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A Letters Journal Exploring the Frontiers of Physics

December 2008

EPL, **84** (2008) 50002
doi: 10.1209/0295-5075/84/50002

www.epljournal.org

Semiclassical quantization of electrons in magnetic fields: The generalized Peierls substitution

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received 22 September 2008; accepted in final form 21 October 2008
published online 26 November 2008

PACS 03.65.Sq – Semiclassical theories and applications
PACS 03.65.Vf – Phases: geometric; dynamic or topological

Abstract – A generalized Peierls substitution which takes into account a Berry phase term must be considered for the semiclassical treatment of electrons in a magnetic field. This substitution turns out to be an essential element for the correct determination of the semiclassical equations of motion as well as for the semiclassical Bohr-Sommerfeld quantization condition for energy levels. A general expression for the cross-sectional area is derived and used as an illustration for the calculation of energy levels of Bloch and Dirac electrons.

Semiclassical approaches are very important in many area of physics for the study of the short-wavelength behavior of quantum systems, including Bloch electrons in crystals or Dirac particles in external fields. An essential ingredient of these approaches is the Bohr-Sommerfeld quantization condition, whose generalization from scalar to vector wave fields has revealed new gauge structures related to Berry's phases [1]. This paper presents a detailed study of the semiclassical quantization for a single quantum particle in a magnetic field, exemplified by electrons in a crystal and by Dirac electrons. This unified description of a particle in a magnetic field is based on a method of semiclassical diagonalization for an arbitrary matrix-valued Hamiltonian developed previously [2] (for a generalization to higher order in $\hbar$ see [3]). This method results in an effective diagonal Hamiltonian in terms of gauge-covariant but noncanonical, actually noncommutative, coordinates. It will be shown that a generalized Berry's phase dependent Peierls substitution is necessary for the establishment of the full equations of motion including Berry's phase terms. This substitution turns out to be also an essential ingredient for the Bohr-Sommerfeld quantization condition of an electron in a magnetic field. Indeed, when reformulated in terms of the generalized Peierls substitution, this condition leads to a modification of the semiclassical quantization rules as well as to a generalization of the cross-sectional area derived independently by Roth [4] and Fal'kovskii [5] in the context of Bloch electrons.

Semiclassical diagonalization. – Let us consider a system of a quantum particle in a uniform external magnetic field $\mathbf{B} = \boldsymbol{\nabla} \times \widetilde{\mathbf{A}}$ described by an arbitrary-matrix–valued Hamiltonian $H(\boldsymbol{\Pi}, \mathbf{R})$, where $\boldsymbol{\Pi} = \mathbf{P} + e\widetilde{\mathbf{A}}(\mathbf{R})$ is the covariant momentum and $e > 0$ is the electric charge. We assume that the system can be separated into two contributions such that $H(\boldsymbol{\Pi}, \mathbf{R}) = H_m(\boldsymbol{\Pi}) + \varphi(\mathbf{R})$, where $H_m(\boldsymbol{\Pi})$ is the pure magnetic part and $\varphi(\mathbf{R})$ is the external electric potential. In this paper we will be mainly interested in the magnetic contribution. The exact diagonalization of this matrix-valued operator through an unitary matrix $U(\boldsymbol{\Pi})$ is in general not known, and in this paper we apply a recursive diagonalization procedure developed previously by two of the authors. This procedure is based on a series expansion in the Planck constant of the required diagonal Hamiltonian [2,3]. By diagonal Hamiltonian it is meant a matrix representation with block-diagonal matrix elements associated with energy band subspaces. The method is based on the knowledge of the zeroth-order diagonal representation $\varepsilon = U_0 H_0 U_0^+$ where U_0 is the zeroth-order transformation matrix, H_0 the Hamiltonian H_m, in which the components Π^i are

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considered formally as classical, and therefore commuting operators. Quantum corrections are then re-introduced to yield the expression for the diagonal Hamiltonian $H_d = U(\mathbf{\Pi}) HU^+(\mathbf{\Pi})$ which, if we limit ourselves to the semiclassical order (the semiclassical condition being that the radius of curvature of the orbit is large in comparison with wavelength), has diagonal operator elements labelled by the energy index n which reads

$$(H_d)_{nn} = \varepsilon_n(\boldsymbol{\pi}_n) + \varphi(\mathbf{r}_n) - e\hbar \mathbf{M}_n \cdot \mathbf{B}. \tag{1}$$

