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1991 J. Phys.: Condens. Matter 3 3047

(http://iopscience.iop.org/0953-8984/3/18/001)

J. Phys.: Condens. Matter 3 (1991) 3047–3064. Printed in the UK

REVIEW ARTICLE

Magnetic gauge transformations in solid-state problems

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Received 15 August 1990, in final form 31 Janury 1991

Abstract. Gauge transformation theory, indispensable in particle physics, is finding a role in magnetic dynamics in the solid state. It can allow for the presence of an imposed magnetic field on the quantum formulation of translational symmetry, thereby extending the range and power of Bloch theory applied to crystalline magnetic phenomena.

The principle is explained and reviewed, along with comments on its application to such features as incommensurate and commensurate enumeration of states, magnetic spectra, quantum phasing and flux quantization.

Notation

a	translating distance in x-direction
$\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$	cell vectors
e	numerical electronic charge
e	algebraic particle charge
$\boldsymbol{k}$	wave vector
l	atomic site vector index
m	(carrier) electron mass
n	magnetic quantum number
$\boldsymbol{p}$	momentum; components p_x, p_y, p_z
p, q	quantizing integers
$\boldsymbol{r}$	vector position
u	envelope function
$\boldsymbol{v}$	velocity $= \dot{\boldsymbol{r}}$
w	atomic wave function
x, y, z	Cartesian coordinates
$\boldsymbol{A}$	vector potential
$\boldsymbol{B}$	magnetic field
C	loop
$\mathscr{C}(\boldsymbol{a})$	translation matrix
E, E_0	energy
$\boldsymbol{E}$	electric field
F	Landau state overlap integral
H	Hamiltonian
I	Hall current
$\boldsymbol{J}$	current density
L_x, L_y, L_z	quantizing lengths; crystal dimensions

0953-8984/91/183047 + 18 $03.50

L	Langrangian
N	number of Landau states
R	Hall constant
U	factor in quantum state
V	sinusoidal potential strength
V_H	Hall voltage
α	$eB/\hbar$
β	unspecified quantum state
γ	phase in Onsager quantizing condition
ε	scaled energy
ζ	Fermi energy
κ	Peierls vector
λ	quantizing integer
ν, ν_s	carrier density
ϕ	Josephson phase
Φ	magnetic flux
χ	single-valued gauge function
ψ	quantum wave function
ω_C	cyclotron frequency

1. Introduction

Gauge transformation theory has for many years provided a principle of considerable formal power in particle physics. More recently it has been discovered by solid-state physicists as a means of symmetrizing quantum states of crystal electrons in a magnetic field. These states are fundamental to the physics of such basic phenomena as magneto-resistance in metals and magneto-optics/transport in semiconductors. Gauge theory is also related to magnetic flux quantization, an indispernsable notion in superconductivity, and possibly the quantum Hall effect. At a more mathematical level gauge theory has also provided a simple model of an aperiodic dynamical system [1], with fractal features.

Gauge refers (in this article) to the vector potential occurring in the dynamics of charge in a magnetic field. Both the Lagrange and Hamilton descriptions demand its use, and yet the potential is not unique. The magnetic flux through any loop gives the loop integral of the potential, and this is recognizably of mechanical significance. However the quantum eigenstates are sensitive to the choice of potential, and not merely to within a phase factor as is sometimes believed. Reconciling these two aspects is the subject of gauge transformation theory; it can impose a translational symmetry, which serves not only to classify and enumerate the quantum states, but also to introduce useful dynamical features.

This article first reviews the elementary quantum mechanics of free charge in a magnetic field, emphasizing gauge features. The translational constraints of a periodic potential, leading to Bloch states, are then considered in the presence of a magnetic field, and the Peierls quantization discussed. The translational gauging transformation is introduced, with an explanation of magnetic Bloch states. Applications to level broadening, magnetic breakdown and flux quantization are discussed. Gauge notions in connection with the quantum Hall effect precede a brief digression on a new approach to that problem. It is emphasized that it is the physics that is of interest here but it is

necessary (with apologies) to employ the elements of quantum mechanics and solid-state theory. A list of symbols is appended.

2. Free charge in a magnetic field

A free particle of charge e moving in a magnetic field $\boldsymbol{B}$ is acted on by the Lorenz force $e\dot{\boldsymbol{r}} \times \boldsymbol{B}$ normal to the velocity $\dot{\boldsymbol{r}}$. A steady uniform field does no work, nor is there any change in kinetic energy, so how therefore are we to explain diamagnetism and other magnetic phenomena? The well known answer is quantization, which determines the energy spectrum, and statistically distributes the available charge. Our starting point therefore is the classical formulation of the charge–field interaction, leading to its quantization.

A magnetic field $\boldsymbol{B}$ is peculiar in that switching it on (and off) is itself appreciably part of the dynamics through the induced electromotive force. Changing the magnetic flux Φ spanning some arbitrary loop C, the EMF is defined and given by

$$\int_C \boldsymbol{E} \cdot \mathrm{d}\boldsymbol{r} = -\mathrm{d}\Phi/\mathrm{d}t. \tag{2.1}$$

The work done in imposing the magnetic field alters the charge energy; indeed, atomic diamagnetism may be introduced in this way, as done, for example, by Feynman [2]. But in the end, the flux loop has to be fixed effectively by quantization. It was in fact established many years ago by Van Leeuwen that, averaged over classical mechanical configurations, the magnetic energy change vanishes.

Assuming then a time-varying field $\boldsymbol{B}$, and an electric field $\mathbf{E}$, the accelerative force equation becomes for a free charged particle of mass m,

$$m\dot{\boldsymbol{r}} = e\dot{\boldsymbol{r}} \times \boldsymbol{B} + e\boldsymbol{E} \tag{2.2}$$

where the induced electric field is to be found from (2.1), that is, by solving $\nabla \times \mathbf{E} = -\dot{\boldsymbol{B}}$. Central to its quantization, equation (2.2) must now be cast in Lagrangian form, and this is done through the introduction of the vector potential $\boldsymbol{A}(r, t)$. A formal solution to the above Maxwell equation can then be written as $\boldsymbol{E} = -\partial\boldsymbol{A}/\partial t$ where $\boldsymbol{B} = \nabla \times \boldsymbol{A}$. Using a simple vector relation, (2.2) becomes

$$\mathrm{d}(m\dot{\boldsymbol{r}} + e\boldsymbol{A})/\mathrm{d}t = \mathrm{e}\nabla(\dot{\boldsymbol{r}} \cdot \boldsymbol{A}) \tag{2.3}$$

where $\mathrm{d}\boldsymbol{A}/\mathrm{d}t$ follows the particle, and is finite even if $\partial\boldsymbol{A}/\partial t = 0$.

The subject of this article can now be introduced. Assume a coordinate frame whose $\boldsymbol{r}$ components are x, y, z, and a uniform field $\boldsymbol{B}$ in the z direction. Then $\boldsymbol{A}$ could be chosen as

$$\boldsymbol{A} = (0, Bx, 0) \tag{2.4}$$

so that from (2.3) a constant of the motion is $m\dot{y} + eBx$ to which any value p_y may be assigned:

$$m\dot{y} + eBx = p_y. \tag{2.5}$$

Now choosing some length a, the effect of the translation $x \rightarrow x + a$ is to replace A_y by $A_y + eBa$, described as a regauging of A, which of course leaves $\boldsymbol{B}$ unaltered. From (2.5) the constant p_y is shifted to $p_y - eBa$. It follows that the magnetic energy, dependent

only upon $\boldsymbol{B}$, must be independent of p_y. This elementary application illustrates the practicality of a gauge argument, but it is in quantum mechanics that its full power is realized.

