. The two branch points of $\varphi_{\boldsymbol{K}}^{(0)}(u)$ are situated on the real u-axis at $u = -K_1 \pm K_{\mathscr{E}\perp}$. They are turning points and keep this character if a weak potential is present. Only their position shifts a little. For a non-zero potential there are further branch points that connect the two-sheeted Riemann surfaces of the functions $\varphi_{\boldsymbol{K}}^{(0)}(u)$ to the many-sheeted Riemann surface of $\varphi(u)$. Among them are (interband) breakdown points whenever two circles with the same q_3, say $\varphi_{\boldsymbol{K}}^{(0)}(u)$ and $\varphi_{\boldsymbol{K}'}^{(0)}(u)$, intersect each other.[9]) That happens in region II of Fig. 8. In the vicinity of such an intersection point $u_{\boldsymbol{K}'\boldsymbol{K}}$ with $\varphi_{\boldsymbol{K}}^{(0)}(u_{\boldsymbol{K}'\boldsymbol{K}}) = \varphi_{\boldsymbol{K}'}^{(0)}(u_{\boldsymbol{K}'\boldsymbol{K}}) = \varphi_{\boldsymbol{K}'\boldsymbol{K}}$ we have a pair of breakdown points. For weak potentials $\varphi(u)$ differs very little from the circles $\varphi_{\boldsymbol{K}}^{(0)}(u)$. From this fact we conclude [22] that the branching of $\varphi(u)$ near $u_{\boldsymbol{K}'\boldsymbol{K}}$ can be derived from the simplified equation

$$B_{\boldsymbol{K}\boldsymbol{K}}(u, \varphi, q_3; \mathscr{E})\, B_{\boldsymbol{K}'\boldsymbol{K}'}(u, \varphi, q_3; \mathscr{E}) - |V_{\boldsymbol{K}'-\boldsymbol{K}}|^2 = 0 \tag{4.44}$$

which is obtained from (4.43) by neglecting all the Fourier coefficients except $V_{\boldsymbol{K}-\boldsymbol{K}'}$. Since this equation holds at the same time in the vicinities of both the intersection points of the circles $\varphi_{\boldsymbol{K}}^{(0)}(u)$ and $\varphi_{\boldsymbol{K}'}^{(0)}(u)$, we can linearize $B_{\boldsymbol{K}\boldsymbol{K}}$ and $B_{\boldsymbol{K}'\boldsymbol{K}'}$ with respect to $u - u_{\boldsymbol{K}'\boldsymbol{K}}$ and $\varphi - \varphi_{\boldsymbol{K}'\boldsymbol{K}}$ in order to study the ramification of φ near $u_{\boldsymbol{K}'\boldsymbol{K}}$ alone. Choosing a frame of reference in which $\boldsymbol{K} + \boldsymbol{K}' = 0$ (Fig. 9), assuming $K_3 = K_3' (= 0)$ for simplicity, and writing $\varphi_{\boldsymbol{K}'\boldsymbol{K}} = \varphi_0$, $u_{\boldsymbol{K}'\boldsymbol{K}} = u_0$, $V_{\boldsymbol{K}-\boldsymbol{K}'} = V$, we find the linearized equation

$$\begin{aligned}&[(\varphi_0 + K_2)(\varphi - \varphi_0) + (u_0 + K_1)(u - u_0)] \times \\ &\quad \times [(\varphi_0 - K_2)(\varphi - \varphi_0) + (u_0 - K_1)(u - u_0)] - \left(\frac{m}{\hbar^2}|V|\right)^2 = 0\,,\end{aligned} \tag{4.45}$$

where $\varphi_0 = K_1 \sqrt{(K_{\mathscr{E}\perp}/|\boldsymbol{K}|)^2 - 1}$ and $u_0 = -K_2 \sqrt{(K_{\mathscr{E}\perp}/|\boldsymbol{K}|)^2 - 1}$. Its solution[10])

$$\varphi - \varphi_0 = (\varphi_0^2 - K_2^2)^{-1}\,[(K_1 K_2 - \varphi_0 u_0)(u - u_0) \pm \Delta \sqrt{(u - u_0)^2 + b^2}] \tag{4.46}$$

is branched at $u = u_0 \pm i\,b$, where

$$b^2 = \frac{|V|^2 (\varphi_0^2 - K_2^2)}{(\hbar^2 \Delta/m)^2} \quad \text{and} \quad \Delta = \varphi_0 K_1 - u_0 K_2\,. \tag{4.47}$$

$|\Delta|$ is the area of the triangle shown in Fig. 9.

To study the behaviour of $C^{\boldsymbol{K}}(u) \equiv C_1(u)$ and $C^{\boldsymbol{K}'}(u) \equiv C_2(u)$ in the vicinity of $u_{\boldsymbol{K}'\boldsymbol{K}} \equiv u_0$ we proceed quite analogously. (4.44) can be interpreted as the determinantal condition of the subsystem

$$\left.\begin{aligned}\frac{\hbar^2}{2m}\left[\left(\frac{1}{i\lambda}\frac{\mathrm{d}}{\mathrm{d}u} + K_2\right)^2 + (u + K_1)^2 - K_{\mathscr{E}\perp}^2\right] C_1(u) + V\, C_2(u) = 0\,,\\ \frac{\hbar^2}{2m}\left[\left(\frac{1}{i\lambda}\frac{\mathrm{d}}{\mathrm{d}u} - K_2\right)^2 + (u - K_1)^2 - K_{\mathscr{E}\perp}^2\right] C_2(u) + V^*\, C_1(u) = 0\end{aligned}\right\} \tag{4.48}$$

[9]) We exclude the case that more than two circles intersect in one point.

[10]) It breaks down if $\varphi_0 = \pm K_2$ because the intersection point then coincides with a turning point. We disregard this unessential case.

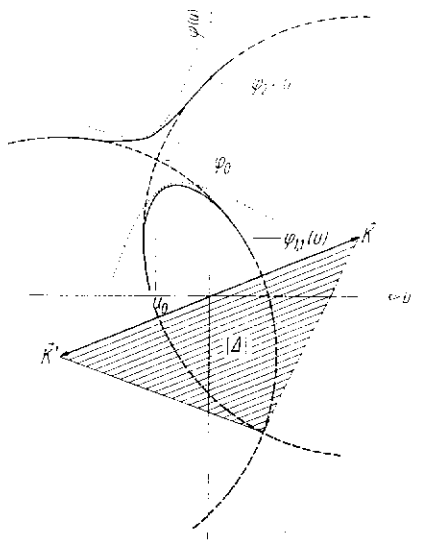

Fig. 9. Branching of $\varphi(u)$ (full lines) near the intersection point u_0 of the circles $\varphi_K^{(u_0)}(u)$ and $\varphi_{K'}^{(u_0)}(u)$ (dashed lines). The approximation (4.46) is depicted by dotted lines

of (4.1). The linearization of (4.44) corresponds to a linearization of (4.48). Equation (4.48) should be written in terms of $C_i(u) = e^{i\lambda\varphi_0(u-u_0)}\,\overline{C}_i\,(u-u_0)$. Neglecting second-order derivatives and powers, we find

$$\left.\begin{aligned}\left[(\varphi_0 + K_2)\frac{1}{i\lambda}\frac{\mathrm{d}}{\mathrm{d}u} + (u_0 + K_1)\,(u-u_0)\right]\overline{C}_1 + \frac{m}{\hbar^2}\,V = 0\,,\\ \left[(\varphi_0 - K_2)\frac{1}{i\lambda}\frac{\mathrm{d}}{\mathrm{d}u} + (u_0 - K_1)\,(u-u_0)\right]\overline{C}_2 + \frac{m}{\hbar^2}\,V^* = 0\,.\end{aligned}\right\} \tag{4.49}$$

Obviously, (4.45) can be considered the determinantal condition of (4.49). By the further transformation

$$C_i(u) \equiv \mathrm{e}^{i\lambda\varphi_0(u-u_0)}\,\overline{C}_i(u) \equiv \mathrm{e}^{\,i\lambda\int_{u_0}^{u}\left[\varphi_0 + \frac{K_1K_2 - \varphi_0 u_0}{\varphi_0^2 - K_2^2}(u'-u_0)\right]\mathrm{d}u'}\,\mathscr{C}_i\,(u-u_0) \tag{4.50}$$

(4.49) goes over into

$$\left.\begin{aligned}\left[\frac{\mathrm{d}}{\mathrm{d}u} + \frac{i\lambda\,\Delta}{\varphi_0^2 - K_2^2}\,(u-u_0)\right]\mathscr{C}_1 + i\lambda\frac{m}{\hbar^2}\frac{V}{\varphi_0 + K_2}\,\mathscr{C}_2 = 0\,,\\ \left[\frac{\mathrm{d}}{\mathrm{d}u} - \frac{i\lambda\,\Delta}{\varphi_0^2 - K_2^2}\,(u-u_0)\right]\mathscr{C}_2 + i\lambda\frac{m}{\hbar^2}\frac{V^*}{\varphi_0 - K_2}\,\mathscr{C}_1 = 0\,.\end{aligned}\right\} \tag{4.51}$$