Here $\varepsilon_n(\boldsymbol{\pi})$ is the zeroth-order matrix element of ε (it can itself be a matrix as for a Dirac Hamiltonian, in which case a block-diagonalization is considered) in which classical variables are now replaced by the quantum operators $\boldsymbol{\pi}_n = \mathbf{\Pi} + \hbar A_\Pi$ and $\mathbf{r}_n = \mathbf{R} + \hbar A_R$, where we have defined the Berry connections as being the projection on the n-th energy band $A_{R/\Pi} = \mathcal{P}_n\left[\mathcal{A}_{R/\Pi}\right]$ of the matrices $\hbar\mathcal{A}_R = U\mathbf{R}U^+$ and $\hbar\mathcal{A}_\Pi = U\mathbf{\Pi}U^+$ (where $\mathbf{R}$ and $\mathbf{\Pi}$ implicitly act only on U^+). The matrix $\hbar\mathcal{A}_R$ can also be written $\hbar\mathcal{A}_R = i\hbar U\boldsymbol{\nabla}_{\mathbf{\Pi}}U^+$ as a consequence of the commutation relation $\left[R^i, \Pi^j\right] = i\hbar\delta^{ij}$. The other matrix $\mathcal{A}_\Pi$ can be expressed in terms of $\mathcal{A}_R$. Indeed, we have $U\mathbf{\Pi}U^+ = U\boldsymbol{\nabla}_{\Pi^i}U^+[\mathbf{\Pi}, \Pi^i] = -e\mathcal{A}_R \times \mathbf{B}$ owing to the fact $\left[\Pi^i, \Pi^j\right] = -ie\hbar\varepsilon^{ijk}B_k$. From this, we deduce, after projection on the n-th energy band the following Berry connection, $A_\Pi = -eA_R \times \mathbf{B}$.

The derivation of the in-band Hamiltonian eq. (1), shows that instead of the Peierls substitution [6], which amounts to replacing the canonical momentum $\mathbf{P}$ by the covariant one $\mathbf{\Pi}$ in the energy band ε_n, the presence of non-zero Berry connections leads to a generalization of the Peierls substitution via a generalized covariant momentum

$$\boldsymbol{\pi}_n = \mathbf{\Pi} - e\hbar A \times \mathbf{B}, \tag{2}$$

where from now we use the notation $A \equiv A_R$ and $\mathcal{A} \equiv \mathcal{A}_R$. The last term in eq. (1) is the coupling between the uniform magnetic field and the magnetic moment which is a vector that reads $\mathbf{M}_n(\pi) = \frac{i}{2\hbar^2}\mathcal{P}_n([\varepsilon, \mathcal{A}] \times \mathcal{A}) = \frac{1}{2\hbar}\mathcal{P}_n(\dot{\mathcal{A}} \times \mathcal{A})$ [2,3] (it can be a matrix-valued vector if the n-th energy band is degenerate). As $\dot{\mathcal{A}}$ has only off-diagonal matrix elements related to the band-to-band matrix elements of $\mathcal{A}$ by the relation $\dot{\mathcal{A}}_{nm} = \frac{i}{\hbar}(\varepsilon_n - \varepsilon_m)\mathcal{A}_{nm}$, we can write the matrix elements of the components of $\mathbf{M}_n$ as

$$(M_x)_{nn} = \frac{i}{2}\sum_{m\neq n}\frac{(\dot{\mathcal{A}}_y)_{nm}(\dot{\mathcal{A}}_z)_{mn}}{\varepsilon_n - \varepsilon_m}, \tag{3}$$

and similarly for the other components M_y and M_z by circular permutation. This is the usual magnetic moment as it is deduced in solid states physics books like [7], but it is actually more general as we can see here. Later, we will use this expression to compute the magnetic moment of a Dirac electron. Note also that $\dot{\mathcal{A}}_{nm}$ are the non-diagonal elements of the velocity matrix $(\dot{\mathbf{r}})_{nm}$ and thus $\mathbf{M}_n$ can be seen as an intrinsic angular momentum. Indeed we can write $\mathbf{M}_n = \frac{1}{2\hbar^2}(\dot{\mathbf{r}} \times (\mathbf{r} - \mathbf{R}))_{nn}$, where it assumed that the diagonal elements of $\dot{\mathbf{r}}$ are excluded (see also [8]).

