GROUND STATES IN A PERIODIC FIELD. MAGNETIC BLOCH FUNCTIONS AND VECTOR BUNDLES

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I. We consider a two-dimensional eigenvalue problem for the nonrelativistic Pauli Hamiltonian which describes an electron with spin 1/2 in a periodic magnetic field directed along the z axis and, possibly, an electric field in the x, y plane

$$H\psi = \epsilon\psi, \quad \psi = (\psi_1, \psi_2),$$

$$H = \frac{1}{2m}\left(-i\hbar\partial_1 - \frac{e}{c}A_1\right)^2 + \frac{1}{2m}\left(-i\hbar\partial_2 - \frac{e}{c}A_2\right)^2 - \frac{e\hbar}{mc}\sigma_3 B(x,y) + v(x,y), \tag{1}$$

$$\partial_1 = \frac{\partial}{\partial x}, \quad \partial_2 = \frac{\partial}{\partial y}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

where B and u are periodic in (x, y) and

$$\begin{gathered} B(x+T_1, y) = B(x, y+T_2) = B(x,y), \\ v(x+T_1, y) = v(x, y+T_2) = v(x,y), \\ B = \partial_1 A_2 - \partial_2 A_1, \quad \partial_1 A_1 + \partial_2 A_2 = 0, \quad \sigma_3 H = H\sigma_3. \end{gathered} \tag{2}$$

We further set $\hbar = m = c = 1$.

On functions with fixed spin $\sigma_2\psi = \kappa\psi$, the operator $H = H_\kappa$ becomes scalar ($\kappa = \pm 1$).

The basic topological characteristic is the magnetic flux

$$\frac{e}{2\pi}\Phi = \frac{e}{2\pi}\int_0^{T_1}\int_0^{T_2} B(x,y)\,dx\,dy; \tag{3}$$

let $\xi = \exp(ie\Phi)$. If $e\Phi/2\pi$ is an integer, this is equivalent to H being defined in a bundle over a compact manifold—the two-dimensional torus T^2. The spectral problem (1) is considered in the Hilbert space $\mathcal{L}_2(\mathbb{R}^2)$ of square-integrable functions on the entire plane $\mathbb{R}^2$. If the magnetic flux is irrational, then the operator H on $\mathcal{L}_2(\mathbb{R}^2)$ does not cover an operator on any compact manifold.

Remark. Problems of this type arise in constructing the quantum theory of an electron in a lattice and a magnetic field (i.e. in a monocrystalline solid situated in a magnetic field which is constant outside the body); here the area of an elementary cell is very small ($T_1T_2 \sim 10^{-16}$ cm^2). The magnetic field must be too strong to accumulate an integral quantum of flux; therefore in this case the flux is fractional and small. Another situation is the case of superconductors of second kind in a magnetic field, where H is the linearized Ginzburg–Landau operator. Here we are dealing with a genuine two-dimensional problem (see [9]); the order of magnitude of the periods is such that the area of an elementary cell is 10^6–10^4 times larger; in this

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case the flux must be an integer and is usually a single-quantum flux with charge $e = 2e_0$, where e_0 is the charge of the electron due to the so-called superconducting pairing in the microscopic Bardeen–Cooper–Schriffer and Bogoljubov theory; if the state describes an electron with charge e_0 we obtain the flux $e_0\Phi/2\pi = 1/2$ (this was indicated to the authors by I. E. Dzjalošinskiĭ and A. I. Larkin).

The so-called magnetic translations which commute with the Hamiltonian comprise the basic algebraic object in problem (1) (see [4]–[6]). Let $\Delta_1 f(x,y) = f(x+T_1,y) - f(x,y)$ and $\Delta_2 f(x,y) = f(x,y+T_2) - f(x,y)$. We have

$$\Delta_1 A_i = \partial_i f_1(x,y), \quad \Delta_2 A_i = \partial_i f_2(x,y).$$

We define the magnetic translations

$$\begin{aligned} T_1^*\psi(x,y) &= \psi(x+T_1,y)\exp[-ief_1(x,y)], \\ T_2^*\psi(x,y) &= \psi(x,y+T_2)\exp[-ief_2(x,y)]. \end{aligned} \tag{4}$$