Comparing this system of equations with the defining equations

$$\left.\begin{aligned}
&\left(\frac{\mathrm{d}}{\mathrm{d}x} - \frac{i\,x}{2}\right) F_1^{(\pm)}(a,x) \pm i\sqrt{a}\, F_2^{(\pm)}(a,x) = 0\,,\\
&\left(\frac{\mathrm{d}}{\mathrm{d}x} \mp \frac{i\,x}{2}\right) F_2^{(\pm)}(a,x) - i\sqrt{a}\, F_1^{(\pm)}(a,x) = 0\,,\\
&\left(\frac{\mathrm{d}}{\mathrm{d}x} - \frac{i\,x}{2}\right) G_1^{(\pm)}(a,x) - i\sqrt{a}\, G_2^{(\pm)}(a,x) = 0\,,\\
&\left(\frac{\mathrm{d}}{\mathrm{d}x} \mp \frac{i\,x}{2}\right) G_2^{(\pm)}(a,x) \mp i\sqrt{a}\, G_1^{(\pm)}(a,x) = 0
\end{aligned}\right\} \qquad (4.52)$$

of the parabolic cylinder functions

$$\begin{aligned}
F_1^{(\pm)}(a,x) &= \mathrm{e}^{i\frac{a}{2}\ln\frac{a}{\mathrm{e}}}\,\mathrm{e}^{-a\left(\frac{\pi}{2}\mp\frac{\pi}{4}\right)}\,D_{-ia}\left(x\,\mathrm{e}^{\pm i\frac{\pi}{4}}\right),\\
F_2^{(\pm)}(a,x) &= \sqrt{a}\,\mathrm{e}^{i\frac{a}{2}\ln\frac{a}{\mathrm{e}}}\,\mathrm{e}^{-(a-i)\left(\frac{\pi}{2}\mp\frac{\pi}{4}\right)}\,D_{-ia-1}\left(x\,\mathrm{e}^{\pm i\frac{\pi}{4}}\right),\\
G_1^{(\pm)}(a,x) &= \sqrt{a}\,\mathrm{e}^{-i\frac{a}{2}\ln\frac{a}{\mathrm{e}}}\,\mathrm{e}^{-(a+i)\left(\frac{\pi}{2}\mp\frac{\pi}{4}\right)}\,D_{ia-1}\left(x\,\mathrm{e}^{\mp i\frac{\pi}{4}}\right),\\
G_2^{(\pm)}(a,x) &= \mathrm{e}^{-i\frac{a}{2}\ln\frac{a}{\mathrm{e}}}\,\mathrm{e}^{-a\left(\frac{\pi}{2}\mp\frac{\pi}{4}\right)}\,D_{ia}\left(x\,\mathrm{e}^{\mp i\frac{\pi}{4}}\right)
\end{aligned}$$

and supposing $\Delta > 0$, we find the solutions

$$\left.\begin{aligned}
\mathscr{E}_1^{(1)} &= \frac{1}{\sqrt{\varphi_0 + K_2}}\,F_1^{(\pm)}\left(a, \frac{2\sqrt{a}}{|b|}(u-u_0)\right),\\
\mathscr{E}_1^{(2)} &= \frac{-\,\mathrm{e}^{i\alpha}}{\sqrt{\varphi_0 + K_2}}\,G_1^{(\pm)}\left(a, \frac{2\sqrt{a}}{|b|}(u-u_0)\right),\\
\mathscr{E}_2^{(1)} &= \frac{\pm\,\mathrm{e}^{-i\alpha}}{\sqrt{|\varphi_0 - K_2|}}\,F_2^{(\pm)}\left(a, \frac{2\sqrt{a}}{|b|}(u-u_0)\right),\\
\mathscr{E}_2^{(2)} &= \frac{1}{\sqrt{|\varphi_0 - K_2|}}\,G_2^{(\pm)}\left(a, \frac{2\sqrt{a}}{|b|}(u-u_0)\right)
\end{aligned}\right\} \qquad (4.53)$$

of (4.51), where

$$a = \frac{\lambda\,(m\,|V|/\hbar^2)^2}{2\,\Delta} \qquad (4.54)$$

and $\alpha = \arg V$. The upper (lower) sign applies if $\varphi_0 - K_2$ is positive (negative). The equations (4.52) are nothing else than a masked form of the well-known recurrence formulas of $D_\nu(z)$ [63]. Regarding (4.7), (4.46), (4.50), (4.53), and

$$\frac{\lambda\,\Delta}{|\varphi_0^2 - K_2^2|}\int_{u_0}^{u}\sqrt{(u'-u_0)^2 \pm |b|^2}\,\mathrm{d}u' \simeq \operatorname{sgn}(u-u_0)\left[\frac{x^2}{4} \pm a\ln\left(x\sqrt{\frac{\mathrm{e}}{a}}\right)\right];$$

$$x = \frac{2\sqrt{a}}{|b|}\,|u-u_0| \gg 2\sqrt{a}$$

we interpret the asymptotic formulas [63] ($x \gtrless 2\,|\,a$)

$$F_2^{(\pm)}(a, x) \simeq \mathrm{e}^{\,a\left(\frac{\pi}{2} \mp \frac{\pi}{2}\right)} \mathrm{e}^{\,i\left[\mp \frac{x^2}{4} - a \ln\left(x\sqrt{\frac{\mathrm{e}}{a}}\right)\right]},$$

$$F_1^{(\pm)}(a, \mathrm{e}^{\mp i\pi} x) \simeq \mathrm{e}^{\,a\left(\frac{\pi}{2} \mp \frac{\pi}{2}\right)} \mathrm{e}^{\,i\left[\mp \frac{x^2}{4} - a \ln\left(x\sqrt{\frac{\mathrm{e}}{a}}\right)\right]} +$$

(4.52)

$$+ \frac{\sqrt{2\pi}\,\mathrm{e}^{-a\frac{\pi}{2}}}{\sqrt{a}\,\Gamma(i\,a)} \mathrm{e}^{\,i\left(a \ln \frac{a}{\mathrm{e}} \mp \frac{\pi}{4}\right)} \frac{\sqrt{a}}{x} \mathrm{e}^{\,i\left[\mp \frac{x^2}{4} - a \ln\left(x\sqrt{\frac{\mathrm{e}}{a}}\right)\right]},$$

$$G_2^{(\pm)}(a, x) \simeq \pm \frac{\sqrt{a}}{x} \mathrm{e}^{\,a\left(\frac{\pi}{2} \mp \frac{\pi}{2}\right)} \mathrm{e}^{\,i\left[\pm \frac{x^2}{4} - a \ln\left(x\sqrt{\frac{\mathrm{e}}{a}}\right)\right]},$$

$$G_1^{(\mp)}(a, \mathrm{e}^{\pm i\pi} x) \simeq \mp \mathrm{e}^{\,a\left(\frac{\pi}{2} \pm \frac{\pi}{2}\right)} \frac{\sqrt{a}}{x} \mathrm{e}^{\,i\left[\pm \frac{x^2}{4} - a \ln\left(x\sqrt{\frac{\mathrm{e}}{a}}\right)\right]} +$$

$$+ \frac{\sqrt{2\pi}\,\mathrm{e}^{-a\frac{\pi}{2}}}{\sqrt{a}\,\Gamma(-i\,a)} \mathrm{e}^{-i\left(a \ln \frac{a}{\mathrm{e}} \mp \frac{\pi}{4}\right)} \mathrm{e}^{\,i\left[\mp \frac{x^2}{4} - a \ln\left(x\sqrt{\frac{\mathrm{e}}{a}}\right)\right]}$$

as connecting relations at the junction u_0, that is

$$C^{(1)\boldsymbol{K}}(u) = \begin{cases} f_{\boldsymbol{K},0}^{(1,1)}\, \mathrm{e}^{\,i\lambda \int_{u_0}^{u} \varphi_{1,1}\,\mathrm{d}u'}; & u > u_0\,, \\ P\, f_{\boldsymbol{K},0}^{(2,1)}\, \mathrm{e}^{\,i\lambda \int_{u_0}^{u} \varphi_{2,1}\,\mathrm{d}u'} + Q\, \mathrm{e}^{i\delta} f_{\boldsymbol{K},0}^{(1,1)}\, \mathrm{e}^{\,i\lambda \int_{u_0}^{u} \varphi_{1,1}\,\mathrm{d}u'}; & u < u_0\,, \end{cases}$$

$$C^{(2)\boldsymbol{K}}(u) = \begin{cases} f_{\boldsymbol{K},0}^{(2,1)}\, \mathrm{e}^{\,i\lambda \int_{u_0}^{u} \varphi_{2,1}\,\mathrm{d}u'}; & u > u_0\,, \\ -P\, f_{\boldsymbol{K},0}^{(1,1)}\, \mathrm{e}^{\,i\lambda \int_{u_0}^{u} \varphi_{1,1}\,\mathrm{d}u'} + Q\, \mathrm{e}^{-i\delta} f_{\boldsymbol{K},0}^{(2,1)}\, \mathrm{e}^{\,i\lambda \int_{u_0}^{u} \varphi_{2,1}\,\mathrm{d}u'}; & u < u_0 \end{cases} \qquad (4.55)$$