The appearance of the Berry connection allows us to define naturally non-Abelian (in general) Berry curvatures $\Theta_{ij}(\boldsymbol{\pi}) = \partial_{\pi^i}A_j - \partial_{\pi^j}A_i + \left[A_i, A_j\right]$, where for simplicity we omit now band indices. Position operators then satisfy an unusual non-commutative algebra $\left[r^i, r^j\right] = i\hbar^2\Theta^{ij}$. The generalized covariant momentum satisfy an algebra $\left[\pi^i, \pi^j\right] = -ie\hbar\varepsilon^{ijk}B_k + ie^2\hbar^2\varepsilon^{ipk}\varepsilon^{jql}\Theta^{pq}B_kB_l$ slightly corrected with respect to the usual one $\left[\Pi^i, \Pi^j\right] = -ie\hbar\varepsilon^{ijk}B_k$ by a term of order $\hbar^2B^2$ which can in general be neglected. The Heisenberg relations between the coordinate and the momentum $\left[r^i, \pi^j\right] = i\hbar\delta^{ij} + ie\hbar^2\varepsilon^{jlk}\Theta^{il}B_k$ is also slightly changed but by a term of order $\hbar^2B$. This contribution which is a direct consequence of introducing the generalized covariant momentum was overlooked in previous works, with the exception of Bliokh's work on the specific case of the Dirac equation [9]. It turns out that this term is essential for the determination of the genuine semiclassical equations of motion which are

$$\begin{aligned}\dot{\mathbf{r}} &= \partial\mathcal{E}/\partial\boldsymbol{\pi} - \hbar\dot{\boldsymbol{\pi}} \times \Theta(\boldsymbol{\pi}),\\ \dot{\boldsymbol{\pi}} &= -e\mathbf{E} - e\dot{\mathbf{r}} \times \mathbf{B},\end{aligned} \tag{4}$$

where we defined $\mathcal{E} \equiv \varepsilon - e\hbar\mathbf{M}\cdot\mathbf{B}$. As consequence of the non-commutative algebra, the velocity equation is corrected by an anomalous velocity term $\dot{\boldsymbol{\pi}} \times \Theta$, where the vector Θ defined as $\Theta_i = \varepsilon_{ijk}\Theta^{jk}/2$ is the Berry curvature of an electronic state in the given n-th band, associated to the electron motion in the n-th energy band. These equations of motion, where first derived in solid-state physics context in [8] (see also [10]) by considering the evolution of the wave packet of a Bloch electron in an electromagnetic field. In this picture, it is the mean over wave packets of the operator $\mathbf{r}$ corresponding thus to the wave packet center r_c and the mean of $\boldsymbol{\pi}$ giving the mean wave vector π_c that are the variables in eq. (4). The operatorial approach reveals first that the operator $\boldsymbol{\pi}$ is in fact a generalized covariant momentum operator which replaces the Peierls substitution, and second, that the operatorial equations of motion are not restricted to Bloch electrons in a magnetic field but are valid for any physical system described by an arbitrary matrix-valued Hamiltonian of the kind $H(\mathbf{\Pi}, \mathbf{R}) = H_m(\mathbf{\Pi}) + \varphi(\mathbf{R})$. In particular they are also valid for Dirac particles moving in an electromagnetic field.

Note that in solids, for crystals with simultaneous time-reversal and spatial inversion symmetry, the Berry curvature and the magnetic moment vanish identically throughout the Brillouin zone [8]. This is the case for most applications in solid-state physics, but there are situations where these symmetries are not simultaneously present as in GaAs, where inversion symmetry is broken, or in

ferromagnets, which break time reversal symmetries. In the same way, the presence of a strong magnetic field, the magnetic Bloch bands corresponding to the unperturbated system breaks the time inversion symmetries. In all these cases the dynamical and transport properties must be described by the full equations of motion given by eq. (4). In the case of Dirac particles, both the Berry curvature and the magnetic moment are non zero and the full equations of motion have to be considered [2,9].