The equation of motion (2.3), being no more than a rewrite of (2.2), is independent of gauge. It derives, using the standard rule, from the Lagrangian L given by

$$L = \tfrac{1}{2}m\dot{\boldsymbol{r}}^2 + e\dot{\boldsymbol{r}}\cdot\boldsymbol{A}. \tag{2.6}$$

Describing the translation $x \to x + a$ by the gauge transformation $A \to A + \nabla\chi$, then $\chi = Bay$. More generally, taking χ as any scalar function of r (which clearly leaves $\boldsymbol{B} = \nabla \times \boldsymbol{A}$ unchanged), then $L \to L + e\,\mathrm{d}\chi/\mathrm{d}t$. This result holds if χ is explicitly time-dependent, though in that case the scalar potential $e\dot{\chi}$ is added to L. Note that χ has the same dimensions as magnetic flux Φ.

Differentiating L with respect to $\dot{x}$, $\dot{y}$, $\dot{z}$ gives the components of momentum $\boldsymbol{p}$,

$$\boldsymbol{p} = m\dot{\boldsymbol{r}} + e\boldsymbol{A}. \tag{2.7}$$

Clearly $\boldsymbol{p}$ depends upon the choice of gauge of $\boldsymbol{A}$, so that adopting (2.4), the y component has been anticipated and appears as (2.5), while $p_x = m\dot{x}$ and $p_z = m\dot{z}$.

3. Magnetic quantization

The next step towards quantization is the construction of the Hamiltonian H, from the canonical definition,

$$H = \boldsymbol{p}\cdot\dot{\boldsymbol{r}} - L \tag{3.1}$$

using L from (2.6), and $m\dot{\boldsymbol{r}} = \boldsymbol{p} - e\boldsymbol{A}$, to give

$$H = (1/2m)(\boldsymbol{p} - e\boldsymbol{A})^2. \tag{3.2}$$

It is unnecessary to consider the classical Hamilton's equations since they can do no more than re-express the Lagrangian equations (2.3). The quantum view of (3.2) is to regard H as a mathematical operator obtained by treating p_x and x as operators satisfying the quantum commutator relation $[p_x, x] = -\mathrm{i}\hbar$, with similar relations for the y and z momenta/coordinate pairs. An immediate consequence is that the transverse velocity components, $v_x \equiv \dot{x}$ and $v_y \equiv \dot{y}$, quite generally, and independent of gauge, satisfy the commutator relation

$$[v_x, v_y] = (\mathrm{i}e\hbar/m^2)B. \tag{3.3}$$

This relation was the model for the Peierls magnetic quantization (see section 4).

The commutation relations are satisfied by representing $\boldsymbol{p}$ in the differential form $-\mathrm{i}\hbar\nabla$. But the gauge discussion raises an ambiguity because (see equation (2.5)) $p_y - eBa$ is exactly equivalent to p_y and could equally be represented as

$$p_y - eBa = -\mathrm{i}\hbar\,\partial/\partial\mathrm{y}. \tag{3.4}$$

This introduces the quantum version of the gauge change, namely as the transformed operator

$$p_y = \exp(-\mathrm{i}e\chi/\hbar)\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial y}\exp(\mathrm{i}e\chi/\hbar) \tag{3.5}$$

where, as earlier, $\chi = Bay$. Quite generally, for any single-valued function $\chi(x, y, z)$ the

gauge change $A \rightarrow A + \nabla\chi$ is represented by the transformation $\exp[(ie/\hbar)\chi]$. It does not follow however that solutions to the Schrödinger equation for different choices of A differ merely by a phase factor; quantum degeneracy complicates the issue. This is the main subject of the article.

Aside from the transformation (3.5), i.e. using $p = -i\hbar\nabla$, the eigenstates of the magnetic Hamiltonian (3.2) depend upon the choice of A, although the energy spectrum of course depends only upon B. A rotation of $\pi/2$ about the field direction provides the alternative choice $A' = (-By, 0, 0)$, the difference $A - A'$ itself being a gauge change, namely, $A' - A = \nabla(Bxy)$. To repeat the above remark, this does not mean that the corresponding eigenstates are convertible by a phase factor. When a cylindrical confining potential is added to (3.2), the combination $\frac{1}{2}(A + A')$ simplifies the azimuthal dependence of the bound-state wavefunctions. Pippard [3] gives an interesting discussion of the geometrical significance of rephasing for this choice of A.

Taking then the Landau gauge (2.4), the Schrödinger equation becomes

$$H\psi = (1/2m)[p_x^2 + (p_y - eBx)^2 + p_z^2]\psi = E\psi. \tag{3.6}$$

Motion in the field (z) direction is independent of B and represented by the plane-wave factor $\exp(ik_z z)$, where k_z provides the eigenvalues $\hbar k_z$ of p_z. Taking a quantizing length L_z gives $k_z = (2\pi/L_z)$ (integer). Omitting the k_z factor, the transverse magnetic motion is represented by the so-called Landau wavefunction, written as

$$\psi_L(x, y; k_y) = \exp(ik_y y)u_n(\alpha^{1/2}(x - p_y/eB)) \tag{3.7}$$

where the scaling area $\alpha^{-1} = (\hbar/eB)$ and $p_y = \hbar k_y$. Each function $u_n(\xi)$ consists of a Hermite polynomial of order n, multiplied by $\exp(-\xi^2/2)$. The symmetry centre $\xi = 0$ thus locates the Landau states at $x = p_y/eB$. The eigenvalue E is independent of p_y, as anticipated by the gauge argument, and takes the allowed values $(n + \frac{1}{2})\hbar eB/m$.

An assumed length L_y now provides the quantized values $k_y = (2\pi/L_y)$ (integer) and thereby a quasi-continuum of Landau centres $(\hbar k_y/eB)$. Confining these to the interval $x = 0, L_x$, it follows that the total number N of Landau states for any E is

$$N = L_x \div (h/L_y eB). \tag{3.8}$$

Defining total magnetic flux $\Phi = BL_xL_y$, N may be usefully expressed as

$$N = \Phi \div h/e. \tag{3.9}$$

The minimum value $N = 1$ requires $\Phi = h/e$, which is therefore a kind of flux 'quantum'. It refers, of course, to a given spin state. There is however no necessity for Φ to be an integral number of such quanta, and, indeed, the above enumeration does not adequately deal with orbital centres $\hbar k_y/eB$ very close to the boundaries. Questions relating to integral and more generally rational values of $e\Phi/\hbar$ are raised more acutely for magnetic states in a regular crystal lattice (sections 6 and 7).

