Bloch electrons in electric and magnetic fields

Alejandro Kunold

Departamento de Ciencias Básicas, Universidad Autónoma Metropolitana-Azcapotzalco, Av. S. Pablo 180, México D.F. 02200, Mexico

Manuel Torres

Instituto de Física, Universidad Nacional Autónoma de México, Aptdo. Postal 20-364, México D.F. 01000, Mexico

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We investigate Bloch electrons in two dimensions subject to constant electric and magnetic fields. The model that results from our pursuit is governed by a finite difference equation with a quasienergy spectrum that interpolates between a butterflylike structure and a Stark ladder structure. These findings ensued from the use of electric and magnetic translation operators.

We consider the problem of an electron moving in a two-dimensional lattice in the presence of applied electric and magnetic fields. We refer to this as the two-dimensional electric-magnetic Bloch problem (EMB). The corresponding magnetic Bloch system (MB) has a long and rich history. An important early contribution to the analysis of the symmetries of the MB problem was made by Zak,[1] who worked out the representation theory of the group of magnetic translations. The renowned Harper equation was derived assuming a tight-binding approximation,[2] and Rauh derived a dual Harper equation[3] in the strong magnetic-field limit. The studies of Hofstadter and others[4] of the Harper equation spectrum have since created an unceasing interest in the problem because of the beautiful self-similar structure of the butterfly spectrum.[5] A remarkable experimental realization of the Hofstadter butterfly was recently achieved, not for an electron system, but in the transmission of microwaves through an array of scatters inside a wave guide.[6] The symmetries of the EMB problem were analyzed some time ago by Ashby and Miller,[7] who constructed the group of electric-magnetic translation operators, and worked out their irreducible representations. In this paper we utilize the properties of the electric-magnetic operators in order to derive a finite difference equation that governs the dynamics of the EMB problem. The numerical solution of this equation displays an interesting pattern which interpolates between a butterflylike structure and a Stark ladder structure.

For the purposes of our research we consider the motion of an electron in a two-dimensional periodic potential, subject to a uniform magnetic field B perpendicular to the plane and to a constant electric field $\vec{E}$, lying on the plane according to $\vec{E}=E(\cos\theta,\sin\theta)$ with θ the angle between $\vec{E}$ and the lattice x_1 axis. The dynamics of the electron is governed by a time-dependent Schrödinger equation that for convenience is written as

$$S\Psi(t,\vec{r})=\left[\pi_0-\frac{\pi_1^2+\pi_2^2}{2m}-U(\vec{r})\right]\Psi(t,\vec{r})=0, \quad (1)$$

where $\pi_0=p_0+A_0$ and $\vec{\pi}=\vec{p}+\vec{A}$, with the momentum operator $p_\mu=[i\partial/\partial t,-i\vec{\nabla}]$. Units have been chosen here in which $\hbar=c=e=1$. Where necessary we use a covariant no-

tation with space-time three vectors $x_\mu=(t,\vec{r})$; $\mu=0,1,2$. Equation (1) can be considered as an eigenvalue equation for the operator S with eigenvalue 0. We adopt a gauge-independent procedure, thus the gauge potential is written as

$$A_0=(\beta-1)\vec{r}\cdot\vec{E},$$

$$A_1=(\alpha-1/2)Bx_2-\beta E_1 t,$$

$$A_2=(\alpha+1/2)Bx_1-\beta E_2 t. \quad (2)$$

This potential yields the correct background fields independent to parameters α and β. A general potential can be represented by its Fourier decomposition, however, for simplicity we shall consider the potential

$$U(x_1,x_2)=U_1\cos(2\pi x_1/a)+U_2\cos(2\pi x_2/a). \quad (3)$$

Let $(t,\vec{r})\rightarrow(t+\tau,\vec{r}+\vec{R})$ be a uniform translation in space and time, where τ is an arbitrary time and $\vec{R}$ is a lattice vector. The classical equations of motion remain invariant under these transformations, whereas the Schrödinger equation does not, the reason being the space and time dependence of the gauge potentials. Nevertheless, quantum dynamics of the system remain invariant under the combined action of space-time translations and gauge transformations. Following Ashby and Miller[7] we define the electric and magnetic translation operators