Bohr-Sommerfeld quantization. – Having shown the necessity of the generalized Peierls substitution for the determination of the semiclassical equations of motion, we now investigate the relevance of this new concept at the level of the semiclassical quantization of the energy levels for an electron motion in an external uniform magnetic field only ($\varphi = 0$), so that eq. (4) becomes $\dot{\mathbf{r}} = D\left(\frac{\partial \mathcal{E}}{\partial \boldsymbol{\pi}}\right)$ and $\dot{\boldsymbol{\pi}} = -eD\left(\frac{\partial \mathcal{E}}{\partial \boldsymbol{\pi}} \times \mathbf{B}\right)$ with $D^{-1} = 1 - e\hbar \mathbf{B}\boldsymbol{\Theta}$. For convenience, $\mathbf{B}$ is chosen to point in the z-direction $\mathbf{B} = B\mathbf{k}$. Consequently the orbits satisfies the conditions $\mathcal{E} = \text{const}$ and $\pi_z = \text{const}$. The semiclassical quantization of energy levels can be done according to the Bohr-Sommerfeld quantization rule

$$\oint P_\perp \mathrm{d}R_\perp = 2\pi\hbar\,(n + 1/2)\,, \tag{5}$$

where $P_\perp$ is the canonical momentum in the plane perpendicular to the axis $\pi_z = \text{const}$. The integration is taken over a period of the motion and n is a large integer. Now, it turns out to be convenient to choose the gauge $\widetilde{A}_y = BX$, $\widetilde{A}_x = \widetilde{A}_z = 0$. In this gauge, one has $\pi_z = P_z = \text{const}$, and the usual covariant momentum $\Pi_y = P_y + eBX$. As $BX = B(x - \hbar A_x)$ the generalized covariant momentum defined as $\pi_y = \Pi_y + e\hbar B A_x$ becomes

$$\pi_y = P_y + eBx, \tag{6}$$

which is formally the same relation as the one between the canonical variables, but now relating the new covariant generalized dynamical operators. This relation with the help of the equations of motion gives $\dot{P}_y = \dot{\pi}_y - eB\dot{x} = 0$, thus P_y is a constant of motion so that $\oint P_y \mathrm{d}Y = P_y \oint \mathrm{d}Y = 0$ and eq. (5) becomes simply $\oint P_x \mathrm{d}X = 2\pi\hbar\,(n + 1/2)$. Now using the definition of the generalized momentum $P_x = \pi_x + e\hbar A_y B$ and the differential of the canonical position $\mathrm{d}X = \mathrm{d}x - \hbar \mathrm{d}A_x = \frac{\mathrm{d}\pi_y}{eB} - \hbar \mathrm{d}A_x$, the Bohr-Sommerfeld condition eq. (5) becomes

$$\oint \pi_x \mathrm{d}\pi_y = 2\pi\hbar eB\left(n + \frac{1}{2} - \frac{1}{2\pi}\oint A_\perp \mathrm{d}\boldsymbol{\pi}_\perp\right), \tag{7}$$

where the integral is now taken along a closed trajectory Γ in the π space and $\frac{1}{2\pi}\oint A_\perp \mathrm{d}\boldsymbol{\pi}_\perp = \phi_B$ is the Berry phase for the orbit Γ. It is interesting to note that in terms of the usual covariant momentum (Peierls substitution) we have instead of eq. (7) the condition $\oint \Pi_x \mathrm{d}\Pi_y = 2\pi\hbar eB\,(n + 1/2)$. The integration in eq. (7) defines the cross-sectional area $S_0(\varepsilon, \pi_z)$ of the orbit Γ which is the intersection of the constant energy surface $\varepsilon(\pi) = \text{const}$ and the plane $\pi_z = \text{const}$. Therefore the condition eq. (7) implicitly determines the energy levels $\varepsilon_n(\pi_z)$. Computing now the cross-sectional area $S_0(\mathcal{E}, \pi_z) = S_0(\varepsilon - e\hbar M_z B, \pi_z) \approx S_0(\varepsilon, \pi_z) + \mathrm{d}S$, with $\mathrm{d}S = \oint \mathrm{d}\kappa \mathrm{d}\boldsymbol{\pi}_\perp$ the area of the annulus between the energy surface $\varepsilon = \text{const}$ and the surface $\varepsilon + \mathrm{d}\varepsilon$ with $\mathrm{d}\varepsilon = -e\hbar M_z B$, and where $\mathrm{d}\kappa = \sqrt{\mathrm{d}\pi_x^2 + \mathrm{d}\pi_y^2}$ is an elementary length of the π orbit. Then, as $\mathrm{d}S$ can be written $\mathrm{d}S = \oint \frac{\mathrm{d}\varepsilon \mathrm{d}\kappa}{|\partial\varepsilon/\partial\boldsymbol{\pi}_\perp|} = -e\hbar B \oint \frac{M_z \mathrm{d}\kappa}{|\partial\varepsilon/\partial\boldsymbol{\pi}_\perp|}$, where the integral is taken over the orbit Γ, one has finally

$$S_0(\mathcal{E}, \pi_z) = 2\pi\hbar eB\left(n + \frac{1}{2} - \phi_B - \frac{1}{2\pi}\oint \frac{M_z(\boldsymbol{\pi})\,\mathrm{d}\kappa}{|\partial\varepsilon/\partial\boldsymbol{\pi}_\perp|}\right). \tag{8}$$