4. Lattice electrons

The preceding section has explained the relations between the translation $x \rightarrow x + a$, the gauge change $A \rightarrow A + \nabla\chi$ and the quantum phase transformation $\exp(-ie\chi/\hbar)$. But all this was for the free charge whose quantum states can in any event be written down explicitly, and where the length a is perfectly arbitrary. These notions can be developed

for the ideal crystal lattice, with the constraint that translations must connect equivalent points in different cells. Before considering these more abstract notions it is worth while reviewing the elements of Bloch theory and some established notions of magnetic motion in real materials.

Transport in metal and semiconductors, as well as optical processes in the latter, are understood in terms of the energy spectra (or electronic band structures) based upon the quantum Bloch functions. These are propagating quantum states characterized by a wavevector k_B, and having the cell-phasing property

$$\psi_{k_B}(r + a) = \exp(ik_B \cdot a)\psi_{k_B}(r). \tag{4.1}$$

The smallest lattice vector a connects equivalent points in adjacent cells, but repetition of (4.1) gives the relative phase for any pair of cells. The wavevectors k_B are enumerated (or quantized) according to the so-called periodic boundary conditions, namely that

$$\psi_{k_B}(r + L) = \psi_{k_B}(r) \tag{4.2}$$

where the cell separation L is of suitably large magnitude. Historically, Peierls and others showed that enumeration using physical boundaries, having electrostatic and other asymmetric effects, would not be appreciably different. Magnetic gauging however requires attention to the use of the periodic boundary condition (section 7).

The general theory of Bloch states shows that, within the Brillouin zone, a polyhedron in k_B-space whose plane boundaries arise from $\exp(ik_B \cdot a) = \pm 1$, there can be many states having a particular k_B. The zone k_B-values broadens each of these into a band of energy values with a characteristic density of states function. Magnetic dynamics has employed a variety of perturbative models based on electronic bands and Bloch state matrix elements. Their utility depends upon both the physical structure, that is, metal or semiconductor, and the effect, which coud be magneto-transport or magneto-optic.

Peierls was the first to direct attention to electronic band diamagnetism, introducing a powerful method of magnetic quantization. In a non-degenerate band, the band energies are a unique function of the quasi-continuous wavevector k_B. Near the centre or edge of a Brillouin zone this dependence is typically quadratic (not necessarily isotropic), but more deeply within, a higher power dependence is appreciable. Alternatively, because the zone structure is repetitive in k_B-space, the band energies can be Fourier-analysed. However represented, Peierls quantization replaces k_B by a vector operator $\boldsymbol{\kappa}$ whose components do not commute but satisfy the relation (3.3), with $m\boldsymbol{v} = \hbar\boldsymbol{\kappa}$, that is to say,

$$[\kappa_x, \kappa_y] = (ie/\hbar)B. \tag{4.3}$$

So long as there is no ambiguity arising from the ordering of κ_x, κ_y, the resulting expression can be used for an effective energy band Hamiltonian operator (see section 8). In connection with the oscillatory diamagnetism in metals (de Haas–van Alphen effect), Onsager [4] ingeniously employed (4.3), making use of the WKB approximation in the form,

$$\int \kappa_x \, d\kappa_y = (n + \gamma)eB/\hbar \tag{4.4}$$

in which the integral is taken over a closed cycle near the Fermi surface, to determine the eigenvalues $E_n(k_z)$. An authoritative account of this basic theory is to be found in Shoenberg [5].

The original arguments for the quantization rule (4.3) were based upon the so-

called 'tight-binding' Bloch function model (9). It is in fact more general, and gauge transformation theory is helpful in revealing this.

In semiconductors, transport and optical properties commonly require multiband models. Their structure is more important than the Fermi surface, and is the subject of extensive computation. The well established semi-empirical $k_B \cdot p$ method was extended by Luttinger and Kohn [6] to include a magnetic field, and has provided a practical way to handle complicated spin–orbital magneto-band structures. An important application to magneto-optics of InSb is due to Pidgeon and Brown [7].

5. Magnetic gauge transformation

The notions of magnetic gauge transformation and Bloch translational theory are now to be combined. It is evident that the imposition of a uniform magnetic field on an ideal crystal does not disturb its repetitive nature: within each cell is the same magnetic field added to the same electrostatic field. But, as for free charge, the electron Hamiltonian is not invariant because, in the translation $r \rightarrow r + a$, the vector potential $A(r)$ is regauged to $A(r) + A(a)$. This change is equivalent to the phase transformation (3.5), $\chi = A(a) \cdot r$, which replaces $-i\hbar\nabla$ by $-i\hbar\nabla + eA(a)$.

Anticipating a similar degree of degeneracy as described above for free electrons, and enumerating the states of common energy by the index β, it follows from (3.5) that $\psi_\beta(r + a)$ satisfies the same equation as any magnetic phased state

$$\exp(ie\chi/\hbar)\,\psi_{\beta'}(r).$$

If these could be equated then the translation $r \rightarrow r + a$, equivalent to a gauge change, would be represented by the magnetic re-phasing. Because of the degeneracy the best that can be asserted is the linear relation,

$$\psi_\beta(r + a) = \exp\left(\frac{ie}{\hbar}A(a) \cdot r\right) \sum_{\beta'} (\beta' | \mathscr{C}(a) | \beta)\psi_{\beta'}(r). \tag{5.1}$$

where the matrix $(\beta' | \mathscr{C}(a) | \beta)$ is yet to be determined. For each basic lattice vector a, b, c there is a matrix $\mathscr{C}(a)$ represented in a space whose dimensions and other features have yet to be determined. The translations $r \rightarrow r + a$ and $r \rightarrow r + b$ of course commute; because of the path-dependent phasing transformation, the matrices $\mathscr{C}(a)$ and $\mathscr{C}(b)$ however may not commute. In fact, it follows from (5.1) that quite generally, and independent of representation,

$$\mathscr{C}(b)\mathscr{C}(a) = \exp[(ie/\hbar)\Phi_c]\mathscr{C}(a)\mathscr{C}(b) \tag{5.2}$$

where $\Phi_c = B \cdot a \times b$ is the magnetic flux through the cell area $a \times b$. Equation (5.2) [8] thus generalizes the commutative identity which in the absence of a magnetic field allows the Abelian representation of the translation matrices, namely $\mathscr{C}(a) = \exp(ik_B \cdot a)$. Of course, closing any sequence of lattice translations, the $\mathscr{C}$ matrices restore the original state but with a relative phase cancelling that due to the phasing factor in (5.1).

The connection of (5.2) with the Peierls quantization can now be seen with the help of a useful algebraic rule (Weyl's identity), which states that if the commutator of two operators P, Q is a c-number, say $[P, Q] = c$, then $\exp(P)\exp(Q) = \exp(c)\exp(Q)\exp(P)$. Putting $\mathscr{C}(a) = \exp(i\kappa \cdot a)$ and $\mathscr{C}(b) = \exp(i\kappa \cdot b)$, then if the operator κ satisfies (4.3), expressed more generally as $\kappa \times \kappa = ieB/\hbar$, it follows that $\exp(i\kappa \cdot a)$, etc., satisfy

(5.2) identically, and can be used to represent $\mathscr{C}(\boldsymbol{a})$, etc. Thus, rather abstractly,

$$\psi(\boldsymbol{r}+\boldsymbol{a}) = \exp[\mathrm{i}(\boldsymbol{\kappa}\cdot\boldsymbol{a} + e\boldsymbol{A}(\boldsymbol{a})\cdot\boldsymbol{r})/\hbar]\psi(\boldsymbol{r}). \tag{5.3}$$

Of course, replacing $\boldsymbol{k}_B$ in a band energy by $\boldsymbol{\kappa}$ is an approximation valid only under special conditions and needing further justification (see section 8).

