BLOCH FUNCTIONS OF A RELATIVISTIC CHARGED PARTICLE IN A MAGNETIC FIELD

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BLOCH FUNCTIONS OF A RELATIVISTIC CHARGED PARTICLE IN A MAGNETIC FIELD

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It is known that the Hamiltonian of a nonrelativistic spinless charged particle in a constant and homogeneous magnetic field is not translationally invariant. However, in this problem, as was shown in works ([1−3]), there is a certain symmetry, analogous to translational invariance, which becomes the latter as the magnetic field tends to zero. This symmetry was called magnetic-translational, and the operators that commute with the Hamiltonian of a charged particle in a field and become shift operators as the field tends to zero were called magnetic-translation operators. The presence of magnetic-translation symmetry in the Hamiltonian makes it possible to construct solutions that realize irreducible representations of the group of magnetic translations ([1−3]). On these solutions the magnetic-translation operators are diagonal, and the solutions themselves are analogues of Bloch functions, realizing irreducible representations of the group of ordinary translations. The purpose of the present work is to prove the existence of magnetic-translation symmetry in the problem of a relativistic charged Dirac particle in a magnetic field, and to construct Bloch quasiperiodic solutions for this particle that realize irreducible representations of the group of magnetic translations. These functions may prove useful in considering physical phenomena in semiconductors and semimetals within the framework of the two-zone model ([4,5]).

The Hamiltonian of a Dirac particle in a magnetic field has the form

$$H_D = \alpha\mathbf{p} + \beta m - e\alpha\mathbf{A} \qquad (\hbar = c = 1), \tag{1}$$

where the matrices α and β are the usual four-row Dirac matrices, and the vector potential is chosen in the form $\mathbf{A} = \frac{1}{2}[\mathbf{H} \times \mathbf{r}]$.

By direct verification one readily sees that the unitary operators

$$T(\mathbf{R}_n) = \exp[-i\mathbf{R}_n(\mathbf{p} + e\mathbf{A})], \tag{2}$$

where $\mathbf{R}_n$ is an arbitrary vector, commute with Hamiltonian (1) and are therefore integrals of motion. The form of these operators is the same as in the nonrelativistic problem ([1−3]). The magnetic-translation operators $T(\mathbf{R}_n)$ satisfy the relations

$$T(\mathbf{R}_1)T(\mathbf{R}_2) = T(\mathbf{R}_1 + \mathbf{R}_2)\exp\left\{\frac{ie}{2}\mathbf{H}\cdot[\mathbf{R}_1\times\mathbf{R}_2]\right\}; \tag{3}$$

this means that they realize a projective representation of the Abelian group of spatial displacements, and this representation, as is easy to show, is irreducible. On any bispinor $\Psi(\mathbf{r},t)$, the magnetic-translation operators (2) act according to the formula

$$T(\mathbf{R}_n)\Psi(\mathbf{r},t) = \exp\left\{\frac{ier}{2}[\mathbf{H}\times\mathbf{R}_n]\right\}\Psi(\mathbf{r}-\mathbf{R}_n,t). \tag{4}$$

We shall solve the eigenvalue equation for Hamiltonian (1) by means of the squaring method ([6]), i.e. we multiply the ordinary equation

Dirac

to the operator

$$O_+\Psi_E = (H_D - E)\Psi_E = 0 \tag{5}$$

$$O_- = \begin{pmatrix} E+m & \sigma(\mathbf{p}-e\mathbf{A}) \\ \sigma(\mathbf{p}-e\mathbf{A}) & E-m \end{pmatrix}. \tag{6}$$

We obtain a new equation, coinciding with the Schrödinger equation for a nonrelativistic particle,

$$\left[\frac{(\mathbf{p}-e\mathbf{A})^2}{2m} - \frac{eH}{2m}\sigma_z - \frac{E^2-m^2}{2m}\right]\Phi_E = 0, \tag{7}$$

where Φ_E is a 4-component bispinor.