$$T_0(\tau)=\exp(-i\tau\mathcal{O}_0), \quad T_j(a)=\exp(ia\mathcal{O}_j), \quad (4)$$

where $j=1,2$ and the symmetry generators are written as new covariant derivatives $\mathcal{O}_\mu=p_\mu+\mathcal{A}_\mu$, with the components of the gauge potentials $\mathcal{A}_\mu$ given by

$$\mathcal{A}_0=\beta\vec{r}\cdot\vec{E},$$

$$\mathcal{A}_1=(\alpha+1/2)Bx_2-(\beta-1)E_1 t,$$

$$\mathcal{A}_2=(\alpha-1/2)Bx_1-(\beta-1)E_2 t. \quad (5)$$

The symmetry operators in Eq. (4) commute with the operator S in Eq. (1). The electric-magnetic operators given by Ashby and Miller include simultaneous space and time translations; we deemed it more convenient to separate the effect

of the time evolution generated by the T_0 to that of the space translations generated by T_j. The following commutators can be worked out with the previous expressions

$$[\pi_0,\pi_j]=-iE_j, \quad [\pi_1,\pi_2]=-iB,$$

$$[\mathcal{O}_0,\mathcal{O}_j]=iE_j, \quad [\mathcal{O}_1,\mathcal{O}_2]=iB, \qquad (6)$$

with all other commutators being zero. The commutators in the second line of Eq. (6) are part of the more general Lie algebra of the magnetic-electric Euclidean two-dimensional group.[8] Schrödinger's equation and the symmetry operators are expressed in terms of covariant derivatives π_μ and $\mathcal{O}_\mu$, respectively. A dual situation in which the roles of π_μ and $\mathcal{O}_\mu$ are interchanged, could be considered. According to Eqs. (2), (5), and (6), the dual problem corresponds to a simultaneous reverse in the directions of B and $\vec{E}$.

The symmetry operators in Eq. (4) commute with S but they do not commute with each other. We follow a three step method to find a set of simultaneously commuting symmetry operators. (1) First we consider a frame rotated at angle θ, with the axis along the longitudinal and transverse direction relative to the electric field. An orthonormal basis for this frame is given by $\hat{e}_L=(\cos\theta,\sin\theta)$ and $\hat{e}_T=(-\sin\theta,\cos\theta)$. We assume a particular orientation of the electric field, for which the following condition holds

$$\rho\equiv\tan\theta=\frac{E_2}{E_1}=\frac{m_2}{m_1}, \qquad (7)$$

where m_1 and m_2 are relatively prime integers. This condition insures that spatial periodicity is also found both along the transverse and the longitudinal directions. Hence, we define a rotated lattice spanned by vectors $\vec{b}_L=b\hat{e}_L$ and $\vec{b}_T=b\hat{e}_T$ where $b=a\sqrt{m_1^2+m_2^2}$. The spatial components of the symmetry generator $\vec{\mathcal{O}}$ are projected along the longitudinal and transverse directions : $\mathcal{O}_L=\hat{e}_L\cdot\vec{\mathcal{O}}$ and $\mathcal{O}_T=\hat{e}_T\cdot\vec{\mathcal{O}}$. It is readily verified that $[\mathcal{O}_0,\ \mathcal{O}_T]=0$.

(2) For the rotated lattice, we regard the number of flux quanta per unit cell to be a rational number p/q, that is

$$\phi\equiv\frac{Bb^2}{2\pi}=\frac{p}{q}. \qquad (8)$$

We can then define the extended supperlattice. A rectangle made of q adjacent lattice cells of side b contains an integer number of flux quanta. The basis vectors of the superlattice are chosen as $q\vec{b}_L$ and $\vec{b}_T$. Under these conditions the longitudinal and transverse magnetic translations $T_L(qb)=\exp(iqb\mathcal{O}_L)$ and $T_T(b)=\exp(ib\mathcal{O}_T)$ define commuting symmetries under displacements $q\vec{b}_L$ and $\vec{b}_T$.