The periodic boundary condition (4.2) cannot be applied to magnetic states because there is a necessary phase factor $\exp[\mathrm{i}e\boldsymbol{A}(\boldsymbol{L})\cdot\boldsymbol{r}/\hbar]$. But it is reasonable to insist that the same state ψ_β be recovered after q translations in a transverse direction $\boldsymbol{a}$ (see section 7 for determination of q):

$$[\mathscr{C}(\boldsymbol{a})]^q = \mathscr{C}(q\boldsymbol{a}) = 1. \tag{5.4}$$

Taking the loop of translations $q\boldsymbol{a}, \boldsymbol{b}, -q\boldsymbol{a}, -\boldsymbol{b}$ (assuming $\boldsymbol{b}$ also transverse) requires that $\exp(\mathrm{i}q\Phi_c/\hbar) = 1$, that is to say

$$Bqab = q\Phi_c = ph/e \qquad p = \text{integer}. \tag{5.5}$$

The periodic condition (5.4) thus requires that the cell flux Φ_c should be a rational fraction p/q of the flux quantum h/e. Now $h/e = 4.136 \times 10^{-15}$ T m^2 so that taking a cell area $ab \sim 10^{-20}$ m^2 and a largish field of $B \leqslant 10$ T, requires $p/q \sim 10^{-4}$.

The interesting question is immediately raised concerning incommensurate values of $e\Phi_c/h$, for which the states can never be repeated by cell translation and would therefore appear to be non-denumerate. The consequences for energy spectra are taken up in sections 7 and 8.

The periodic boundary condition (5.4) may be applied along one axis, but what of the other two? For an arbitrary orientation of the magnetic field, further difficulties of commensurability arise and do not appear to have been thoroughly examined. Most theory in fact relates only to $\boldsymbol{B}$ aligned with an axis (the z direction) with assumed orthorhombic structure, that is $\boldsymbol{a} \perp \boldsymbol{b} \perp \boldsymbol{c}$. Pippard [3] however has a thorough discussion of non-cubic crytals. These limitations in fact have been tacitly imposed in the preceding discussion, and will continue so. Thus the non-magnetic periodic conditions will be used for motion in the y and z directions along with a particular gauge choice, namely $\boldsymbol{A} = (0, Bx, 0)$.

The dimensions of the $\mathscr{C}$ matrices are more directly dealt with from the particular representation introduced in the following section.

6. The *k*-representation

The gauge transformation matrices $\mathscr{C}(\boldsymbol{a})$, $\mathscr{C}(\boldsymbol{b})$ and $\mathscr{C}(\boldsymbol{c})$ introduced in (5.1) and operationally defined by (5.2) have already been related to the Peierls quantization through the correspondence or isomorphism $\mathscr{C}(\boldsymbol{a}) \rightarrow \exp(\mathrm{i}\boldsymbol{\kappa}\cdot\boldsymbol{a})$, etc. But this abstraction leaves their dimensionality and space undefined, and although a differential representation of the commutator $[\kappa_x, \kappa_y] = \mathrm{i}eB/\hbar$ is easily constructed (see section 8), it is preferable to find matrices enabling the construction of the magnetic states.

The above form suggests that the unspecified β label should in fact be a wavevector $\boldsymbol{k}$ (not to be immediately identified with Bloch $\boldsymbol{k}_B$), $\mathscr{C}(\boldsymbol{a})$ being necessarily non-diagonal. The matrices are easily discovered, and may be written

$$(\boldsymbol{k}'|\mathscr{C}(\boldsymbol{a})|\boldsymbol{k}) = \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a})\delta[\boldsymbol{k}' - \boldsymbol{k} + e\boldsymbol{A}(\boldsymbol{a})/\hbar] \tag{6.1}$$

with similar expressions for $\mathfrak{C}(\boldsymbol{b})$ and $\mathfrak{C}(\boldsymbol{c})$. Simple matrix multiplication confirms the non-commutative rule (5.2), recognizing that $\boldsymbol{A}(\boldsymbol{a})\cdot\boldsymbol{b}-\boldsymbol{A}(\boldsymbol{b})\cdot\boldsymbol{a}=\boldsymbol{B}\cdot\boldsymbol{a}\times\boldsymbol{b}$.

Denoting the $\boldsymbol{k}$-labelled magnetic states by $\varphi(\boldsymbol{r};\boldsymbol{k})$ (omitting any other quantum labels), then for any basic lattice vector, the translation $\boldsymbol{r}\rightarrow\boldsymbol{r}+\boldsymbol{a}$ is represented explicitly by

$$\psi(\boldsymbol{r}+\boldsymbol{a}:\boldsymbol{k})=\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a})\exp[(\mathrm{i}e/\hbar)\boldsymbol{A}(\boldsymbol{a})\cdot\boldsymbol{r}]\psi(\boldsymbol{r};\boldsymbol{k}-e\boldsymbol{A}(\boldsymbol{a})/\hbar). \tag{6.2}$$

The expression (6.2) holds generally for any type of crystal, and for any orientation of $\boldsymbol{B}$, represented by any gauge of $\boldsymbol{A}$. But as earlier explained, it is simpler to suppose that $\boldsymbol{a}=(a,0,0)$, $\boldsymbol{b}=(0,b,0)$, $\boldsymbol{c}=(0,0,c)$ with $\boldsymbol{A}=(0,Bx,0)$. Setting out (6.2) for each direction, the translations become

$$\psi(x+a,y,z;k_{\mathrm{B}})=\exp(\mathrm{i}k_x a)\exp[(\mathrm{i}e/\hbar)Bay]\psi(x,y,z;k_x,k_y-eBa/\hbar,k_z) \tag{6.3a}$$

$$\psi(x,y+b;z;\boldsymbol{k})=\exp(\mathrm{i}k_y b)\psi(x,y,z;\boldsymbol{k}) \tag{6.3b}$$

$$\psi(x,y,z+c;\boldsymbol{k})=\exp(\mathrm{i}k_z c)\psi(x,y,z;\boldsymbol{k}). \tag{6.3c}$$

Evidently (6.3*b*) and (6.3*c*) resemble the non-magnetic Bloch relations (4.1), allowing us to use conventional y, z dependence such as plane-wave or tight-binding models, taking $k_z=(k_z)_{\mathrm{B}}$.

Regarding (6.3*a*), the shift $k_y\rightarrow k_y-\mathrm{e}Ba/\hbar$ required by the translation $x\rightarrow x+a$ resembles (3.4) namely $p_y\rightarrow p_y-\mathrm{e}Ba$, and suggests that the non-magnetic correspondence of the free particle p_y with the Bloch state $\hbar k_y$ holds also in the magnetic domain for $\hbar k_y$. This relation can be pursued by considering the translational behaviour (6.3*a*) in free-space motion, where of course the displacement a is arbitrary.