The one-to-one relation between the solutions of equation (7) Φ_E and the solutions of equation (5) Ψ_E is given by the formula [6]

$$\Psi_E = O_-\Phi_E, \qquad \Phi_E = \begin{pmatrix} 0 \\ \varphi_E \end{pmatrix}, \tag{8}$$

where φ_E is a two-component spinor satisfying the nonrelativistic equation (7). Since the magnetic-translation operators (2) commute with the operator O_-, it is easy to see that the problem of constructing Bloch functions for a relativistic charged particle is solved if such functions are constructed for a nonrelativistic particle. Solving equation (5) by the method of squaring makes it possible to carry over all results obtained for the nonrelativistic Schrödinger equation to the case of the Dirac equation.

Let us consider, as solutions of equation (5), such functions $\Psi^s_{Ek_xk_z}$ for which the function $\varphi^s_{Ek_xk_z}$ has the form (7)

$$\varphi^s_{Ek_xk_z} = C\chi_s^{1/2} \exp\left\{ i\left[k_{xx} + k_{zz} + \omega m \frac{xy}{2}\right] - \frac{\omega m}{2}\left(y + \frac{k_x}{m\omega}\right)^2 \right\} H_n\left[\sqrt{m\omega}\left(y + \frac{k_x}{m\omega}\right)\right], \tag{9}$$

where C is a normalization constant; $\chi_s^{1/2}$ is a 2-component spinor; $\omega = eH/m$; $s = \pm 1/2$; H_n is a Hermite polynomial, and the energy does not depend on the momentum k_x, i.e., the energy levels are infinitely degenerate, with

$$E^2 = [k_z^2 + m^2 + \omega m(2n - s + 1)] \qquad (n = 0, 1, 2, ...). \tag{10}$$

The functions $\Psi^s_{Ek_xk_z}$ form a complete set. On these functions the magnetic-translation operators $T(\mathbf{R}_n)$ act according to the formulas

$$T(R_x\mathbf{i})\Psi^s_{Ek_xk_z} = \exp(-ik_{xR}x)\Psi^s_{Ek_xk_z}; \tag{11}$$

$$T(R_y\mathbf{j})\Psi^s_{Ek_xk_z} = \Psi^s_{E\,(k_x - m\omega R_y)\,k_z}; \tag{12}$$

$$T(R_z\mathbf{k})\Psi^s_{Ek_xk_z} = \exp(-ik_{zR}z)\Psi^s_{Ek_xk_z}. \tag{13}$$

In formulas (11)–(13) we impose no conditions on the displacement parameters $\mathbf{R}$.

Let us now consider the question of the possibility of isolating finite-dimensional irreducible representations of the group of spatial displacements realized by the operators (2). Let, in formula (3), the operators $T(\mathbf{R}_n)$ be replaced by finite-dimensional square matrices $N \times N$. Taking the determinant of the right- and left-hand sides of the equality and changing the order of matrix multiplication, which does not change the value of the determinant, we have

$$\exp\left\{\frac{ieH}{2}\mathbf{H}\cdot[\mathbf{R}_1 \times \mathbf{R}_2]\right\} = \exp\left\{-\frac{ieH}{2}N\cdot[\mathbf{R}_1 \times \mathbf{R}_2]\right\}. \tag{14}$$

Hence follow the quantization conditions for the magnetic flux,

$$eH \cdot [\mathbf{R}_1 \times \mathbf{R}_2] = \frac{2\pi l}{N} \qquad (l = 0, \pm 1, \pm 2, ...). \tag{15}$$

It should be noted that the quantization conditions for the magnetic flux are connected precisely with the finite-dimensionality of the loaded representations of the group of spatial translations. A particular case of such representations is given by representations realized on functions satisfying analogues of the Born-von Karman conditions ([2]), i.e., cyclicity conditions with respect to a magnetic translation. The number of different matrices of such representations is finite, and they may be regarded as a finite group commuting with the Hamiltonian (1) operators. Representations of such finite groups were considered in ([1−3]).