It is easy to verify that the group (4) commutes with the Hamiltonian H; the commutator of the basic translations has the form

$$T_1^*T_2^* = T_2^*T_1^*\exp\{ie\Phi\}, \quad \exp\{ie\Phi\} = \xi. \tag{5}$$

There arises the group with basis T_1^*, T_2^*, ξ and relations

$$T_1^*T_2^* = T_2^*T_1^*\xi, \quad \xi T_1^* = T_1^*\xi, \quad \xi T_2^* = T_2^*\xi. \tag{6}$$

If $e\Phi/2\pi = N/M$, where $M < \infty$, then $\xi^M = 1$. If $\xi = 1$ or $e\Phi/2\pi = N$ there arise the magnetic Bloch eigenfunctions and quasimomenta (p_1, p_2):

$$\begin{aligned} T_1^*\psi &= \exp(ip_1T_1)\psi, \quad |\exp(ip_1T_1)| = 1, \\ T_2^*\psi &= \exp(ip_2T_2)\psi, \quad |\exp(ip_2T_2)| = 1. \end{aligned} \tag{7}$$

For rational fluxes $e\Phi/2\pi = N/M$ the irreducible representations of the group of magnetic translations (6) with condition (5) have dimension M.

For irrational fluxes the irreducible representations with condition (5) are infinite-dimensional; the decomposition of a unitary representation into irreducible representations is not unique even in the simplest examples. This complicates the question and prevents indicating the quantum numbers which define the state of the electron in the magnetic field.

II. We now assume that $v(x,y) = 0$; we make use of a result of [1] on the ground states of an electron in a localized magnetic field on the plane $\mathbb{R}^2$ (in the theory of instantons an analogous fact was known earlier). Let H_κ be the operator H on the subspace $\sigma_3\psi = \kappa\psi$, and let A be the operator of first order $A = -i(\partial_1 - eA_2) - (\partial_2 + eA_1)$. We have

$$\begin{aligned} H_1 &= AA^*, \quad \kappa = 1, \\ H_{-1} &= A^*A, \quad \kappa = -1. \end{aligned} \tag{8}$$

Since $\langle H_\kappa\psi, \psi\rangle \geq 0$, it follows that $\epsilon \geq 0$. We rigorously prove this for the ground state $\epsilon = 0$ by finding nontrivial square-integrable solutions of the equation $H_\kappa\psi = 0$. Since $H_1 = AA^*$, the condition $\langle AA^*\psi, \psi\rangle = 0$ implies that $A^*\psi = 0$ (similarly, for $\kappa = -1$ we obtain $A\psi = 0$). The ground states are all such that $\kappa e\Phi > 0$. If $e\Phi/2\pi > 0$, then $\kappa = 1$.

We set $A_1 = -\partial_2\phi$; then $A_2 = \partial_1\phi$ because of condition (2): $\partial_1 A_1 + \partial_2 A_2 = 0$. For ϕ we have $\Delta\phi = \partial_1^2\phi + \partial_2^2 = B(x,y)$. By the substitution $\psi = \exp(-e\phi)f(x,y)$

we demonstrate the validity of the following important fact: if $H_\kappa\psi = 0$, $e\Phi/2\pi > 0$, and ψ is square-integrable, then $\kappa = 1$, $A^*\psi = 0$, and $f(x, y) = f(x + iy)$ is an analytic (entire) function. In a localized field on the plane this together with the choice of if in the form

$$\phi = \frac{1}{\pi} \iint \ln|r - r'|\, B(r')\, dx'\, dy', \quad r = (x, y), \quad r' = (x', y'),$$

implies that $f(x + iy)$ is a polynomial of degree $k \le [e\Phi/2\pi] - 1$. For an integral flux the required states also give polynomials of degrees $k = 0, 1, \ldots, N - 1$, but the last of these is not square-integrable (it is probably for this reason that integral fluxes are excluded in [1]). From this we draw the conclusion that the ground state is the endpoint of the continuous spectrum. In the fractional case $e\Phi/2\pi = N + \delta$, $0 < \delta < 1$, there is a nontrivial gap between the ground state and the remainder of the spectrum (this can probably be proved rigorously).