For the present limited application of (6.2), the field direction motion may be disregarded, and only the k_x, k_y dependence of $\psi(\boldsymbol{r};\boldsymbol{k})$ retained, writing $\psi(\boldsymbol{r};\boldsymbol{k})\equiv\psi(x,y;k_x,k_y)$. As has been explained, equation (3.7), a Landau free-particle magnetic state ψ_{L} is localized about $x=\hbar k_y/\mathrm{e}B$, so that there is positional degeneracy $N=\mathrm{e}\Phi/h$ where Φ is the magnetic flux over the quantizing area. *The localized Landau state is therefore only one of many choices, with the possibility of other spatially prescribed forms.* Now the translation $x\rightarrow x+a$ shifts p_y to p_y-eBa, formally described in terms of ψ_{L} by

$$\psi_{\mathrm{L}}(x+a,y;k_y)=\exp[(\mathrm{i}eBa/\hbar)y]\psi_{\mathrm{L}}(x,y;k_y-eBa/\hbar). \tag{6.4}$$

This expression differs from (6.3*a*) by the absence of k_x in ψ_{L} and the propagating phase factor $\exp(\mathrm{i}k_x a)$. With one provision (see section 7), the degeneracy now allows the construction of alternative free-particle states,

$$\psi(x,y;k_x,k_y)=\sum_r\exp(\mathrm{i}k_x ra)\psi_{\mathrm{L}}\left(x,y;k_y+\frac{eBra}{\hbar}\right) \tag{6.5}$$

where ra must lie in the quantizing length L_x and the ψ-notation has anticipated the translational property (6.3*a*). Such a combination of phased Landau states has the potential to describe a transverse current; but that requires an energy coupling, provided by the lattice potential (section 8). These considerations suggest that $\boldsymbol{k}_{\mathrm{B}}$ and $\boldsymbol{k}$ may be safely equated.

7. Commensurability

Elementary statistical mechanics supposes that all spectral energy densities are the consequence of denumerable quantum levels. But ergodic or aperiodic quantum systems studied at a computational level can show remarkable and unexpected structures of a chaotic or fractal character [1, 9]. The quantum magnetic motion dealt with here can provide a tractable instance of such an aperiodic action and has received some attention. It is essentially a mathematical topic, outside the intentions of this article; no more than its background is sketched here.

The periodic boundary conditions discussed in section 5 place a constraint on the k_y-values. It is necessary that the displaced value $k_y - eBa/\hbar$ should be a permitted quantized value, that is to say

$$eBa/\hbar = \lambda 2\pi/L_y \tag{7.1}$$

where λ is some integer. This is additional to the flux requirement (5.5), expressed here as

$$\Phi_c = Bab = (p/q)h/e. \tag{7.2}$$

Evidently (7.1) and (7.2) are compatible only if

$$q = (p/\lambda)L_y/b \tag{7.3}$$

and this fixes the quantizing length $L_x = qa$. For example, a square section $L_x = L_y$ of a cubic lattice, $b = a$, requires $\lambda = p$.

The number of degenerate Landau states was shown, equation (3.9), to be equal to the number of flux quanta N. From (7.3), it is seen that

$$N = \frac{e}{h} Bab \frac{L_x}{a} \frac{L_y}{b} = \lambda \frac{L_x}{a}. \tag{7.4}$$

It follows that a commensurate system, where p, q, λ and N are all integral, is periodic in its spatial behaviour.

Under these commensurate conditions, the quantized values of k_x, k_y are enumerated as

$$\begin{aligned} k_x &= (2\pi/L_x)(1, 2, 3, \ldots, q) \\ k_y &= (2\pi/L_y)(1, 2, 3, \ldots, N/q). \end{aligned} \tag{7.5}$$

The integral values of p, q, λ and N needed to satisfy (7.1)–(7.4) are unlikely to be found in a material sample in an arbitrary field. Mathematical periodicity is thus not guaranteed and it would seem an open question whether measurable dynamic effects arise. To deal with the problem requires numerical investigation of an actual system, and this is the subject of the succeeding section.

8. Magnetic energy broadening

The k-state translation (6.2) dictated by the gauge transformation allows a formal representation of $\psi(r; k)$, namely

$$\psi(r; k) = \exp(ik \cdot r)U(r; k - (e/\hbar)A(r)) \tag{8.1}$$

where $U(\boldsymbol{r}+\boldsymbol{a};\boldsymbol{k}) = U(\boldsymbol{r};\boldsymbol{k})$, that is to say, $U(\boldsymbol{r};\boldsymbol{k})$ has the periodicity of the lattice, and could be written as a Fourier series. It is easily confirmed that if the magnetic free-particle state (6.5) is presented in this way, there is no periodic dependence. An alternative to Fourier representation is an expansion based on Bloch states of the lattice, and it has been shown [10] that this is equivalent to the Luttinger–Kohn theory [6] mentioned in section 4.

At any rate, to study the magnetic energy levels, some model conforming to (8.1) is needed, and the choice depends upon the crystal (metal, semiconductor), and physical features of interest (Fermi surface, band structure).

With the possible exception of the quantum Hall effect (section 9), semiconductor magneto-optics has not drawn much upon gauge theory, although, as mentioned, the quantum states conform entirely to its requirements. For metals, the early interest was in steady and oscillatory diamagnetism [5], with developments in magneto-resistance, largely the work of Pippard [3]. In metals, and semi-metals such as Bi, the consequences of electron drift, mentioned in section 6, seemed particularly interesting.

Before examining models of the form (8.1) for their energy eigenvalues, some features can be anticipated. Since $\boldsymbol{k}$ and $\boldsymbol{k} - e\boldsymbol{A}(a)/\hbar$ refer to degenerate states, the relation $E(\boldsymbol{k} - e\boldsymbol{A}(a)/\hbar) = E(\boldsymbol{k})$, implies a periodic dependence of $E(\boldsymbol{k})$ upon $\boldsymbol{k}$. In the present gauge (2.4), this would provide the period $eBa/\hbar$ for k_y, and since the gauge $\boldsymbol{A}' = (-By, 0, 0)$ is equally acceptable, k_x must have the identical period.

A simple application of (6.5) confirms this energy periodicity in k_x, k_y. Since the states already have the correct translational symmetry corresponding to an isotropic lattice period a, the energy due to a weak lattice potential can be immediately calculated from first-order perturbation theory. Assume then a weak lattice potential of the separable model form,

$$V(x, y) = V[\cos(2\pi x/a) + \cos(2\pi y/a)] \tag{8.2}$$

and consider

$$E(k_x, k_y) = \int \mathrm{d}x\, \mathrm{d}y\, |\psi(x, y; k_x, k_y)|^2 V(x, y). \tag{8.3}$$

Recollecting that the Landau states are centred at $x = \hbar k_y/eB$ then the contribution to (8.3) from $\cos(2\pi x/a)$ is given by

$$V \cos\left(\frac{2\pi\hbar k_y}{eBa}\right) \int_{-\infty}^{\infty} \mathrm{d}x\, |\psi_L(x, y; 0)|^2 \cos\left(\frac{2\pi x}{a}\right) \tag{8.4}$$

showing the expected periodic dependence upon k_y, with the period $eBa/\hbar$. For the second term in (8.2) the y-integration of $\cos(2\pi y/a)$ must phase-match with $\exp(\mathrm{i}k_y y)$, $\exp[\mathrm{i}(k_y \pm 2\pi/a)y]$, and therefore connects the Landau states with centres separated by $\hbar(2\pi/a)/eB$ and with the relative phase factor (from (6.5)) of $\exp[\mathrm{i}k_x\hbar(2\pi/a)/eB]$ to give the contribution

$$V \cos\left(\frac{2\pi\hbar k_x}{eBa}\right) \int_{-\infty}^{\infty} \mathrm{d}x\, \psi_L\left(x - \frac{2\pi\hbar}{eBa}\right) \psi_L(x). \tag{8.5}$$