(3) We observe that T_0 and $T_L(qb)$ commute with T_T. Yet they fail to commute with each other: $T_0(\tau)T_L(qb)=T_L(qb)T_0(\tau)\exp(-iqb\tau E)$. However the operators T_0 and $T_L(qb)$ will commute with one another by restricting time, in the evolution operator, to discrete values with period

$$\tau_0=\frac{2\pi}{qbE}=\frac{1}{p}\left(\frac{b}{v_d}\right), \qquad (9)$$

where $v_d=E/B$ and we utilized Eq. (8) to write the second equality. b/v_d is the period of time it takes an electron with drift velocity v_d to travel between lattice points. Hence, the meaning of Eq. (9) is that the ratio of the Stark ladder spacing (bE) to the Brillouin zone for the quasienergy ($2\pi v_d/b$) is given by the rational number $\phi=p/q$.

We henceforth consider that the three conditions (7), (8), and (9) hold simultaneously. In this case the three EMB operators—the electric evolution $\mathcal{T}_0\equiv T_0(\tau_0)$ and the magnetic translations $\mathcal{T}_L\equiv T_L(qb)$, and $\mathcal{T}_T\equiv T_T(b)$—form a set of mutually commuting symmetry operators. In addition to the symmetry operators, we can define the energy translation operator[9]

$$\mathcal{T}_E=\exp\left(-i\frac{2\pi}{\tau_0}t\right), \qquad (10)$$

that produces a finite translation in energy by $2\pi/\tau_0\equiv qbE$. $\mathcal{T}_E$ commutes with the three symmetry operators but not with S. Its eigenfunction $\exp(-iqbE\xi)$ defines a quasi-time ξ modulo τ_0.

Having defined $\mathcal{T}_0$, $\mathcal{T}_L$, and $\mathcal{T}_T$ that commute with each other and that also commute with S, we can look for solutions of the Schrödinger equation characterized by the quasienergy $\mathcal{E}$ and quasimomentum k_L and k_T quantum numbers according to

$$\mathcal{T}_0\Psi=\exp(-i\tau\mathcal{E})\psi,$$

$$\mathcal{T}_L\Psi=\exp(ik_Lqb)\psi,$$

$$\mathcal{T}_T\Psi=\exp(ik_Tb)\psi. \qquad (11)$$

In particular, the previous relations imply that if a simple space-time translation acts on the wave function, the latter satisfy the generalized Bloch conditions

$$\Psi(t+\tau_0,\vec{r})=\exp\{-i\tau_0(\mathcal{E}+\mathcal{A}_0(t,\vec{r}))\}\Psi(t,\vec{r}),$$

$$\Psi(t,\vec{r}+q\vec{b}_L)=\exp\{iqb(k_L+\mathcal{A}_L(t,\vec{r}))\}\Psi(t,\vec{r}),$$

$$\Psi(t,\vec{r}+\vec{b}_T)=\exp\{ib(k_T+\mathcal{A}_T(t,\vec{r}))\}\Psi(t,\vec{r}). \qquad (12)$$

We now find convenient to apply a transformation to new variables given by

$$X_0=-t, \quad P_0=\mathcal{O}_0,$$

$$X_1=\pi_T+m\frac{E}{B}, \quad P_1=\pi_L/B,$$

$$X_2=\mathcal{O}_L/B, \quad P_2=\mathcal{O}_T+m\frac{E}{B}, \qquad (13)$$

that satisfy $[X_\mu,P_\mu]=i$ for $\mu=0,1,2$. The explicit relation between $(X_\mu,\ P_\mu)$ and (x_μ,p_μ) can be worked out using the definition of π_μ, and $\mathcal{O}_\mu$ and Eqs. (2) and (5). The transformation is not canonical because of commutator $[P_0,X_2]=iE/B$, all others being zero. Applied to Eq. (1) the transformation yields for the Schrödinger equation