(4.53)

in case of the upper sign ($\varphi_0 > K_2$) and $\Delta > 0$ (cf. Fig. 9) and

$$C^{(1)\boldsymbol{K}}(u) = \begin{cases} P\, f_{\boldsymbol{K},0}^{(2,2)}\, \mathrm{e}^{\,i\lambda \int_{u_0}^{u} \varphi_{2,2}\,\mathrm{d}u'}; & u > u_0\,, \\ f_{\boldsymbol{K},0}^{(1,1)}\, \mathrm{e}^{\,i\lambda \int_{u_0}^{u} \varphi_{1,1}\,\mathrm{d}u'} + Q\, \mathrm{e}^{\,i\left(\delta + \frac{\pi}{2}\right)} f_{\boldsymbol{K},0}^{(1,2)}\, \mathrm{e}^{\,i\lambda \int_{u_0}^{u} \varphi_{1,2}\,\mathrm{d}u'}; & u < u_0\,, \end{cases}$$

(4.54)

$$C^{(2)\boldsymbol{K}}(u) = \begin{cases} -P\, f_{\boldsymbol{K},0}^{(2,1)}\, \mathrm{e}^{\,i\lambda \int_{u_0}^{u} \varphi_{2,1}\,\mathrm{d}u'}; & u > u_0\,, \\ f_{\boldsymbol{K},0}^{(1,2)}\, \mathrm{e}^{\,i\lambda \int_{u_0}^{u} \varphi_{1,2}\,\mathrm{d}u'} + Q\, \mathrm{e}^{-i\left(\delta + \frac{\pi}{2}\right)} f_{\boldsymbol{K},0}^{(1,1)}\, \mathrm{e}^{\,i\lambda \int_{u_0}^{u} \varphi_{1,1}\,\mathrm{d}u'}; & u < u_0 \end{cases} \qquad (4.56)$$

gative).
-known
3), and

in case of the lower sign ($\varphi_0 < K_2$) and $\Delta > 0$ (cf. Fig. 10), where

$$P = \mathrm{e}^{-a\pi}, \qquad Q = \frac{\sqrt{2\pi}\,\mathrm{e}^{-a\frac{\pi}{2}}}{\sqrt{a}\,|\Gamma(\pm i\,a)|} = \sqrt{1 - P^2}, \qquad \delta = a \ln \frac{a}{\mathrm{e}} - \frac{\pi}{4} - \arg \Gamma(i\,a). \qquad (4.57)$$

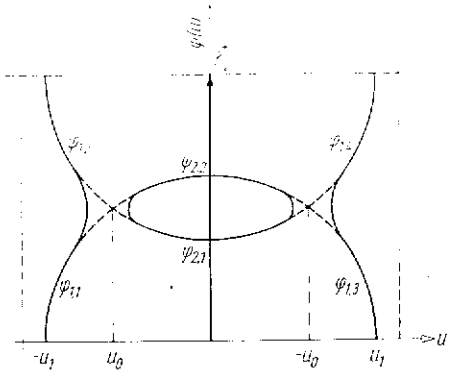

Fig. 10. Linear network

If $\Delta < 0$, the connecting relations come out quite analogously, but the signs of P are reversed if the same notation of ascending and descending branches of φ is used. It should be noted that both the intersection points of two circles are distinguished by the sign of $\Delta = \pm |\Delta|$. P and Q are Pippard's probability amplitudes, and δ is the phase change accompanying a Bragg switching. From Stirling's formula we learn that $\arg \Gamma(i\,a) \approx a \ln (a/\mathrm{e}) - \pi/4$ for large a so that $\delta \to 0$ in the low-field limit. In our gauge-independent formalism we have no evidence [49] of a phase change $\delta' = \pm \lambda \Delta$ that Pippard deduced from regauging orbit phases on switching [27]. As mentioned by R. G. Chambers [68] such phase changes δ' prove to be immaterial because, on the rationality condition supposed, they cancel in the final energy expression. Another minor point of difference is that in our formalism a minus sign appears in one of the connecting relations (4.55) or (4.56) [49] instead of a purely imaginary breakdown amplitude originally assumed by Pippard [51, 27]. The extra phase $\pi/2$ occuring in (4.56) accounts for the fact that in this case ($\varphi_0 < K_2$) the switching is combined with passing a turning point.

The breakdown parameters (4.57) depend on the quantity (4.54). Let $\hat{\boldsymbol{K}} = \boldsymbol{K} - \boldsymbol{K}'$ be one of the shortest reciprocal lattice vectors in the plane perpendicular to the field, then

$$a = \frac{|V_{\hat{\boldsymbol{K}}}|^2}{4\,\hbar\,\omega_c^{(0)}\,\mathscr{E}_0^{1/2}\,(\mathscr{E}_\perp - \mathscr{E}_0)^{1/2}}\,.$$

$\mathscr{E}_0$ and $\mathscr{E}_\perp$ have been defined in connecting with (4.41) and (4.42). The condition $a \ll \pi/2$ for almost complete breakdown is identical with (4.42).

The breakdown probability P^2 was derived first by Blount [10] with regard to Zener breakdown and later by R. G. Chambers [68] with more general arguments.

To derive the Pippard relations (4.55) and (4.56), systems of linearized first-order differential equations similar to (4.51) were considered by W. G. Chambers [44], who referred to an unpublished work of Upadhyaya [69], Slutskin and Kadigrobov [70], Slutskin [49, 71], Ruvalds and McClure [50] and W. G. Chambers [72]. In most cases [44, 49, 50] they are obtained from secular Hamiltonians of two-band models based on the $\boldsymbol{k}, \boldsymbol{p}$ approximation by replacing $\boldsymbol{k}$ by $\tilde{\boldsymbol{w}}$. Outside the validity region of the two-band model a Peierls Hamiltonian is taken. In this way one obtains a field-independent band coupling just as in the

present calculation but avoids the assumption of weak binding. This procedure, however, is not proved in a closed form in contrast to Roth's many-band Hamiltonian. A derivation of the breakdown effect from a two-band Roth Hamiltonian undertaken by Schulz [47] and the author [48] yielded somewhat different results because the Roth coupling terms are field-dependent and vanish for $B \to 0$. From another point of view, R. G. Chambers [68] discussed the question to what extent Pippard's results are independent of the nearly-free approximation.

In concluding this section we want to show how to derive the Pippard energy quantization [27, 51] from the subsidiary condition (2.47). We first consider the simplest example of interband breakdown, i.e. the linear network [51] (Fig. 10). The general solution (4.14) of the linear network left and right of the breakdown points $\pm u_0 = \mp |u_0|$ with $\Delta = \pm |\Delta|$ ($u_0 < 0$) looks as follows:

$$C^{\boldsymbol{K}}(u) = \sum_{l=-\infty}^{+\infty} \begin{cases} \alpha_{1,1}^{(l)} f_{\boldsymbol{K},0}^{(1,1,l)} \, \mathrm{e}^{\,i\lambda \int_{u_0}^{u} \varphi_{1,1}^{(l)} \mathrm{d}u'} + \alpha_{1,2}^{(l)} f_{\boldsymbol{K},0}^{(1,2,l)} \, \mathrm{e}^{\,i\lambda \int_{u_0}^{u} \varphi_{1,2}^{(l)} \mathrm{d}u'} ; & -u_1 < u < u_0 , \\ \alpha_{2,1}^{(l)} f_{\boldsymbol{K},0}^{(2,1,l)} \, \mathrm{e}^{\,i\lambda \int_{u_0}^{u} \varphi_{2,1}^{(l)} \mathrm{d}u'} + \alpha_{2,2}^{(l)} f_{\boldsymbol{K},0}^{(2,2,l)} \, \mathrm{e}^{\,i\lambda \int_{u_0}^{u} \varphi_{2,2}^{(l)} \mathrm{d}u'} ; & u_0 < u < -u_0 , \\ \alpha_{1,3}^{(l)} f_{\boldsymbol{K},0}^{(1,3,l)} \, \mathrm{e}^{\,i\lambda \int_{-u_0}^{u} \varphi_{1,3}^{(l)} \mathrm{d}u'} + \alpha_{1,4}^{(l)} f_{\boldsymbol{K},0}^{(1,4,l)} \, \mathrm{e}^{\,i\lambda \int_{-u_0}^{u} \varphi_{1,4}^{(l)} \mathrm{d}u'} ; & -u_0 < u < u_1 , \end{cases} \tag{4.58}$$