The integrals in (8.4) and (8.5) are identical (a Fourier transform property of Hermite polynominals), and denoting the value by F, then

$$E(k_x, k_y) = FV[\cos(\hbar k_x/eBa) + \cos(\hbar k_y/eBa)]. \tag{8.6}$$

In this expression the values of k_x and k_y are given by (7.5) (assuming the commensurate relations (7.1)–(7.4)), and are quasi-continuous. From the limits in (7.5), the full cycle of values is permitted. Thus each discrete Landau level is broadened, with a width set dimensionally by the lattice potential, but reduced by the overlap integral (8.5). This lattice broadening is additional to collision broadening described by Dingle [11].

One of the benefits of the free-space magnetic states (6.5) is that, although not yet current-carrying states, the gauge translation symmetry organizes their degeneracy into the current-carrying form. It was shown [8] that the mean velocities $\langle v_x \rangle$, $\langle v_y \rangle$ are quite generally given as

$$\langle v_x \rangle = \hbar^{-1} (\partial E/\partial k_x) \qquad \langle v_y \rangle = \hbar^{-1} \partial E/\partial k_y. \tag{8.7}$$

Direct calculation of $\langle v_y \rangle = \langle p_y - eBx \rangle/m$ would in fact require at least first-order perturbed gauged functions, but (8.7) gets there more quickly.

Formula (8.5) shows that the current is proportional to the overlap of Landau states separated by $2\pi\hbar/eBa$. The integral F in (8.6) describes a quantum tunnelling and increases with orbital radius $(n\hbar/2eB)^{1/2}$. The latter approaches the semi-separation at an orbital energy $n\hbar\omega_c = (\hbar^2/2m)(\pi/a)^2$, that is to say, at the energy needed for Bragg reflection. Here quantum tunnelling between orbits becomes easy and it is this aspect, from the analogy with Zener tunnelling, that provides the misleading name 'magnetic breakdown'. The effect assumes a special importance in connection with magnetoresistance, an area of solid-state physics much developed by Pippard.

The weak potential model serves to estimate the k_x, k_y level broadening but is inadequate for further development. Atomic tight-binding [12] is a complementary model that often produces useful and credible results even though it is somewhat far-fetched. It resembles molecular orbital theory in that the wavefunction is composed of local atomic states regarded as approximately orthogonal. Used to model Bloch functions, each lattice cell is phased according to (4.1), but for magnetic states based on (8.1), U effectively appears as an envelope function, defined only at lattice points.

The model supposes a cubic lattice, each cell containing one non-degenerate atomic state, written as w_l, where $(l_1, l_2, l_3)a$ locates the atomic centre. Most metals are close-packed structures but hexagonal symmetry complicates the commensurability restrictions (7.1)–(7.4), and obscures more elementary features.

For each state w_l the vector potential is gauged to its local cell value providing the overall phase factor

$$\exp(i\boldsymbol{k} \cdot \boldsymbol{la}) \exp[\hbar^{-1} ie\boldsymbol{A}(\boldsymbol{la}) \cdot (\boldsymbol{r} - \boldsymbol{la})] \tag{8.8}$$

and modulated by an envelope function, written as

$$u(\boldsymbol{k} - e\boldsymbol{A}(\boldsymbol{la})\hbar). \tag{8.9}$$

Using the simpler notation of section 6, and omitting the k_z dependence, i.e. the sum over l_3, the transverse k_x, k_y state becomes, making use of $\alpha = eB/\hbar$,

$$\psi(x, y; k_x, k_y) = \sum_{l_1, l_2} \exp(ik_x l_1 a) u(k_x, k_y - \alpha l_1 a) \exp[i(k_y - \alpha l_1 a]$$
$$\times \exp(i\alpha l_1 a y) w_{l_1, l_2}. \tag{8.10}$$

The translation $x \to x + a$ equivalently replaces the site l_1 by $l_1 - 1$. Rewriting the index l_1 as $l_1 + 1$ everywhere in the sum effectively changes k_y into $k_y - \alpha a$ and prefaces

the sum with the factors $\exp(ik_x a)\exp(i\alpha a y)$, thus meeting the gauge transformation requirement (6.3*a*).

The problem then is to determine u regarded as a function of k_y, with a parametric dependence on k_x. In calculating $H\psi$ as in (3.6), the effect of the gauge factor in (8.8) is to replace $p_y - eBx$ by $p_y - eB(x - l_1 a)$, which, since w_{l_1,l_2} is localized about $x = l_1 a$, is approximated by p_y. The kinetic energy of the state (8.10) is thus taken as its unperturbed crystal value, E_0, though there are clearly small magnetic corrections. Tight binding supposes that the lattice potential connects cell state l_1, l_2 with nearest neighbours $l_1 \pm 1$, l_2 and $l_1, l_2 \pm 1$. The factor $\exp(i\alpha l_1 a y)$ is assumed not to impede this selection rule.

The magnitude of the matrix element coupling neighbouring sites is the atomic overlap integral (denoted by $E_1/2$), which provides the electronic band width. The amplitude $u(k_x, k_y - \alpha l_1 a)$ is then coupled to each neighbouring amplitude $u(k_x, k_y - a(l_1 \pm 1)a)$ with the phased element $\frac{1}{2}E_1 \exp(\pm ik_x a)$. The phasing comes from the form (8.10), which meets the gauging requirement and comes into effect in expressing the magnetic periodic boundary condition. Nearest neighbours $(l_2, l_2 \pm 1)$ in the y direction take the same amplitude $u(k_x, k_y - \alpha l_1 a)$ but now become coupled with a position-dependent magnetic phase, thus providing the important modulating factor

$$\cos[(k_y - \alpha l_1 a)a].$$

The resulting eigen-equation can be written

$$\exp(-ik_x a)u_{l+1} + \exp(ik_x a)u_{l-1} + 2\cos(l\alpha a^2 - k_y a)u_l = \varepsilon u_l \qquad (8.11)$$

where for simplicity u_l stands for $u(k_x, k_y - \alpha l_1 a)$, and ε is a dimensionless eigenvalue, namely the energy difference $E - E_0$ in units of the bandwidth energy $E_1/2$. The equation, originally introduced in this magnetic context [8], in fact has a wider physical significance and has provided a useful instance of phase holonomy [1, 22].

Recollecting the definition of α,

$$\alpha a^2 = 2\pi(e/h)\Phi_c \qquad (8.12)$$

the discussion on the commensurability condition $e\Phi/h = p/q$ (equation (7.2)) is illustrated by the form of (8.11). The cyclic boundary applies to u_l in that u_{l-q} satisfies the same equation as u_l. In dealing with (8.11) it is common to take $k_x = 0$, but this merely amounts to a redefinition of u_l to include the phase factor $\exp(ik_x la)$. With the choice, u_{l+q} must be taken as $\exp(ik_x qa)u_l$. Either way, k_x enters parametrically into ε, and from the earlier discussion, (8.6) plays a broadening role.