$$\left(P_0 + \frac{E}{B}P_2\right)\Psi = \left[\frac{B^2 P_1^2 + X_1^2}{2m} + \frac{mv_d^2}{2} + U(x_1, x_2)\right]\Psi, \tag{14}$$

where x_1 and x_2 have to be written in terms of the new variables as

$$\frac{x_1}{a} = \frac{m_2}{b}(P_1 - BX_2 - EX_0) + \frac{m_1}{b}(BX_1 - P_2),$$

$$\frac{x_2}{a} = -\frac{m_1}{b}(P_1 - BX_2 - EX_0) + \frac{m_2}{b}(BX_1 - P_2). \tag{15}$$

For $U=0$ the dynamics is cyclic in coordinates X_2 and X_0. The appearance of the time variable X_0 introduced by the periodic potential suggests that an approximation is required to solve the problem (e.g., adiabatic approximation). However, as we show below the use of an appropriate representation makes such an approximation unnecessary. We adopt the P_0, P_1, P_2 representation $\Psi_{\mathcal{E}, k_L, k_T}(P) = \langle P_0, P_1, P_2 | \mathcal{E}, k_L, k_T \rangle$ with quasienergy $\mathcal{E}$ and quasimomentum k_L and k_T. In this representation the X_μ operators act as $X_0 = i\partial/\partial P_0$, $X_1 = i\partial/\partial P_1$, and $X_2 = -i(E/B)\partial/\partial P_0 + i\partial/\partial P_2$. It is readily clear that the substitution of these relations in Eq. (15) eliminates the $\partial/\partial P_0$ contribution. For finding solutions of Eq. (14) we split the phase space (X_μ, P_μ) in the (X_1, P_1) and the $(X_0, P_0; X_2, P_2)$ variables. For the first set of variables we choose a set of basis functions in P_1 given by the Landau wave functions $\chi_n(P_1)$; these functions yield exact eigenvalues of the kinetic part of the right-hand side of Eq. (14): $(n+1/2)\omega_c$, with the cyclotron frequency $\omega_c = B/m$. For the subspace generated by the variables $(X_0, P_0; X_2, P_2)$, we notice that the four operators $(\mathcal{T}_0^i, \mathcal{T}_L^j, \mathcal{T}_T^k, \mathcal{T}_E^l)$ with all possible integer values of (i,j,k,l) form a complete set of operators. The demonstration follows similar steps as those presented by Zak in Ref. 10. Hence a complete set of functions, for the subspace $(X_0, P_0; X_2, P_2)$, is provided by the eigenfunctions of the operators $(\mathcal{T}_0^i, \mathcal{T}_L^j, \mathcal{T}_T^k, \mathcal{T}_E^l)$, we write them down and verify their correctness:

$$\phi_{k_L, k_T, \epsilon, \xi}(P_0, P_2) = \sum_{l,m} c_m e^{i\xi\sigma bE(pl-m)} e^{i(2\pi/b)mk_L}$$

$$\times \delta(P_0 - \mathcal{E} - lqbE)$$

$$\times \delta\left(P_2 - k_T + \frac{2\pi}{b}m\right), \tag{16}$$

where we defined $\sigma \equiv 1/\phi = q/p$. It is easy to check that this function automatically satisfies the first and third EMB translations in Eqs. (11), whereas the second equation is satisfied by imposing the periodicity condition $c_{m+p} = c_m$. In addition, ϕ is also eigenfunction of the energy translation operator Eq. (10) with eigenvalue $\exp(-iqbE\xi)$. The wave function Ψ is then expanded in terms of χ_n and $\phi_{k_L, k_T, \epsilon, \xi}$. The operator $\mathcal{T}_E$ is not a symmetry of the problem, so we have to multiply ϕ by a coefficient d_ξ and add over all possible values of ξ; the resulting wave function can be recast as

$$\Psi_{k_L, k_T, \epsilon}(P) = \sum_{n,l,m} a_n \chi_n(P_1) h_{m-pl} c_m e^{i(2\pi/b)mk_L}$$