where $\varphi_{\nu,i}^{(l)} = \varphi_{\nu,i}^{(0)} + l\,K_{22}$ and $f_{\boldsymbol{K},0}^{(\nu,i,l)} = \left(\partial E_\nu / \partial \varphi_{\nu,i}^{(0)}\right)^{-1/2} c_\nu \left(\widetilde{\boldsymbol{w}}_{\nu,i}^{(0)} + \boldsymbol{K} + l\,\boldsymbol{K}_2\right)$. The subsidiary condition (2.47),

$$B_0(\boldsymbol{K}_2)\, C^{\boldsymbol{K}_\mathrm{r} + \boldsymbol{K}_2} = \mathrm{e}^{i\lambda u K_{22}}\, C^{\boldsymbol{K}_\mathrm{r} + \boldsymbol{K}_2} = \mathrm{e}^{i\,(\boldsymbol{q} + n\,\boldsymbol{K}_1,\, \boldsymbol{K}_2 \times \lambda)}\, C^{\boldsymbol{K}_\mathrm{r}} ,$$

is obviously fulfilled if

$$\alpha_{\nu,i}^{(l-1)} \, \mathrm{e}^{\pm i\lambda K_{22} u_0} = \mathrm{e}^{i\,(\boldsymbol{q} + n\,\boldsymbol{K}_1,\, \boldsymbol{K}_2 \times \lambda)}\, \alpha_{\nu,i}^{(l)} . \tag{4.59}$$

At the turning points $-u_1$ and $+u_1$ the respective branches $\varphi_{1,1}^{(l)}$ and $\varphi_{1,3}^{(l)}$ join the branches $\varphi_{1,2}^{(l-1)}$ and $\varphi_{1,4}^{(l-1)}$. Neglecting intraband coupling between the open orbits, we apply the WKB boundary condition

$$\left.\begin{aligned} \alpha_{1,1}^{(l)} \, \mathrm{e}^{\,i\lambda \int_{u_0}^{-u_1} \varphi_{1,1}^{(l)} \mathrm{d}u} \, \mathrm{e}^{\,-i\frac{\pi}{4}} &= \alpha_{1,2}^{(l-1)} \, \mathrm{e}^{\,i\lambda \int_{u_0}^{-u_1} \varphi_{1,2}^{(l-1)} \mathrm{d}u} \, \mathrm{e}^{\,i\frac{\pi}{4}} , \\ \alpha_{1,3}^{(l)} \, \mathrm{e}^{\,i\lambda \int_{-u_0}^{u_1} \varphi_{1,3}^{(l)} \mathrm{d}u} \, \mathrm{e}^{\,i\frac{\pi}{4}} &= \alpha_{1,4}^{(l-1)} \, \mathrm{e}^{\,i\lambda \int_{-u_0}^{u_1} \varphi_{1,4}^{(l-1)} \mathrm{d}u} \, \mathrm{e}^{\,-i\frac{\pi}{4}} \end{aligned}\right\} \tag{4.60}$$

at these points (cf. (4.23) and (4.24)). Combining (4.59) and (4.60), we get

$$\left.\begin{aligned} \alpha_{1,1}^{(l)} &= \alpha_{1,2}^{(l)} \, \mathrm{e}^{\,i\,(\boldsymbol{q} + n\,\boldsymbol{K}_1,\, \boldsymbol{K}_2 \times \lambda)}\, \mathrm{e}^{\,i(\lambda \mathcal{A}_1 + \pi)/2} , \\ \alpha_{1,3}^{(l)} &= \alpha_{1,4}^{(l)} \, \mathrm{e}^{\,i\,(\boldsymbol{q} + n\,\boldsymbol{K}_1,\, \boldsymbol{K}_2 \times \lambda)}\, \mathrm{e}^{\,-i\,(\lambda \mathcal{A}_1 + \pi)/2} , \end{aligned}\right\} \tag{4.61}$$

where $\mathcal{A}_1$ is the area between the open orbits within a Brillouin zone. From the

relations (4.56) and the corresponding ones holding at u_0 ($\lambda < 0$) we obtain

$$\mathfrak{a}_{2,1} = Q\,\mathrm{e}^{i\left(\delta - \frac{\pi}{2}\right)}\mathfrak{a}_{2,2} - P\,\mathfrak{a}_{1,2}\,,$$

$$\mathfrak{a}_{1,1} = P\,\mathfrak{a}_{2,2} + Q\,\mathrm{e}^{-i\left(\delta - \frac{\pi}{2}\right)}\mathfrak{a}_{1,2}\,,$$

$$\mathfrak{a}_{1,3} = Q\,\mathrm{e}^{i\left(\delta + \frac{\pi}{2}\right)}\mathfrak{a}_{1,4} + P\,\mathfrak{a}_{2,2}\,\mathrm{e}^{i\lambda\int_{u_0}^{u_0} q_{2,2}\,\mathrm{d}u}\,,$$

$$\mathfrak{a}_{2,1}\,\mathrm{e}^{i\lambda\int_{u_0}^{-u_0} q_{2,1}\,\mathrm{d}u} = -P\,\mathfrak{a}_{1,4} + Q\,\mathrm{e}^{-i\left(\delta + \frac{\pi}{2}\right)}\mathfrak{a}_{2,2}\,\mathrm{e}^{i\lambda\int_{u_0}^{u_0} q_{2,2}\,\mathrm{d}u}\,.$$

Eliminating $\mathfrak{a}_{2,1}$ and $\mathfrak{a}_{2,2}$ from these equations and using (4.61), we find a homogeneous system of equations for $\mathfrak{a}_{1,2}$ and $\mathfrak{a}_{1,4}$. Its solvability condition

$$-2\,Q\cos\left(\frac{\lambda}{2}\,\mathcal{A}_2 - \delta\right)\cos\left(\boldsymbol{q} + n\,\boldsymbol{K}_1,\,\boldsymbol{K}_2\times\boldsymbol{\lambda}\right) =$$

$$= \cos\frac{\lambda}{2}\,(\mathcal{A}_1 + \mathcal{A}_2) + Q^2\cos\left(\frac{\lambda}{2}\,(\mathcal{A}_1 - \mathcal{A}_2) + 2\,\delta\right) \qquad (4.62)$$

is the quantum condition of the energy [51, 48, 70, 49, 50, 73], where $\mathcal{A}_2$ is the area of the closed lens orbit. This expression is exhaustively discussed by Pippard [51]. It exhibits no subband splitting and no q_2-dependence as we have neglected the (intraband) coupling between neigbouring linear networks. As expected, it gives the Onsager condition $\cos(\lambda/2)\,(\mathcal{A}_1 + \mathcal{A}_2) = 0$ of the broken down orbit in case of total breakdown ($Q = 0$) and the respective quantum conditions $\cos(\lambda/2)\mathcal{A}_2 = 0$ and $-\cos(\boldsymbol{q} + n\,\boldsymbol{K}_1,\,\boldsymbol{K}_2\times\boldsymbol{\lambda}) = \cos(\lambda/2)\mathcal{A}_1$ of the lens orbit and the open orbit in absence of breakdown ($Q = 1$). In view of (2.13) the latter is easily shown to be identical with (4.32).