When $e\Phi_c/h$ is not a simple rational fraction p/q, the cyclic boundary condition cannot be applied, quantum phase is not repeated, and the system is described as non-holonomic. It is here perhaps that (8.11) becomes of greatest mathematical interest. The computations of Wilkenson [13] show the strange 'butterfly' spectral patterns that have been computed. Stinchcombe and Bell [14] have discussed the categorization of the various spectral bands, allowing for a scaling factor λ, which physically corresponds to a lattice anisotropy. Lovesay [25] has also treated solutions of (8.11).

There is yet another view of (8.11). Formally $u(k_x, k_y \pm \alpha)$ can be written as

$$u(k_x, k_y \pm \alpha a) = \exp(\pm \alpha a\, \partial/\partial k_y)u(k_x, k_y) \qquad (8.13)$$

which enables (8.10) to be presented in the operator form,

$$\tfrac{1}{2}E_1\{\cos[a(k_x + i\alpha\, \partial/\partial k_y)] + \cos(ak_y)\}\, u(k_x, k_y) = (E - E_0)u(k_x, k_y). \qquad (8.14)$$

Effectively, in the non-magnetic band energy k_x has been replaced by the operator κ_x,

$$\kappa_x = k_x + i\alpha\,\partial/\partial k_y. \tag{8.15}$$

Thus for the simple cubic band, Peierls' intuitive notion is confirmed, with the κ-representation fully justified and explained. In the Onsager method for finding its eigenvalues, formula (4.4), the value of the phase constant γ is to be found from a more detailed examination of the turning points WKB theory. Wilkenson has discussed this in connection with the solution of (8.11). Pippard [3] has also discussed its physical significance.

9. Quantum Hall effect

Some explanation is needed for this section, which is somewhat peripheral to the main theme of the review. But existing Hall effect theories have drawn upon gauge notions, typified by that of Thouless *et al* [15], which work with extended wavefunctions satisfying the translational conditions (6.2). Other theories [23] have emphasized magnetic flux conservation, viewed as a gauge property. Current-carrying states, already discussed in the gauge context, are used here to provide a view of the quantum Hall effect.

Metals and semiconductors are characterized by their resistivity and mobility, and transport theory is therefore a major study in solid-state physics. The addition of a magnetic field can assist to measure parameters such as effective band mass. Pippard [3] has dealt comprehensively with this topic. The Hall effect in semiconductors is particularly useful in distinguishing the sign and density of charge carriers, and the elements of the theory (though sometimes complicated by multiband effects) could hardly be simpler. Regarded as a conductor, a current in a perpendicular magnetic field, under open-circuit conditions, can produce a transverse voltage proportional to current and field. Using (2.2), then under stationary conditions, $\dot{x} = 0$, the Lorenz force must be balanced by a reactive electric field namely, $E_x = B\dot{y}$. Denoting the carrier density by ν, then the current density J_y is simply $ve\dot{y}$, giving the Hall field E_x *as* BJ/ve, that is, the Hall constant $R = 1/ve$. There is particular interest in very thin samples, where the field direction $L_z \ll L_x, L_y$. Taking the surface current as $I = L_x J_y$, and supposing ν to denote now the surface carrier density with the Hall voltage $V_H = \mathbf{E}_x L_x$, then the Hall conductance (actually a non-diagonal element of the conductance tensor), becomes

$$I/V_H = e\nu/B. \tag{9.1}$$

In the quantized version, including the reactive electric field, the two-dimensional magnetic free-carrier Hamiltonian (3.2), (3.6), becomes

$$H_E = (1/2m)[p_x^2 + (p_y - eBx)^2] + eE_x x \tag{9.2}$$

whence

$$[v_x, H_E] = i\hbar e(Bv_y - E_x). \tag{9.3}$$

For every eigenstate of H_E, the expectation value of the commutator is identically zero so that $\langle v_y \rangle$ has the fixed value

$$\langle v_y \rangle = E_x/B. \tag{9.4}$$

Regardless of level density, the current is $\nu e v_y$ so that magnetic quantization would appear to have no effect.

The startling result of von Klitzing [16] showed that, at low temperatures, in thin samples of low mobility (disordered structures), and sufficiently large L_x, instead of the monotonic field dependence of (9.1) there could occur a discontinuous, step behaviour, very accurately expressed as

$$I/V_H = (e^2/h) \text{ integer} \tag{9.5}$$

with the discontinuities occurring when the Fermi energy ζ is a half-integral multiple of $\hbar eB/m \equiv \hbar\omega_c$. The physics of this 'quantum Hall effect' is further complicated by later discoveries that simple fractional values of e^2/h can also occur.

Theories of (9.5) invoke flux quantization, i.e. the notion (3.9) that if N is to be integral, then the flux Φ can change only by the minimum fixed amount h/e. As explained, this is true in the sense that to accommodate in additional electron, $N = e\Phi/h$, must change by unity. Thus Laughlin [17] argues that eV_H is the energy needed to transfer one mobile carrier across the sample, i.e. the translation $x \to x + L_x$. But this is also a gauge change $A_y \to A_y + eBL_x$, which, since $\Phi = \int \boldsymbol{A} \cdot d\boldsymbol{r}$, is equivalent to a flux change. Taking this as h/e their ratio gives immediately $I = (e^2/h)V_H$ per transferred electron. Localized electrons can provide a source/sink, and it is concluded that the explanation of the quantum Hall effect lies in gauge invariance.

The difficulty is that flux is independent of gauge and that for electron transfer (as distinct from adding/removing an electron) its quantization, like the other commensurability relations of section 7, is only a useful idealization.

The Hamiltonian H_E remains a stumbling block since it provides the same velocity $\langle v_y \rangle = E_x/B$ for every electron. This stubborn feature can be modified if a localizing potential is added which serves as a source or sink of electrons to provide the observed flat behaviour of I/V_H. Other Hamiltonians have been used to calculate the conductivity tensor [15]. One can argue however that Laughlin's transfer energy is better described as the difference in chemical potential (Fermi energy) across the sample due to the imposed current I. That is to say

$$\zeta(\nu, B, I) = \zeta_0(\nu, B) + eV_H(I). \tag{9.6}$$

The Fermi energy ζ is now calculated in the conventional way as the population limit (at zero temperature) of levels defined not by H_E but by a Hamiltonian describing an *imposed coherent current*. The necessary Lagrangian is most directly obtained in the present Landau gauge from the replacement $\dot{y} \to \dot{y} + v$, where as before the surface current I is related to v through $I = e\nu L_x v$. From its definition (3.1) the resulting Hamiltonian H_v becomes, in contrast to (9.2),

$$H_v = (1/2m)[p_x^2 + (p_y - eBx)^2] - vp_y. \tag{9.7}$$

The identity $\langle [y, H_v] \rangle = 0$ gives $\langle v_y \rangle = v$ for every eigenstate of (9.7). Since p_y remains a constant of the motion the eigenvalues of (9.7) are

$$(n + \tfrac{1}{2})\hbar\omega_c - v\hbar k_y. \tag{9.8}$$

Thus, for the current Hamiltonian H_v, the k_y degeneracy is removed. By populating the current states $n = 0$, $k_y = (-2\pi L_y)(1, 2, 3, \ldots)$, the Fermi energy ζ can now be varied continuously between $\frac{1}{2}\hbar\omega_c$ and $\frac{3}{2}\hbar\omega_c$, though to attain the $\frac{3}{2}\hbar\omega_c$ value, the N value (3.8) requires a minimum strip width L_x,

$$L_x \geqslant h/mv. \tag{9.9}$$

Since the oscillator centres are at $\hbar k_y/eB$ then for positive carriers, $e > 0$, $x = -L_x$ is at

a positive potential relative to $x = 0$. This agrees with the sense defined by the classical model.