It is common to write $S_0(\mathcal{E}, \pi_z) = 2\pi\hbar eB\,(n + \gamma)$ defining thus the coefficient $\gamma - \frac{1}{2} = -\phi_B - \frac{1}{2\pi}\oint \frac{M_z \mathrm{d}\kappa}{|\partial\varepsilon/\partial\boldsymbol{\pi}_\perp|}$. This coefficient can also be written in a different form

$$\gamma - \frac{1}{2} = -\frac{1}{2\pi}\oint \frac{[\widetilde{\mathbf{v}} \times A + \mathbf{M}]_z\,\mathrm{d}\kappa}{|\partial\varepsilon/\partial\boldsymbol{\pi}_\perp|} \tag{9}$$

with $\widetilde{\mathbf{v}} \equiv \partial\varepsilon/\partial\boldsymbol{\pi}$. Equation (9) is a generalization of a previous result found by Roth [4] and Fal'kovskii [5], in the specific context of Bloch electrons in a magnetic field. The connection with Berry's phase was seen later by Mikitik and Sharlai [11]. In both [4] and [11], the term $[\widetilde{\mathbf{v}} \times A + \mathbf{M}]$ was written as $\frac{1}{2}\mathcal{P}_n\left[\left(\frac{\boldsymbol{\Pi}}{m} + \mathbf{v}\right) \times \mathcal{A}\right]$, where $\mathbf{v} = \frac{\boldsymbol{\Pi}}{m} + \hbar\dot{\mathcal{A}}$ is the velocity operator before projection on a band, and $\Pi = m\dot{\mathbf{R}}$, a relation valid only for a Hamiltonian whose kinetic energy is $\Pi^2/2m$. Therefore eq. (8) is more general and has a broader field of application, as it is a general result which applies for any kind of single quantum particle system in a magnetic field, including Bloch and Dirac electrons. Importantly the derivation provided here is new, and it turns out to be the result of the generalized Peierls substitution in the Bohr-Sommerfeld condition.

Bloch electron. – In a crystal, the Berry gauge $A(\mathbf{k})$ is Abelian (a scalar operator), written in terms of the periodic part of the Bloch wave $|u_n(\mathbf{k})\rangle$ as $A(\mathbf{k}) = i\langle u_n(\mathbf{k})|\partial_{\mathbf{k}}|u_n(\mathbf{k})\rangle$, where $\mathbf{k}$ is the generalized covariant pseudo momentum ($\mathbf{k} = \boldsymbol{\pi}/\hbar$). Application of eq. (8) for electron trajectories in a crystal with time reversal and spatial inversion symmetry, where it is expected that, both $\boldsymbol{\Theta}$ and $\mathbf{M}$ vanish in the Brillouin zone, has been studied by Mikitik and Sharlai [11]. But these authors also pointed out the fact that the Berry's phase is non-zero when the electron orbit surrounds the band-contact line of a metal, actually $\phi_B = \pm 1/2$. Consequently, $\gamma = 0$ in this case, instead of the previously

supposed constant value $\gamma = 1/2$ which is commonly used in describing oscillation effect in metals. As these authors mentioned, measurements of γ can allows the detection of band contact lines.

As a simple application of eq. (8) consider a crystal with time reversal and spatial inversion symmetry, and where the Fermi surface is an ellipsoid of revolution characterized by two effective masses, a transverse $m_\perp$ and a longitudinal m_l one. The energy levels can easily be deduced. Indeed $\mathcal{E} = \hbar^2 \left(\frac{\mathbf{k}_\perp^2}{2m_\perp} + \frac{K_z^2}{2m_l} \right)$ and the cross-sectional area $S_0(\mathcal{E}, K_z)$ is a disc of radius square $\mathbf{k}_\perp^2 = 2m_\perp \left(\mathcal{E}/\hbar^2 - \frac{K_z^2}{2m_l} \right)$, so that the energy levels are $\mathcal{E}_n = \frac{eB\hbar}{m_\perp}\left(n + \frac{1}{2}\right) + \frac{\hbar^2 K_z^2}{2m_l}$, which actually coincide with the exact ones because the energy levels of an harmonic oscillator keep their form at large n.