III. In a periodic magnetic field ($v(x, y) = 0$) the situation is topologically more complicated. For an integral (or rational) flux it is found possible to compute in terms of elliptic functions a magnetic Bloch basis in the Hilbert space of ground states. If $e\Phi/2\pi > 0$, then $\kappa = 1$; we seek a solution in the form

$$\begin{gathered} \psi = \exp(-e\phi)/f(x + iy), \\ \frac{\partial f}{\partial x} + i\frac{\partial f}{\partial y} = 0, \quad \partial_1^2\phi + \partial_2^2\phi = B(x, y). \end{gathered} \tag{9}$$

The functions (9) are always solutions of the equation $H_1\psi = 0$ (this is a local assertion). Suppose for simplicity that the lattice is rectangular with periods T_1 and T_2 in x and y and that the flux is integral: $e\Phi/2\pi = N$. The points of the lattice have the form $z_{m,n} = mT_1 + inT_2$. The so-called σ function is given by the product ([8], §13.12, formula (11))

$$\sigma(z) = z \prod_{m^2+n^2\ne 0} \left(1 - \frac{z}{z_{m,n}}\right) \exp\left\{\frac{z}{z_{m,n}} + \frac{1}{2}\frac{z^2}{z_{m,n}^2}\right\}.$$

For the translations we have

$$\begin{aligned} \sigma(z + T_1) &= -\sigma(z)\exp\{2\eta_1(z + T_1/2)\}, \quad \eta_1 = \zeta(T_1/2), \\ \sigma(z + iT_2) &= -\sigma(z)\exp\{2\eta_2(z + iT_2/2)\}, \quad \eta_2 = \zeta(iT_2/2), \quad \zeta(z) = \sigma'/\sigma. \end{aligned} \tag{10}$$

We choose ϕ in the form

$$\phi(x, y) = \frac{1}{2\pi} \iint_K \ln|\sigma(z - z')|\, B(x', y')\, dx'\, dy', \quad z = x + iy, \quad z' = x' + iy', \tag{11}$$

where Kxs is the elementary cell of area $K = T_1T_2$. We make the following important "Ansatz": we seek the states in the form

$$\psi_A = \lambda \exp(-e\phi) \prod_{j=1}^{N} \sigma(z - a_j) \exp(az), \tag{12}$$

where the conditions on the set of constants $A = (a, a_1, \ldots, a_N)$ will be indicated later (see (14)); λ is an arbitrary constant. On the basis of (4), according to (10) and (11), the magnetic translations have the form

$$
\begin{gathered}
T_1^*\colon \psi(x,y) \to \psi(x+T_1,y)\exp\{-ie\eta_1\Phi y/\pi\},\\
T_2^*\colon \psi(x,y) \to \psi(x,y+T_2)\exp\{-ie\eta_2\Phi y/\pi\},\\
T_2^*T_1^*\exp\{ie\eta_2 T_1\Phi/\pi\} = T_1^*T_2^*\exp\{ie\eta_1 T_2\Phi/\pi\}, \quad \eta_1 T_2 - \eta_2 T_1 = \pi.
\end{gathered} \tag{13}
$$

We have the following result.

Lemma. *All the functions* (12) *are eigenfunctions for the magnetic translations* T_1^* *and* T_2^*. *The functions* (12) *are magnetic Bloch functions* (*i.e., the eigenvalues of* T_1^* *and* T_2^* *are unimodular*) *if and only if*

$$
\begin{aligned}
\operatorname{Re} a &= \operatorname{Re}\left\{\frac{\eta_1}{T_1}\left[2\sum_{j=1}^N a_j - \frac{e}{\pi}\iint_K z\,B(x,y)\,dx\,dy\right]\right\},\\
\operatorname{Im} a &= \operatorname{Im}\left\{\frac{\eta_2}{T_2}\left[2\sum_{j=1}^N a_j - \frac{e}{\pi}\iint_K z\,B(x,y)\,dx\,dy\right]\right\}, \quad z = x+iy.
\end{aligned} \tag{14}
$$

For the quasimomenta (p_1,p_2) *the following formulas hold*:

$$
\begin{aligned}
p_1 + \frac{N\pi}{T_1} &= \operatorname{Im}\left(a - \frac{2\eta_1}{T_1}\sum_{j=1}^N a_j\right),\\
p_2 + \frac{N\pi}{T_2} &= \operatorname{Re}\left(a - \frac{2\eta_2}{T_2}\sum_{j=1}^N a_j\right).
\end{aligned} \tag{15}
$$

The proof of the lemma proceeds by direct computation from the preceding formulas.