Assuming (9.9), and spin-polarized states (but neglecting Zeeman level splitting), then equating the number of available states, namely $(\zeta - \frac{1}{2}\hbar\omega_c)L_y/hv$, to the number of surface carriers $\nu L_x L_y$, and using $I = e\nu v L_x$, it follows that for $\frac{1}{2}\hbar\omega_c \leqslant \zeta \leqslant \frac{3}{2}\hbar\omega_c$,

$$\zeta - \tfrac{1}{2}\hbar\omega_c = (h/e)I. \tag{9.10}$$

Populating beyond $\frac{3}{2}\hbar\omega_c$ brings in the $n = 1$ levels, providing a further number of states, $(\zeta - \frac{3}{2}\hbar\omega_c)L_y/hv$, which added to (9.9) gives for $\frac{3}{2}\hbar\omega_c \leqslant \zeta \leqslant \frac{5}{2}\hbar\omega_c$

$$\zeta - \hbar\omega_c = (h/2e)I. \tag{9.11}$$

Quite generally for $(n + \frac{1}{2})\hbar\omega_c < \zeta < (n + \frac{3}{2})\hbar\omega_c$, the Fermi energy is obtained as

$$\zeta - \tfrac{1}{2}(n + 1)\hbar\omega_c = [h/e(n + 1)]I. \tag{9.12}$$

In accordance with (9.6), the I dependence of ζ is to be attributed to the induced Hall voltage V_H, establishing that I/V_H takes the quantum values (9.5), namely

$$I/V_H = (e^2/h)(n + 1) \tag{9.13}$$

where $n = 0, 1, 2, \ldots$ is now identified as the Landau quantum number. The Fermi energy ζ is continuous, but $\partial\zeta/\partial I$ changes discontinuously at $\zeta = (n + \frac{1}{2})\hbar\omega_c$.

Carrier localization, regarded as necesary for localization, does not directly appear on this model. However, the dimensional condition (9.9) evidently excludes the zero-current configuration $v = 0$ for which the k_y states are all degenerate. To avoid unphysical discontinuities in ζ_0 it would seem necessary to assume that a realistic two-dimensional Hamiltonian should permit non-current-carrying states with energies in the mobility gap as Laughlin supposes.

The gauging translation $x \rightarrow x + a$ accompanied by the replacement $p_y \rightarrow p_y - eBa$ does not leave the current Hamiltonian H_o invariant but shifts it by $eBav$. This is expected in view of the potential difference transverse to the current. The fundamental gauging relation (5.2) appears to remain intact provided that the energy shift $eBav$ corresponds to a permitted energy. With the periodic lattice potential present, taking a as a cell translation, the commensurability conditions (7.1) and (7.3) may need re-examining, and may throw light on the difficult problem of the fractional quantum Hall effect.

10. Other gauge considerations

This article may be concluded with brief comments on the use, in other solid-state contexts, of gauge invariance. It refers to the notion, introduced in section 2, that the quantum relation $\boldsymbol{p} = m\boldsymbol{v} + e\boldsymbol{A}$ remains unaltered under the gauge change $\boldsymbol{A} \rightarrow \boldsymbol{A} + \nabla\chi$, and transformation $\exp(ie\chi/\hbar)$. One of the criticisms of the BCS theory of superconductivity [24, 26] was the extent of its disregard of the principle.

In the early theories of superconductivity it was proposed by Bloch that in the ground state, the statistical expectation value of $\boldsymbol{p}$ should vanish, that is

$$\langle \boldsymbol{p}_s \rangle = 0 \tag{10.1}$$

giving a supercurrent velocity $\boldsymbol{v}_s$,

$$\boldsymbol{v}_s = -(e/m)\boldsymbol{A}. \tag{10.2}$$

which in terms of the supercurrent density $J_s = \nu_s e v_s$ provides the Meissner relation

$$J_s = -(\nu_s e^2/m)A. \tag{10.3}$$

The quantum mechanical relation between A and current density J for a single electron is provided as

$$J = (e\hbar/m)\,\mathrm{Im}(\psi^*\nabla\psi) - (e^2/m)\,|\psi|^2 A. \tag{10.4}$$

Under the general gauge change, $A \to A + \nabla\chi$, the current density $J(r)$ remains invariant, provided that in (10.4),

$$\psi \to \psi \exp(ie\chi/\hbar). \tag{10.5}$$

This gauging freedom is incompatible with (10.1)–(10.3), which require $\nabla\psi = 0$ with $\nu_s = |\psi|^2, J_s = J$. It was in fact shown, (Buckingham [27]), that in (10.4) a sum rule, itself derived from gauge considerations, ensures that the final term is cancelled identically from the $\nabla\psi$ terms, leaving only a normal diamagnetic contribution to J proportional to $\nabla^2 A$.

More realistically, to fit his penetration depth data, Pippard [19] found it necessary to replace (10.3) with a non-local relation, later confirmed by the microscopic BCS theory, which was itself shown to be consistent with the Ginsburg–Landau order theory (Tinkham [18]), at least near the critical temperature.

The phase of ψ, the basis of the interferrometric flux properties of Josephson junctions, is directly displayed by writing the complex order parameter as,

$$\psi_S = |\psi_S| \exp(i\varphi) \tag{10.6}$$

giving the supercurrent velocity from (10.4) with $\psi \to \psi_S$, as

$$v = m^{-1}(\hbar\nabla\varphi - eA). \tag{10.7}$$

The phase $\varphi(xyz)$ need not be single-valued so that $\nabla\varphi$ is (in general) irrotational, that is, $\nabla \times \nabla\varphi \neq 0$; for example, $\psi = x + iy$ for which $\nabla\varphi = (-y, x, 0)(x^2 + y^2)^{-1}$. For a loop C about the origin the circuit integral of $\nabla\varphi$ is 2π and, quite generally, the circulation phase change is a multiple of 2π,

$$\int_C \nabla\varphi \cdot \mathrm{d}r = 2\pi(\text{integer}). \tag{10.8}$$

The gauge transformation $\varphi \to \varphi + e\chi/\hbar$, $A \to A + \nabla\chi$ leaves (10.6) and (10.7) unchanged, and fluxoid (so-called) quantization then follows from (10.6) by consideration of $\Phi = \int_c A \cdot \mathrm{d}r$.

As a final thought it has been suggested (Zak [21]) that the Berry geometric phase [20] is connected with gauge rephasing. It would be interesting to confirm this and establish the precise relation.

Acknowledgments

The author acknowledges helpful comments from colleagues and referees.

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