The simplest example of a two-dimensional interband network is W. G. Cham-

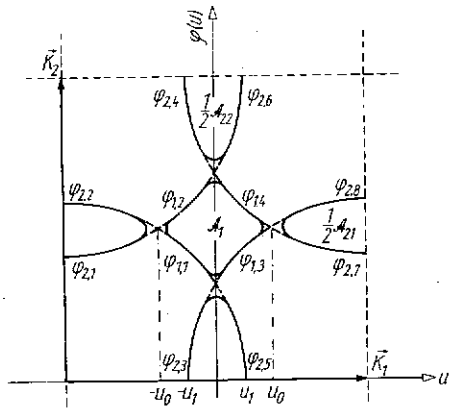

Fig. 11. Tetragonal network

bers' tetragonal network [29]. With regard to Fig. 11 its general solution (4.14) reads

$$C^{K}(u \quad j\,K_{11}) =$$

$$= \sum_{l} \begin{cases} \sum_{i=1,2} \alpha_{2,i}^{(j,l)} f_{K,0}^{(2,i,l)} \, e^{i\lambda \int_{u_0}^{u} \varphi_{2,i}^{(j)} du'} ; & -\frac{K_{11}}{2} < u < -u_0 , \\ \sum_{i=3,4} \alpha_{2,i}^{(j,l)} f_{K,0}^{(2,i,l)} \, e^{i\lambda \int_{0}^{u} \varphi_{2,i}^{(j)} du'} + \sum_{i=1,2} \alpha_{1,i}^{(j,l)} f_{K,0}^{(1,i,l)} \, e^{i\lambda \int_{0}^{u} \varphi_{1,i}^{(j)} du'} ; & -u_0 < u < 0 , \\ \sum_{i=5,6} \alpha_{2,i}^{(j,l)} f_{K,0}^{(2,i,l)} \, e^{i\lambda \int_{0}^{u} \varphi_{2,i}^{(j)} du'} + \sum_{i=3,4} \alpha_{1,i}^{(j,l)} f_{K,0}^{(1,i,l)} \, e^{i\lambda \int_{0}^{u} \varphi_{1,i}^{(j)} du'} ; & 0 < u < u_0 , \\ \sum_{i=7,8} \alpha_{2,i}^{(j,l)} f_{K,0}^{(2,i,l)} \, e^{i\lambda \int_{u_0}^{u} \varphi_{2,i}^{(j)} du'} ; & u_0 < u < \frac{K_{11}}{2} , \end{cases} \tag{4.63}$$

where $f_{K,0}^{(\nu,i,l)}(u - j\,K_{11}) = (\partial E_\nu / \partial \varphi_{\nu,i}^{(0)})^{-1/2}\, c_\nu\, (\widetilde{\boldsymbol{w}}_{\nu,i}^{(0)} + \boldsymbol{K} - j\,\boldsymbol{K}_1 + l\,\boldsymbol{K}_2)$. The subsidiary conditions (2.47)

$$B_0(\boldsymbol{K}_2)\, C^{\boldsymbol{K}_\nu + \boldsymbol{K}_2} = e^{i(\boldsymbol{q},\, \boldsymbol{K}_2 \times \lambda)}\, C^{\boldsymbol{K}_\nu}, \quad B_0(\boldsymbol{K}_0)\, C^{\boldsymbol{K}_\nu + \boldsymbol{K}_0} = e^{i(\boldsymbol{q},\, \boldsymbol{K}_0 \times \lambda)}\, C^{\boldsymbol{K}_\nu}$$

connect the coefficients [11])

$$\alpha_{2,i}^{(j,\,l-1)} = e^{i\,(\boldsymbol{q} + j\,\boldsymbol{K}_1,\, \boldsymbol{K}_2 \times \lambda)}\, \alpha_{2,i}^{(j,\,l)}; \quad i = 4,6\,, \tag{4.64}$$

$$\alpha_{2,i}^{(j+q,\,l)} = e^{i(\boldsymbol{q},\, \boldsymbol{K}_0 \times \lambda)}\, \alpha_{2,i}^{(j,\,l)}; \qquad i = 7,8 \tag{4.65}$$

of different Brillouin zones marked by the indices j, l. The coefficients of one Brillouin zone are linked by Pippard's relations of the junctions at $u = \mp u_0$ ((4.56); $\Delta \lessgtr 0$):

$$\alpha_{1,1}\, e^{i\lambda \int_{0}^{-u_0} \varphi_{1,1}\, du} = Q_1\, e^{i\left(\delta_1 + \frac{\pi}{2}\right)} \alpha_{1,2}\, e^{i\lambda \int_{0}^{-u_0} \varphi_{1,2}\, du} + P_1\, \alpha_{2,2}\,,$$

$$\alpha_{2,1} = -P_1\, \alpha_{1,2}\, e^{i\lambda \int_{0}^{-u_0} \varphi_{1,2}\, du} + Q_1\, e^{-i\left(\delta_1 + \frac{\pi}{2}\right)} \alpha_{2,2}\,,$$

$$\alpha_{2,7} = Q_1\, e^{i\left(\delta_1 + \frac{\pi}{2}\right)} \alpha_{2,8} - P_1\, \alpha_{1,4}\, e^{i\lambda \int_{0}^{u_0} \varphi_{1,4}\, du},$$

$$\alpha_{1,3}\, e^{i\lambda \int_{0}^{u_0} \varphi_{1,3}\, du} = P_1\, \alpha_{2,8} + Q_1\, e^{-i\left(\delta_1 + \frac{\pi}{2}\right)} \alpha_{1,4}\, e^{i\lambda \int_{0}^{u_0} \varphi_{1,4}\, du}$$

and $u = 0$ ((4.55); $\Delta \lessgtr 0$):

$$\alpha_{2,4} = Q_2\, e^{-i\,\delta_2}\, \alpha_{2,6} - P_2\, \alpha_{1,4}\,, \qquad \alpha_{1,1} = Q_2\, e^{-i\,\delta_2}\, \alpha_{1,3} + P_2\, \alpha_{2,5}\,,$$

$$\alpha_{1,2} = P_2\, \alpha_{2,6} + Q_2\, e^{i\,\delta_2}\, \alpha_{1,4}\,, \qquad \alpha_{2,3} = -P_2\, \alpha_{1,3} + Q_2\, e^{i\,\delta_2}\, \alpha_{2,5}\,,$$

where the indices j, l have been omitted. We now eliminate the "inner" coefficients $\alpha_{1,i}$ from these relations and insert (4.64) in the form

$$\alpha_{2,3}^{(j,l)} = e^{i\,(\boldsymbol{q} + j\,\boldsymbol{K}_1,\, \boldsymbol{K}_2 \times \lambda)}\, e^{i\,(\lambda\, \mathcal{A}_{22} + \pi)/2}\, \alpha_{2,4}^{(j,l)}\,, \qquad \alpha_{2,5}^{(j,l)} = e^{i\,(\boldsymbol{q} + j\,\boldsymbol{K}_1,\, \boldsymbol{K}_2 \times \lambda)}\, e^{-i\,(\lambda\, \mathcal{A}_{22} + \pi)/2}\, \alpha_{2,6}^{(j,l)}$$

[11]) Note that the variable u is taken in the reduced form $u - j\,K_{11}$ ($-K_{11}/2 < u < K_{11}/2$).

which results from the WKB boundary condition at $u = \mp u_1$ as before. From the remaining four equations we eliminate $\alpha_{2,4}$ and $\alpha_{2,6}$ and make use of the relations

$$\alpha_{2,7}^{(j+1,l)} = e^{i(\lambda/2)\mathcal{A}_{21}} e^{2i\lambda l u_0 K_{22}} e^{-i2\pi l p/q} \alpha_{2,1}^{(j,l)},$$
$$\alpha_{2,8}^{(j+1,l)} = e^{-i(\lambda/2)\mathcal{A}_{21}} e^{2i\lambda l u_0 K_{22}} e^{-i2\pi l p/q} \alpha_{2,2}^{(j,l)}.$$

to warrant (4.63) continuous. In this way we obtain a linear relation

$$\begin{pmatrix} \alpha_{2,7}^{(j+1,l)} \\ \alpha_{2,8}^{(j+1,l)} \end{pmatrix} = e^{-i2\pi l p/q} M_j(\boldsymbol{q}) \begin{pmatrix} \alpha_{2,7}^{(j,l)} \\ \alpha_{2,8}^{(j,l)} \end{pmatrix}$$

between the coefficients of adjacent Brillouin zones, where

$$M_j(\boldsymbol{q}) = \frac{1}{2\,Q_2\,(1-Q_1^2)\cos\left(\frac{\lambda}{2}\mathcal{A}_{22} - \delta_2\right)} \begin{pmatrix} a & b \\ b^* & a^* \end{pmatrix}; \tag{4.66}$$

$$a = e^{i\frac{\lambda}{2}\mathcal{A}_{21}}\Big[Q_1^2\, e^{-2i\delta_1} e^{i\frac{\lambda}{2}\mathcal{A}_1}\Big(e^{-i\frac{\lambda}{2}\mathcal{A}_{22}} + Q_2^2\, e^{-2i\delta_2} e^{i\frac{\lambda}{2}\mathcal{A}_{22}}\Big) +$$
$$+ 2\,Q_1 e^{-i\delta_1}(1-Q_2^2)\cos(\boldsymbol{q}+j\boldsymbol{K}_1, \boldsymbol{K}_2\times\boldsymbol{\lambda}) + e^{-i\frac{\lambda}{2}\mathcal{A}_1}\Big(e^{i\frac{\lambda}{2}\mathcal{A}_{22}} + Q_2^2\, e^{2i\delta_2} e^{-i\frac{\lambda}{2}\mathcal{A}_{22}}\Big)\Big],$$