We now construct from the bispinors $\Psi^s_{Ek_xk_z}$ (see (8), (9)) the Bloch relativistic functions. For this purpose we choose a sublattice of vectors $R_x\mathbf{i}, R_y\mathbf{j}$, where $R_x = na,\ R_y = mb$ $(n, m = 0, \pm 1, \pm 2, ...)$, and require that the operators $T(a\mathbf{i})$ and $T(b\mathbf{j})$ commute. The operators $T(na\mathbf{i}), T(mb\mathbf{j})$ realize a unitary infinite-dimensional irreducible representation of the group of translations by the vectors of the rectangular lattice $na + mb$. Since all irreducible unitary representations of a commutative translation group are one-dimensional, the problem of constructing Bloch functions corresponding to translations by vectors of the chosen lattice reduces to restricting the loaded representation of the group of all two-dimensional spatial translations (2) to the subgroup of translations by the vectors of the sublattice satisfying the condition

$$eHab = 2\pi l \qquad (l = 0, \pm 1, \pm 2, ...). \tag{16}$$

The number $N = 1$, since the representations considered are one-dimensional.

The quasimomentum k_x lies in the interval $|k_x| \leq \pi/a$; in this case it follows from formula (11) that the function (8) realizes a one-dimensional irreducible representation of the group of translations by the vectors $na\mathbf{i}$. However, as is seen from formula (12), this function is not an eigenfunction of the operator $T(mb\mathbf{j})$. The construction of the eigenfunction is carried out analogously to the nonrelativistic case ([2]). Consider the case of a unit quantum of magnetic flux (in (16), $l = 1$). Using the complete system of functions $\Psi^s_{Ek_xk_z}$ (see (8), (9)) and the operator

$$\hat{V}_{k_y} = \sum_{m=-\infty}^{\infty} \exp(imk_yb)\, T(mb\mathbf{j}), \tag{17}$$

which, as is easily verified, satisfies the condition

$$T(b\mathbf{j})\hat{V}_{k_y} = \exp(-ik_yb)\hat{V}_{k_y}, \tag{18}$$

where the quasimomentum k_y lies in the interval $|k_y| \leq \pi/b$, we construct the bispinor $U^s_{Ek_xk_yk_z}$ by the formula

$$U^s_{Ek_xk_yk_z} = \hat{V}_{k_y} \Psi^s_{Ek_xk_z}. \tag{19}$$

The complete system of functions (19) thus constructed solves the problem posed. Indeed, the following relations hold:

$$H_D U^s_{Ek_xk_yk_z} = E U^s_{Ek_xk_yk_z}; \tag{20}$$

$$T(na\mathbf{i})\, U^s_{Ek_xk_yk_z} = \exp(-ik_x na)\, U^s_{Ek_xk_yk_z}; \tag{21}$$

$$T(mb\mathbf{j})\, U^s_{Ek_xk_yk_z} = \exp(-ik_y mb)\, U^s_{Ek_xk_yk_z}. \tag{22}$$

The functions $U^s_{Ek_xk_yk_z}$ are quasiperiodic in the plane perpendicular to the magnetic field, with periods a and b. One quantum of magnetic flux passes through the area of the primitive cell. An electron in the state described by the function (19) has quasimomentum $k_\perp(k_x, k_y)$, and the modulus of the quasimomentum lies within

$$|k_x| \leq \pi/a, \qquad |k_y| \leq \pi/b. \tag{23}$$

The energy of the electron does not depend on the quasi-momenta k_x and k_y. The functions $U^s_{Ek_xk_yk_z}$ realize one-dimensional irreducible representations of the discrete group of two-dimensional magnetic translations. Each such representation, as can be shown, enters the induced irreducible representation of this group (2) once. One can compute the explicit form of the functions $U^s_{Ek_xk_yk_z}$. Thus, for the ground state one obtains an expression in terms of a theta function, and for excited states—in terms of derivatives of theta functions, reducible to algebraic expressions in theta functions. It is convenient to construct such functions using the relation of magnetic translations to coherent states ([8]). The quasiperiodic solutions of the exact Dirac equation for an electron in a magnetic field (and also for an electron in crossed electric and magnetic fields, $\mathbf{E} \cdot \mathbf{H} = 0$, $E < H$) can be used as the zeroth approximation in problems solved within the framework of the two-zone model of semiconductors and semimetals ([4,5]), described by the exact Dirac equation. The case of solutions corresponding to a larger number of magnetic-flux quanta, as well as the case of solutions corresponding to an oblique lattice, is considered in an analogous way. The representations of the magnetic-translation group that arise in this case are more complicated; however, all the results obtained in ([1–3]) for the nonrelativistic equation remain fully valid for the Dirac equation as well.

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Note: Figure translations are in progress. See original paper for figures.