Theorem. a) *For an integral* (*and hence rational*) *flux* $e\Phi/2\pi = N > 0$ *the functions* ψ_A *under conditions* (12), (14), *and* (15) *give a complete magnetic Bloch basis in the space of ground states* (*i.e. the eigenfunctions with the lowest level*) *which is defined by the equation* $H\psi = 0$ *and separates out as a direct factor in the Hilbert space* $\mathcal{L}_2(\mathbb{R}^2)$ *of all square-integrable, vector-valued functions on the plane.*

b) *The space of parameters* $(a_1,\dots,a_N)$ *indexing the functions* ψ_A *of* (12) *forms a vector bundle* E *with base which is the torus of the inverse lattice and fiber which is the* N*-dimensional space* $\mathbb{C}^N(p_1,p_2)$ *of Bloch functions with fixed quasimomenta,*

$$
\begin{gathered}
E \underset{p}{\to} T^2, \quad F = \mathbb{C}^N(p_1,p_2),\\
p(a_1,\dots,a_N,\lambda) = p_1 + ip_2 = -\frac{2\pi i}{T_1T_2}\sum_{j=1}^N a_j + \text{const}.
\end{gathered} \tag{16}
$$

The points of E *are the symmetrized aggregates*

$$
(a_1,\dots,a_N,\lambda) \sim (a_{i_1},\dots,a_{i_N},\lambda).
$$

For the proof we use the general fact that a complete basis of states $H\psi = \epsilon\psi$ can be formed from the magnetic Bloch functions for all real p_1 and p_2. For $\epsilon = 0$ we obtain the Atiyah–Singer theorem [2] for the operator $A^*\colon H_1 \to H_{-1}$ together with the remark (above) that the index of A^* reduces to the kernel of A^*, since the kernel of Axs is trivial. It follows from [2] that for fixed (p_1,p_2) the index of the operator is equal to N. Thus, the dimension of the kernel of A^* is N. Formulas (12), (14), and (15) give the required quantity, and this completes the argument.

From rough considerations without any formulas it is already evident that the degeneracy of the ground state is the same as in a homogeneous field $B = B_0 =$ const.

Conclusions. 1) For a periodic perturbation of the magnetic field the bottom Landau level of the homogeneous field does not spread out into a magnetic zone, in contrast to all the higher levels. This result is also true for all rational (and therefore generally all) magnetic fluxes. (Construction of an analogue of the basis ψ_A in the irrational case is of interest.)

2) The gap between the ground state and the remaining spectrum persists under a small perturbation of the homogeneous field B_0. A simple argument makes it clear that the gap is always present: the gap is a continuous function on the torus (p_1, p_2) and has on it a minimum which is nonzero (this can be shown).

IV. When the operator H is perturbed by a small electric potential $v(x, y)$ with the same periods T_1 and T_2, the "spreading out" of the ground state into magnetic zones and the formation of a dispersion law occur already in the first order of perturbation theory. The potential v generates a Hermitian form $\hat{v}$ on the fibers $\mathbb{C}^N(p_1, p_2)$ of the bundle E

$$\hat{v}(\psi_A) = \iint_K \bar{\psi}_A v(x, y)\, \psi_A \, dx\, dy.$$

The eigenvalues $\epsilon_j(p_1, p_2)$, $j = 1, \ldots, N$, of this form are, in general, distinct for all points of the torus (p_1, p_2) for an integral flux $e\Phi/2\pi = N$. For a rational flux $e\Phi/2\pi = N/M$ it is necessary to enlarge the lattice: $T_1 \to MT_1$, $T_2 \to MT_2$. A lattice of area $M^2 T_1 T_2$ is then obtained with flux $e\Phi^*/2\pi = MN = N^*$. It is easily proved that the form $\bar{\hat{v}}$ on the fibers consists of N blocks. All the eigenvalues $\epsilon_j(p_1, p_2)$ are M-fold degenerate, and $\epsilon_j \neq \epsilon_k$ pairwise for the blocks (in general position, for all p_1, p_2). Permutation of the eigenvalues ϵ_j (monodromy) occurs on passing around the torus (p_1, p_2) along an element of $\pi_1(T^2)$. A commutative pair of basic permutations of N elements (γ_1, γ_2), $\gamma_1\gamma_2 = \gamma_2\gamma_1$, arises. The pair (γ_1, γ_2) leads to a collection of general cycles $(n_1, \ldots, n_k)$, $\sum n_j = N$. In this case we can obtain k magnetic zones (there will be a total of k connected components in the dispersion law $\epsilon(p)$). For large N ($N \to \infty$ for the approximation of an irrational number by rational numbers) it would be interesting to clarify the statistical weights of the various topological types of decompositions into magnetic zones.

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