$$b = -i\, e^{i\frac{\lambda}{2}\mathcal{A}_{21}}\Big[2\,Q_1\cos\Big(\frac{\lambda}{2}(\mathcal{A}_1 - \mathcal{A}_{22}) - \delta_1\Big) +$$
$$+ 2\,Q_1 Q_2^2\cos\Big(\frac{\lambda}{2}(\mathcal{A}_1 + \mathcal{A}_{22}) - \delta_1 - 2\,\delta_2\Big) +$$
$$+ (1-Q_2^2)\,(e^{-i(\boldsymbol{q}+j\boldsymbol{K}_1, \boldsymbol{K}_2\times\boldsymbol{\lambda})} + Q_1^2\, e^{i(\boldsymbol{q}+j\boldsymbol{K}_1, \boldsymbol{K}_2\times\boldsymbol{\lambda})})\Big]$$

and $\det M_j(\boldsymbol{q}) = 1$. $\mathcal{A}_1$ and $\mathcal{A}_{21}$, $\mathcal{A}_{22}$ are the areas of the quadrangular and the lens-shaped orbits respectively. The subsidiary condition (4.65) is saying that the coefficients $\alpha_{2,7}^{(j,l)}$, $\alpha_{2,8}^{(j,l)}$ must form eigenvectors of the 2×2 matrix product $\prod_{j'=0}^{q-1} M_{j+j'}(\boldsymbol{q})$, the factors of which are arranged with the values of j' decreasing from the left to the right. The corresponding eigenvalues are given by the secular equation

$$\det\left(\prod_{j'=0}^{q-1} M_{j+j'}(\boldsymbol{q}) - e^{i(\boldsymbol{q}, \boldsymbol{K}_0\times\boldsymbol{\lambda})}\right) = 0.$$

Because of $\det M_j(\boldsymbol{q}) = 1$ it can be written as

$$\cos(\boldsymbol{q}, \boldsymbol{K}_0\times\boldsymbol{\lambda}) = \frac{1}{2}\operatorname{tr}\prod_{j'=0}^{q-1} M_{j+j'}(\boldsymbol{q}) = \frac{1}{2}\operatorname{tr}\prod_{j=0}^{q-1} M_j(\boldsymbol{q}). \tag{4.67}$$

This quantum condition exhibits two periods in $\boldsymbol{K}_1$-direction. The first one, $\boldsymbol{M}_j(\boldsymbol{q} + (q/p)\boldsymbol{K}_1) = \boldsymbol{M}_j(\boldsymbol{q})$, is well-known to us (cf. (2.49)) and follows from (4.66). The other one is obvious from $M_j(\boldsymbol{q} + n\boldsymbol{K}_1) = M_{j+n}(\boldsymbol{q})$ and the invariance of the trace under cyclic permutations of the factors. The real periodicity of the energy is the greatest common measure $(1/p)\boldsymbol{K}_1$ of both periods.

This indicates the splitting of the energy bands into q subbands (cf. Fig. 2). In the simple case $q = 1$ equation (4.67) reduces to

$$2\,Q_2\,(1 - Q_1^2)\cos\left(\frac{\lambda}{2}\,\mathcal{A}_{22} - \delta_2\right)\cos\,(\boldsymbol{q}, \boldsymbol{K}_1\times\boldsymbol{\lambda}) -$$

$$- 2\,Q_1\,(1 - Q_2^2)\cos\left(\frac{\lambda}{2}\,\mathcal{A}_{21} - \delta_1\right)\cos\,(\boldsymbol{q}, \boldsymbol{K}_2\times\boldsymbol{\lambda}) =$$

$$= Q_1^2\cos\left(\frac{\lambda}{2}\,(\mathcal{A}_1 + \mathcal{A}_{21} - \mathcal{A}_{22}) - 2\,\delta_1\right) + Q_2^2\cos\left(\frac{\lambda}{2}\,(\mathcal{A}_1 + \mathcal{A}_{22} - \mathcal{A}_{21}) - 2\,\delta_2\right) +$$

$$+ Q_1^2\,Q_2^2\cos\left(\frac{\lambda}{2}\,(\mathcal{A}_1 + \mathcal{A}_{21} + \mathcal{A}_{22}) - 2\,\delta_1 - 2\,\delta_2\right) + \cos\frac{\lambda}{2}\,(\mathcal{A}_{21} + \mathcal{A}_{22} - \mathcal{A}_1)\,. \tag{4.68}$$

This expression includes several linear networks as special cases. With $Q_2 = 0$ and $Q_1 = Q \neq 0$ we come back to (4.62). Putting $Q_1 = 1$, $\delta_1 = 0$, we get another type

$$(1 - Q_2^2)\cos\,(\boldsymbol{q}, \boldsymbol{K}_2\times\boldsymbol{\lambda}) = Q_2^2\cos\left(\frac{\lambda}{2}\,(\mathcal{A}_1 + \mathcal{A}_{22}) - 2\,\delta_2\right) + \cos\frac{\lambda}{2}\,(\mathcal{A}_1 - \mathcal{A}_{22})$$

of a linear network which has been considered by Slutskin [49]. The Onsager conditions in the cases of zero breakdown ($Q_1 = Q_2 = 1$) and total breakdown ($Q_1 = Q_2 = 0$) are easily obtained. It should be noted that the zone part $|\boldsymbol{K}_1\times\boldsymbol{K}_2|$ of the whole area of the broken-down orbit fails in the last cosine term of (4.68). But that does not count because $\lambda\,|\boldsymbol{K}_1\times\boldsymbol{K}_2| = 2\,\pi\,p$ for $q = 1$ (cf. (2.13)).

For further details of the tetragonal network we refer the reader to Chambers' original work [29] which also contains results of numerical computations of magnetic energy bands based on an expression equivalent to (4.67).

The basic idea of breakdown theory is the network model. This concept has been developed by Pippard [27, 51, 74, 75] in a physically illustrative rather than mathematical way. Some of his notions such as magnetic wave vector, magnetic energy band, group velocity, orbit lattice prove to be inherent in the general theory we have outlined in Section 2. Especially, Pippard has investigated the hexagonal network [27] occurring in the basal plane of Mg and Zn. He has derived its quantization condition for $q = 1$ and calculated the corresponding magnetic band structure. The various experimental aspects of magnetic breakdown, which we have not taken into consideration no more than all other applications of the theory, have been reviewed by Stark and Falicov [76].

5. Concluding Remarks

We have shown that the Bloch electron in a magnetic field behaves like a quasi-particle, with the wave vector $\boldsymbol{q}$, the dispersion law $\mathscr{E} = \mathscr{E}_\alpha(\boldsymbol{q})$, the velocity $\hbar\,\boldsymbol{v}_\alpha(\boldsymbol{q}) = \nabla_{\boldsymbol{q}}\,\mathscr{E}_\alpha(\boldsymbol{q})$, and the effective mass $\hbar^2\,(\boldsymbol{m}_\alpha^*(\boldsymbol{q}))^{-1} = \nabla_{\boldsymbol{q}}\,\nabla_{\boldsymbol{q}}\,\mathscr{E}_\alpha(\boldsymbol{q})$. It is a rather anisotropic entity as its motion perpendicular to the field distinctively differs from the one parallel to the field. This inheres in our whole analysis but is already reflected e.g. by the shape of the magnetic Brillouin zone. The most striking feature of the theory is the strange dependence of energies and wave functions on q and p, which spasmodically change with the field strength varying monotonously. How after all a continuous dependence of measurable quantities on field strength comes about is not clearly understood as yet.

The higher the experimental fields grow the more important the quasi-particle aspects become. The asymptotic solution methods, however, gradually lose their validity with increasing fields so that new approaches would be desirable. The only method available at present whose validity range enlarges with increasing fields is the nearly free approximation (cf. Fig. 8). It should be reformulated in terms of pseudopotential theory. A first step in this direction is made by Misra and Roth [77].