Dirac electron. – Let us consider the Dirac Hamiltonian $H = \boldsymbol{\alpha} \cdot \boldsymbol{\Pi} + \beta m$ in the presence of an uniform magnetic field, with α and β the usual (4×4) Dirac matrices. The semiclassical block-diagonalization followed by a projection on, say, the positive energy subspace, leads to the (2×2)-matrix–valued energy operator $\mathcal{E} = \varepsilon - e\hbar \mathbf{M} \cdot \mathbf{B}$, where $\varepsilon = \sqrt{\boldsymbol{\pi}^2 + m^2}$ $(c = 1)$ and the magnetic moment is given by $\mathbf{M} = \frac{\boldsymbol{\sigma}}{2\varepsilon} - \frac{\mathbf{L}}{\varepsilon}$, with $\mathbf{L} = \boldsymbol{\pi} \times A$ representing the intrinsic orbital angular momentum [2,9]. It turns out that for Dirac, the magnetic moment can also be expressed as $\mathbf{M} = \varepsilon \boldsymbol{\Theta}$, with the curvature vector given by the matrix [2,9]

$$\boldsymbol{\Theta}(\boldsymbol{\pi}) = -\frac{1}{2\varepsilon^3} \left[m\boldsymbol{\sigma} + \frac{(\boldsymbol{\sigma} \cdot \boldsymbol{\pi})\, \boldsymbol{\pi}}{\varepsilon + m} \right],$$

with $\boldsymbol{\sigma}$ the Pauli matrices. Berry's connection is defined as $A = i \langle +, \boldsymbol{\pi} | \, \partial_{\boldsymbol{\pi}} \, | +, \boldsymbol{\pi} \rangle$ where $|+, \boldsymbol{\pi}\rangle$ is the two-components spinor of the positive-energy subspace. Consider $\mathbf{B}$ pointing in the z-direction so that $\pi_z = P_z = \text{const}$, with the goal to compute the Landau energy levels (LEL) as an application of eq. (8). As the cross-sectional area $S_0(\varepsilon, P_z)$ is a disc of radius square $\boldsymbol{\pi}_\perp^2 = \varepsilon^2 - m^2 - P_z^2$, the application of eq. (8) consists in replacing ε by $\mathcal{E}$ in $\boldsymbol{\pi}_\perp^2$, so that we have $S_0(\mathcal{E}, P_z) = \pi \left(\mathcal{E}_n^2 - m^2 - P_z^2 \right)$, which yields the semiclassical quantized LEL through the relation

$$\mathcal{E}_n^2 - m^2 - P_z^2 = 2\hbar eB \left(n + \frac{1}{2} - \phi_B - \frac{1}{2\pi} \oint \frac{M_z \mathrm{d}\kappa}{|\partial\varepsilon/\partial \boldsymbol{\pi}_\perp|} \right).$$

Now from the Berry connection $A = \frac{\boldsymbol{\pi} \times \boldsymbol{\sigma}}{2\varepsilon(\varepsilon + m)}$ we deduce Berry's phase $\phi_B = -\frac{\tau}{2} + \tau \left(\frac{m}{2\varepsilon} + \frac{P_z^2}{2\varepsilon(\varepsilon+m)} \right)$, where $\tau = \pm 1$ are the eigenvalues of the Pauli matrix σ_z. Berry's phase is the sum of a topological part $-\frac{\tau}{2}$ and a non-topological $\tau \left(\frac{m}{2\varepsilon} + \frac{P_z^2}{2\varepsilon(\varepsilon+m)} \right)$ one. The contribution from the magnetic moment yields $\frac{1}{2\pi} \oint \frac{M_z \mathrm{d}\kappa}{|\partial\varepsilon/\partial \boldsymbol{\pi}_\perp|} = -\tau \left(\frac{m}{2\varepsilon} + \frac{P_z^2}{2\varepsilon(\varepsilon+m)} \right)$ a term which exactly cancels the non-topological contribution of ϕ_B, so that finally

$$\mathcal{E}_n = \sqrt{m^2 + 2\hbar Be \left(n + \frac{1}{2} + \frac{\tau}{2} \right) + P_z^2}.$$