$$\times \delta(P_0 - \mathcal{E} - lqbE)\delta\left(P_2 - k_T + \frac{2\pi}{b}m\right), \tag{17}$$

where $h_{m-pl} = \Sigma_\xi d_\xi e^{i\xi\sigma bE(pl-m)}$. Of particular interest are the following Bloch conditions obeyed by Ψ with respect to the eigenvalues:

$$\Psi(\mathcal{E}, k_L + bB, k_T) = \Psi(\mathcal{E}, k_L, k_T),$$

$$\Psi(\mathcal{E}, k_L, k_T + qbB) = e^{iqbk_L}\Psi(\mathcal{E} + qbE, k_L, k_T). \tag{18}$$

These conditions are quite different from those satisfied by the usual Bloch and magnetic Bloch functions;[1] the second one is not periodic, because in addition to the Bloch phase e^{iqbk_L} the $k_T \to k_T + qb$ shift leads to the change in energy $\mathcal{E} \to \mathcal{E} + qbE$.

Based on wave function (17) it is possible to work out a complete solution of the EMB problem, similar to what has been achieved for the magnetic-Bloch problem.[11] This will be analyzed elsewhere.[12] Nevertheless, the approximated solution wherein the coupling between different Landau levels is neglected is interesting enough, and probably more illuminating. Within this approximation the Landau number n is also a conserved quantum number and the substitution of Eqs. (17) in (14) yields the secular equation

$$\left(\Delta - \frac{Eb}{2\pi}\Sigma_m\right)\widetilde{c}_m$$

$$= f_n(\sigma)\left[U_1\lambda(e^{-im_1\Sigma_m}\widetilde{c}_{m+m_2} + e^{im_1\Sigma_m}\widetilde{c}_{m-m_2})\right.$$

$$\left. + U_2\lambda^*(e^{im_2\Sigma_m}\widetilde{c}_{m+m_1} + e^{-im_2\Sigma_m}\widetilde{c}_{m-m_1})\right], \tag{19}$$

where we defined $\widetilde{c}_m = e^{i(2\pi/b)mk_L}h_m c_m$, $\Sigma_m = (2\pi m - k_T b)\sigma$, $\lambda = \exp\{-i\pi m_1 m_2 \sigma\}$, $f_n(\sigma) = e^{-\pi\sigma/2}L_n(\pi\sigma)$ and L_n are the Laguerre polynomials. The quasienergy $\mathcal{E}$ is related to the eigenvalue Δ according to $\mathcal{E} = (n+1/2)\omega_c + mv_d^2/2 + \Delta$.

The dynamics of the system is then described by Eq. (19), a finite difference equation with distant neighbor couplings m_1 and m_2, which also includes a linear term proportional to $\vec{E}$. This equation generalizes Harper's equation to include the effect of an electric field of arbitrary intensity. If the electric field is switched off, it can be set $m_1 = 1$, $m_2 = 0$ in which case Eq. (19) reduces to Harper's equation.

We present results for particular cases when the electric field is aligned along the axis of the original lattice (i.e., $m_1 = 1$, $m_2 = 0$). It is known that the experimental observation of the butterfly spectrum could possibly be achieved in lateral surface superlattices,[4,11] given that a value for $\sigma \sim 1$ can be obtained for feasible magnetic fields, due to the large dimensions of the unit cell. Hence we select the following values: $a \sim 100$ nm, $U_0 \equiv U_1 = U_2 = 0.5$ meV, $m = 0.07m_e$, and $E = 0.05$ V/cm, which can be satisfied in current experiments.[13] For these values, $\sigma = 1$ corresponds to a magnetic field of 10T, hence $U_0/\omega_c \sim 0.05$ and the condition required for weak periodic potential is satisfied. Figures 1
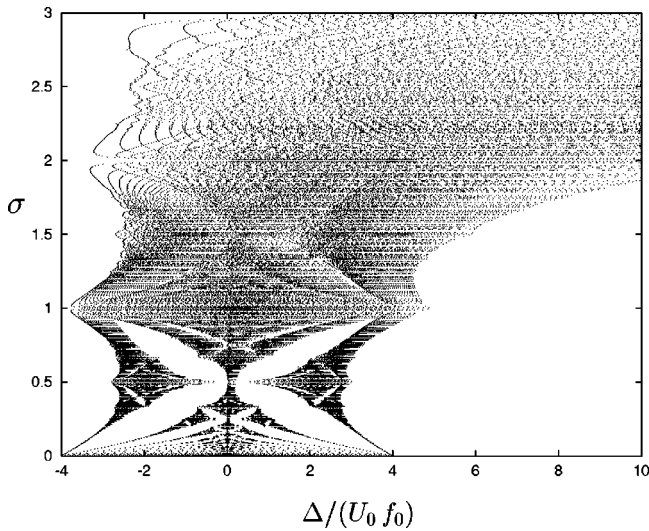
FIG. 1. Quasienergy spectrum for the lowest Landau level. The energy axis is rescaled to $\Delta/[U_0 f_0(\sigma)]$, the parameters selected are $a \sim 100$ nm, $U_0 = 0.5$ meV, $m = 0.07 m_e$, $E = 0.05$ V/cm and $k_T = 0$.