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Appendix 1

We collect a lot of useful formulas that are derived from (2.6) and (2.7) by using the well-known relation

$$e^{B}\, e^{A} = e^{-[A,\,B]/2}\, e^{A+B} \tag{A 1}$$

which holds if $[A, B]$ commutes with both A and B:

$$e^{-i(\boldsymbol{w},\,\boldsymbol{k}\times\boldsymbol{\lambda})}\, \boldsymbol{w}_{\perp}\, e^{i(\boldsymbol{w},\,\boldsymbol{k}\times\boldsymbol{\lambda})} = \boldsymbol{w}_{\perp} + \boldsymbol{k}_{\perp}\,, \tag{A 2}$$

$$e^{-i(\boldsymbol{w},\,\boldsymbol{k}\times\boldsymbol{\lambda})}\, (\boldsymbol{w}\times\boldsymbol{\lambda})\, e^{i(\boldsymbol{w},\,\boldsymbol{k}\times\boldsymbol{\lambda})} = (\boldsymbol{w}+\boldsymbol{k})\times\boldsymbol{\lambda}\,, \tag{A 3}$$

$$\begin{aligned} e^{i(\boldsymbol{w},\,\boldsymbol{k}\times\boldsymbol{\lambda})}\, e^{i(\boldsymbol{w},\,\boldsymbol{k}'\times\boldsymbol{\lambda})} &= e^{-(i/2)\,(\boldsymbol{k}\times\boldsymbol{k}',\,\boldsymbol{\lambda})}\, e^{i\,(\boldsymbol{w},\,(\boldsymbol{k}+\boldsymbol{k}')\times\boldsymbol{\lambda})} \\ &= e^{-i(\boldsymbol{k}\times\boldsymbol{k}',\,\boldsymbol{\lambda})}\, e^{i(\boldsymbol{w},\,\boldsymbol{k}'\times\boldsymbol{\lambda})}\, e^{i(\boldsymbol{w},\,\boldsymbol{k}\times\boldsymbol{\lambda})}\,, \end{aligned} \tag{A 4}$$

$$e^{i(\widetilde{\boldsymbol{w}},\,\boldsymbol{x})}\, \widetilde{\boldsymbol{w}}\, e^{-i(\widetilde{\boldsymbol{w}},\,\boldsymbol{x})} = \widetilde{\boldsymbol{w}} + \boldsymbol{x}\times\boldsymbol{b}\,, \tag{A 5}$$

$$e^{i(\widetilde{\boldsymbol{w}},\,\boldsymbol{x})}\left(\widetilde{\boldsymbol{w}} + \frac{1}{i}\,\nabla_{\boldsymbol{x}}\right) e^{-i(\widetilde{\boldsymbol{w}},\,\boldsymbol{x})} = \frac{1}{i}\,\nabla_{\boldsymbol{x}} + \frac{1}{2}\,\boldsymbol{x}\times\boldsymbol{b}\,, \tag{A 6}$$

$$\begin{aligned} e^{i(\widetilde{\boldsymbol{w}},\,\boldsymbol{x})}\, e^{i(\widetilde{\boldsymbol{w}},\,\boldsymbol{x}')} &= e^{-(i/2)\,(\boldsymbol{x}\times\boldsymbol{x}',\,\boldsymbol{b})}\, e^{i(\widetilde{\boldsymbol{w}},\,\boldsymbol{x}\times\boldsymbol{x}')} \\ &= e^{-i(\boldsymbol{x}\times\boldsymbol{x}',\,\boldsymbol{b})}\, e^{i(\widetilde{\boldsymbol{w}},\,\boldsymbol{x}')}\, e^{i(\widetilde{\boldsymbol{w}},\,\boldsymbol{x})}\,, \end{aligned} \tag{A 7}$$

$$e^{i\,(\boldsymbol{w},\,\boldsymbol{k}\times\boldsymbol{\lambda})}\, e^{i(\widetilde{\boldsymbol{w}},\,\boldsymbol{x})} = e^{-i(\boldsymbol{k}_{\perp},\,\boldsymbol{x})}\, e^{i(\widetilde{\boldsymbol{w}},\,\boldsymbol{x})}\, e^{i(\boldsymbol{w},\,\boldsymbol{k}\times\boldsymbol{\lambda})}\,. \tag{A 8}$$

$\boldsymbol{x}$ and $\boldsymbol{k}$ are arbitrary vectors in the direct and the reciprocal space respectively. $\boldsymbol{k}_{\perp}$ and $\boldsymbol{w}_{\perp}$ are the projections of $\boldsymbol{k}$ and $\boldsymbol{w}$ on the plane perpendicular to the field (1, 2 plane).

The symmetric operator $A(\widetilde{\boldsymbol{w}})$ formed from the function $A(\boldsymbol{k}) = \int e^{i(\boldsymbol{k},\boldsymbol{x})}\, A(\boldsymbol{x})\, \mathrm{d}^3\boldsymbol{x}$ can be generally represented by

$$A(\widetilde{\boldsymbol{w}}) = \int e^{i(\widetilde{\boldsymbol{w}},\,\boldsymbol{x})}\, A(\boldsymbol{x})\, \mathrm{d}^3\boldsymbol{x}\,.$$

Because of (A 7) the product

$$A(\widetilde{\boldsymbol{w}})\, B(\widetilde{\boldsymbol{w}}) = \iint A(\boldsymbol{x})\, B(\boldsymbol{x}')\, e^{-(i/2)\,(\boldsymbol{x}\times\boldsymbol{x}',\,\boldsymbol{b})}\, e^{i(\widetilde{\boldsymbol{w}},\,\boldsymbol{x}+\boldsymbol{x}')}\, \mathrm{d}^3\boldsymbol{x}\, \mathrm{d}^3\boldsymbol{x}'$$

of two symmetric operators is again a symmetric operator $C(\widetilde{\boldsymbol{w}})$. The identity

$$e^{-(i/2)\,(\boldsymbol{x}\times\boldsymbol{x}',\,\boldsymbol{b})}\, e^{i(\boldsymbol{k},\,\boldsymbol{x}+\boldsymbol{x}')} = e^{(i/2)\,(\nabla_{\boldsymbol{k}}\times\nabla_{\boldsymbol{k}'},\,\boldsymbol{b})}\, e^{i(\boldsymbol{k},\,\boldsymbol{x})}\, e^{i(\boldsymbol{k}',\,\boldsymbol{x}')}\big|_{\boldsymbol{k}'=\boldsymbol{k}}$$

is saying that $C(\widetilde{\boldsymbol{w}})$ is formed from

$$C(\boldsymbol{k}) = e^{(i/2)\,(\nabla_{\boldsymbol{k}}\nabla\times\nabla_{\boldsymbol{k}'},\,\boldsymbol{b})}\, A(\boldsymbol{k})\, B(\boldsymbol{k}')\big|_{\boldsymbol{k}'=\boldsymbol{k}}\,. \tag{A 9}$$

This is Roth's multiplication formula [12].

Appendix II

For deriving (2.61) we need the expression

$$\sum_{s=0}^{p-1} \varphi^*_{\boldsymbol{q}s}(\boldsymbol{K}'_{\mathrm{r}};\boldsymbol{s}')\,\varphi_{\boldsymbol{q}s}(\boldsymbol{K}_{\mathrm{r}};\boldsymbol{s})$$

$$= \mathrm{e}^{i(\lambda/2)[2q_2(K'_{\mathrm{r}1}-K_{\mathrm{r}1})+K'_{\mathrm{r}1}K'_{\mathrm{r}2}-K_{\mathrm{r}1}K_{\mathrm{r}2}]}\,\frac{p}{(2\pi)^2}\sum_{k=-\infty}^{+\infty}\mathrm{e}^{(i/2)k^2K_{02}K_{02}}\mathrm{e}^{ik(q_2+K'_{\mathrm{r}2})K_{02}}\times$$

$$\times\,\mathrm{e}^{i(\bar{\boldsymbol{q}}+\bar{\boldsymbol{K}}_{\mathrm{r}},\bar{\boldsymbol{s}})}\,\mathrm{e}^{-i(\bar{\boldsymbol{q}}+\bar{\boldsymbol{K}}'_{\mathrm{r}}+k\bar{\boldsymbol{K}}_0,\bar{\boldsymbol{s}}')}\sum_{l=-\infty}^{+\infty}\delta\,(u_{(2)}-u'_{(2)}+K'_{\mathrm{r}2}-K_{\mathrm{r}2}+k\,K_{02}+l\,K_{22})\,.$$

It is obtained from (2.33), where a shift of the summation indices is made and one of the resulting sums is joined with the s-summation. The latter gives the δ-function. We now insert this expression into

$$A=\sum_{s,s'=0}^{p-1}\int\!\!\int\varphi^*_{\boldsymbol{q}s}(\boldsymbol{K}_{\mathrm{r}};\bar{\boldsymbol{s}})\,\mathrm{e}^{-i(\boldsymbol{\varkappa},\boldsymbol{s})}\varphi_{\boldsymbol{q}'s'}(\boldsymbol{K}'_{\mathrm{r}};\bar{\boldsymbol{s}})\varphi^*_{\boldsymbol{q}'s'}(\boldsymbol{K}''_{\mathrm{r}};\bar{\boldsymbol{s}}')\,\mathrm{e}^{i(\boldsymbol{\varkappa},\boldsymbol{s}')}\varphi_{\boldsymbol{q}s}(\boldsymbol{K}'''_{\mathrm{r}};\bar{\boldsymbol{s}}')\,\mathrm{d}^2\bar{\boldsymbol{s}}\,\mathrm{d}^2\bar{\boldsymbol{s}}'\,,$$

write $\mathrm{e}^{i(\boldsymbol{\varkappa},\boldsymbol{s})}=\mathrm{e}^{-i(\lambda/2)\varkappa_1\varkappa_2}\mathrm{e}^{i(\boldsymbol{\varkappa},\bar{\boldsymbol{s}})}\mathrm{e}^{-i(\bar{\boldsymbol{t}},\boldsymbol{\varkappa}\times\boldsymbol{\lambda})}$ (cf. (2.29)), and perform the integrations. Whenever possible we convert sums over exponential functions into δ-functions in which case (2.30) is used several times. Finally, the tiresome calculation yields