and 2 show plots for the scaled Δ spectrum as function of σ. We recall that for $\vec{E} = 0$ the spectrum for $\Delta/[U_0 f_n(\sigma)]$ is invariant under the substitution $\sigma \rightarrow \sigma + N$ with N an integer.

In Fig. 1 for the lowest Landau level we observe that for a strong magnetic field the Hofstadter butterfly is clearly shown for σ in the interval $[0,1]$. However, as the magnetic field decreases (σ increases), some of the fine-grained structures of the spectrum are smeared by the effect of the electric field. A weak distorted replica of the butterfly is still observed for σ in the interval $[1,2]$. Finally, for bigger values of σ, the spectrum is strongly distorted by the electric field and the butterfly ''flies away.'' At this limit the effect of the periodic potential is negligible and the spectrum consists of equally spaced levels with separation σEb, i.e., a Stark lad-
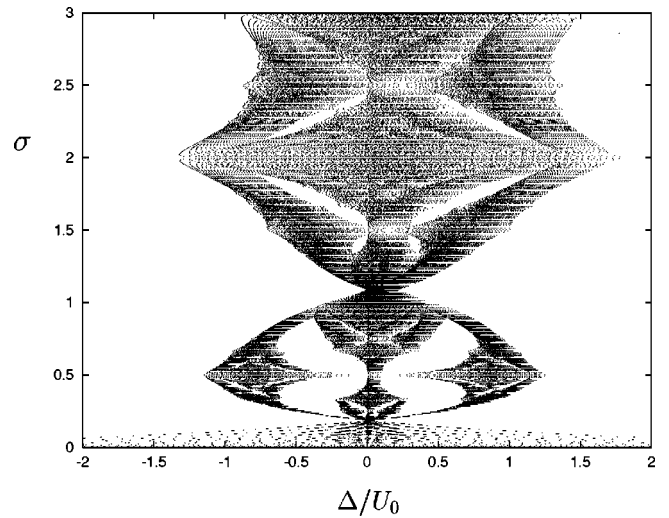

FIG. 2. Quasienergy spectrum of the second Landau level ($n = 2$). In this case the energy axis is rescaled to $\Delta/(U_0)$, the other parameters are the same as in Fig. 1.

der. For the $n = 2$ Landau level (Fig. 2) three smeared replicas of the butterfly can be observed, the narrow waist segments of the plot corresponds to the flat band condition given by $\sigma = \gamma_n/\pi$, with γ_n a zero of the Laguerre polynomial.

In conclusion, the electric and magnetic translation symmetries are utilized to analyze the EMB problem. Bloch functions are derived and their properties established in Eqs. (12) and (18). The system is governed by Eq. (19), the spectrum of which interpolates between a butterflylike structure and a Stark ladder structure. This equation offers a very interesting model, susceptible to analysis in terms of dynamical systems. We finally remark that the present formalism should set the basis for the study of Hall conductivity beyond the linear response approximation.

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