$$A=\mathrm{e}^{(i/2)((\boldsymbol{K}_{\mathrm{r}}-\boldsymbol{K}'_{\mathrm{r}})\times(\boldsymbol{K}''_{\mathrm{r}}-\boldsymbol{K}'''_{\mathrm{r}}),\,\lambda)}\,\mathrm{e}^{(i/2)(\boldsymbol{K}'_{\mathrm{r}}\times\boldsymbol{K}_{\mathrm{r}},\,\lambda)}\,\mathrm{e}^{(i/2)(\boldsymbol{K}'''_{\mathrm{r}}\times\boldsymbol{K}''_{\mathrm{r}},\,\lambda)}\,\mathrm{e}^{i((\boldsymbol{q}-\boldsymbol{q}'+\boldsymbol{\varkappa})\times(\boldsymbol{K}''_{\mathrm{r}}-\boldsymbol{K}'_{\mathrm{r}}),\,\lambda)}\times$$

$$\times\,p\sum_{\boldsymbol{K}_{\mathrm{c}}}\delta\left(\boldsymbol{q}-\boldsymbol{q}'+\boldsymbol{\varkappa}+\boldsymbol{K}'''_{\mathrm{r}}-\boldsymbol{K}''_{\mathrm{r}}+\frac{1}{p}\boldsymbol{K}_{\mathrm{c}}\right)\sum_{k=-\infty}^{+\infty}\delta(\boldsymbol{K}_{\mathrm{r}}-\boldsymbol{K}'_{\mathrm{r}}+\boldsymbol{K}''_{\mathrm{r}}-\boldsymbol{K}'''_{\mathrm{r}}+k\,\boldsymbol{K}_0)\,. \tag{A 10}$$

We need this expression when inserting (2.36) into

$$\sum_{s,s'=0}^{p-1}(\psi_{\mu n\boldsymbol{q}s}\,|\,\mathrm{e}^{-i(\boldsymbol{\varkappa},\boldsymbol{r})}\,\psi_{\mu'n'\boldsymbol{q}'s'})\,(\psi_{\mu'n'\boldsymbol{q}'s'}\,|\,\mathrm{e}^{i(\boldsymbol{\varkappa},\boldsymbol{r})}\,\psi_{\mu n\boldsymbol{q}s})\,;\qquad \boldsymbol{r}=\boldsymbol{s}-\boldsymbol{w}\times\boldsymbol{\lambda}\,.$$

According to the δ-functions of (A 10) we have $K''_{\mathrm{r}3}=K'''_{\mathrm{r}3}$ and $K_{\mathrm{r}3}=K'_{\mathrm{r}3}$ in the optical region $|\boldsymbol{\varkappa}|\ll|\boldsymbol{K}|$. Hence, $\boldsymbol{K}_{\mathrm{r}}-\boldsymbol{K}'_{\mathrm{r}}=n''\,\boldsymbol{K}_1-k_0\,\boldsymbol{K}_0$ and $\boldsymbol{K}'''_{\mathrm{r}}-\boldsymbol{K}''_{\mathrm{r}}=n''\,\boldsymbol{K}_1-k'_0\,\boldsymbol{K}_0$, where $k_0-k'_0=k$ and $n''=0,\ldots,q-1$. Thus, the fourfold sum over $\boldsymbol{K}_{\mathrm{r}},\boldsymbol{K}'_{\mathrm{r}},\boldsymbol{K}''_{\mathrm{r}},\boldsymbol{K}'''_{\mathrm{r}}$ reduces to two sums over $\boldsymbol{K}_{\mathrm{r}},\boldsymbol{K}'''_{\mathrm{r}}$ (which we include in the symbols $\langle|\rangle$ and a sum over n''. Using (A 4) the occurring exponentials can be arranged so that (2.53) becomes applicable. In the final result (2.61) we utilize the fact that $C_{\mu,n,\boldsymbol{q}+(1/p)\boldsymbol{K}_{\mathrm{c}}}$ differs from $C_{\mu n\boldsymbol{q}}$ only by a phase factor which cancels out here.

Appendix III

Using (2.43), (A 1), (2.30), and $\boldsymbol{K}_{\mathrm{c}}=k\,\boldsymbol{K}_0+l\,\boldsymbol{K}_2$ we write the projectors (3.31) in the form

$$P'^{\boldsymbol{q},1}_{n}=\frac{p^2}{q\,|\boldsymbol{K}_1\times\boldsymbol{K}_2|}\sum_{k,l=-\infty}^{+\infty}\mathrm{e}^{-i(\boldsymbol{q}+n\boldsymbol{K}_1,\boldsymbol{K}_{\mathrm{c}}\times\boldsymbol{\lambda})}\,\mathrm{e}^{i(\lambda/2)k^2K_{01}K_{02}}\mathrm{e}^{-i\lambda kK_{01}v_{(1)}}\mathrm{e}^{i\lambda(kK_{02}+lK_{22})u_{(1)}}\,.$$

Applying this to (3.32) and performing the l-summation with regard to (2.30), we obtain

$$P''_{\boldsymbol{q}'} \frac{1}{\sqrt{2\pi}} \mathrm{e}^{-i\lambda\left[q_1' - \left(\frac{n'}{q'} - \frac{m'}{p'} + k'\right) K_{01}\right] v_{(1)}'} =$$

$$= \delta\,(q_1' - q_1)\,\delta_{n'n}\,\mathrm{e}^{-i\,(\lambda/2)\left(k' + \frac{n}{q} + \frac{m}{p}\right)^2 K_{01} K_{02}}\,\mathrm{e}^{-i\lambda\left(k' + \frac{n}{q} + \frac{m}{p}\right) q_2 K_{01}} \times$$

$$\times \frac{p}{K_{22}} \sum_{k=-\infty}^{-\infty} \mathrm{e}^{i\,(\lambda/2)\left(k + \frac{n}{q} + \frac{m'}{p}\right)^2 K_{01} K_{02}}\,\mathrm{e}^{i\lambda\left(k + \frac{n}{q} + \frac{m}{p}\right) q_2 K_{01}} \frac{1}{\sqrt{2\pi}}\,\mathrm{e}^{-i\lambda\left[q_1 + \left(k + \frac{n}{q} - \frac{m}{p}\right) K_{01}\right] v_{(1)}}.$$

Apparently, the projections of basis functions with different k' differ from each other only by phase factors. Selecting the ones with $k' = 0$, we get the complete orthonormal set of partner functions (3.33). We now calculate the matrix element of

$$C_0(\boldsymbol{R}) = \mathrm{e}^{i\,\pi\,j\,k\,q/p}\,\mathrm{e}^{i\,(\widetilde{\boldsymbol{w}},\,\boldsymbol{R})}\;; \quad \boldsymbol{R} = j\,\boldsymbol{R}_1 + k\,\boldsymbol{R}_2 + l\,\boldsymbol{R}_3 \tag{A 11}$$

with these functions. With the aid of (A 1) and (2.30) we write

$$C_0(\boldsymbol{R}) = \mathrm{e}^{i\,(\lambda/2)\,(k/p)^2\,K_{01}\,K_{02}}\,\mathrm{e}^{i\,q_2\,R_2}\,\mathrm{e}^{i\,\lambda\,(k/p)\,K_{01}\,v_{(1)}}\,\mathrm{e}^{i\,(j\,R_{11} + k\,R_{21})\,u_{(1)}}$$

and obtain

$$C_0(\boldsymbol{R})\,\chi_{n\boldsymbol{q}}(m;\,v_{(1)}) = \mathrm{e}^{i\,(\boldsymbol{q} + (m/p)\,\boldsymbol{K}_0,\,\boldsymbol{R})}\,\chi_{n\boldsymbol{q}}\left((m-k)_p;\,v_{(1)}\right)$$

after some obvious manipulations, in which (2.30) is needed. Thus, (3.34) gives

$$(\chi_{n'\boldsymbol{q}'}(m';\,v_{(1)}) \mid C_0(\boldsymbol{R})\,\chi_{n\boldsymbol{q}}(m;\,v_{(1)})) = \mathrm{e}^{i\,(\boldsymbol{q} + (m/p)\,\boldsymbol{K}_0,\,\boldsymbol{R})}\,\delta_{n'n}\,\delta_{m',\,(m-k)_p}\,\delta\,(\boldsymbol{q}'_\perp - \boldsymbol{q}_\perp)\,. \tag{A 12}$$

Note that $\chi_{n\boldsymbol{q}}$ is an eigenfunction of $C_0(\widetilde{\boldsymbol{R}})$ (cf. (2.22)).

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