It turns out in this example that the semiclassical energy quantization coincides also with the exact result. It is usually expected that for a massless Dirac particle Berry's phase takes the topological value $\phi_B = \pm 1/2$, as a consequence of the band degeneracy at zero momentum [12]. This is not the case here because the magnetic field lifts this degeneracy as P_z is not zero in, general. But it turns out that the magnetic-moment contribution exactly compensates for the non-topological Berry's phase contribution. This cancellation can be easily understood from the expression, eq. (9), for the coefficient γ. Indeed from the equality $[\widetilde{\mathbf{v}} \times A + \mathbf{M}]_z = \left[\frac{\boldsymbol{\pi} \times A}{\varepsilon} \right]_z + \frac{\tau}{2\varepsilon} - \frac{\mathbf{L}_z}{\varepsilon} = \frac{\tau}{2\varepsilon}$ we deduce the expected result $\gamma = \frac{1}{2} + \frac{\tau}{2} = 0$ or 1.

For a two-dimensional Dirac system it is therefore expected that the magnetic moment for massless particles exactly vanishes, and that Berry's phase takes the topological value $\phi_B = \pm 1/2$. The electron motion in graphene is an interesting physical situation which illustrates this assertion. Indeed, graphene is a two-dimensional carbon crystalline honeycomb structure with inversion symmetry so that $\mathbf{M} = 0$. The hexagonal Brillouin zone has two distinct and degenerate Dirac points or valleys (labelled by $\tau \pm 1$) where the conduction and valence bands meet and the electronic excitations behave like massless relativistic fermions, so that $\phi_B = \pm 1/2$ and consequently $\mathcal{E}_n = \pm\sqrt{2\hbar eB \left(n + \frac{1}{2} + \frac{\tau}{2} \right)}$ [13]. Therefore the ground state is not degenerate as there is only one possibility to realize it $n = 0$ and $\tau = -1$. This result explains the peculiar quantum Hall effect of graphene [14].

Summary. – We have shown that a generalized Peierls substitution including a Berry phase term must be considered for a correct semiclassical treatment of electrons in a magnetic field. This substitution is essential for the determination of the full semiclassical equations of motion, as well as for the semiclassical Bohr-Sommerfeld quantization condition for energy levels. Indeed, the substitution in the Bohr-Sommerfeld condition leads to an expression for the cross-sectional area which in some sort generalizes the formula found by Roth and Fal'kovskii in the context of Bloch electrons in a crystal. Application of this formula to Dirac electrons shows the subtle cancellation mechanism between the magnetic moment and the non-topological part of Berry's phase, which yields the Landau energy levels.

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The authors acknowledge fruitful discussions with F. Piéchon and J. N. Fuchs. We also thank L. A. Fal'kovskii for having drawn our attention to his own work on this subject.

REFERENCES

[1] Flynn W. G. and Littlejohn R. G., *Phys. Rev. Lett.*, **66** (1991) 2839; Littlejohn R. G. and Flynn W. G., *Phys. Rev. A*, **44** (1991) 5239.

[2] Gosselin P., Bérard A. and Mohrbach H., *Eur. Phys. J. B*, **58** (2007) 137.

[3] Gosselin P., Hanssen J. and Mohrbach H., *Phys. Rev. D*, **77** (2008) 085008; Gosselin P. and Mohrbach H., arXiv:0801.0940.

[4] Roth L. M., *Phys. Rev.*, **145** (1966) 434.

[5] Fal'kovskii L. A., *JETP*, **22** (1966) 423; *Usp. Fiz. Nauk*, **94** (1968) 1.

[6] Peierls R., *Z. Phys.*, **80** (1933) 763.

[7] Lifshitz E. M. and Pitaevskii L. P., *Statistical Physics*, Vol. **9** (Pergamon Press) 1981.

[8] Chang M. C. and Niu Q., *Phys. Rev. Lett.*, **75** (1995) 1348; *Phys. Rev. B*, **53** (1996) 7010; Sundaram G. and Niu Q., *Phys. Rev. B*, **59** (1999) 14915.

[9] Bliokh K. Y., *Europhys. Lett.*, **72** (2005) 7.

[10] Gosselin P., Ménas F., Bérard A. and Mohrbach H., *Europhys. Lett.*, **76** (2006) 651.

[11] Mikitik G. P. and Sharlai Yu. V., *Phys. Rev. Lett.*, **82** (1999) 2147.

[12] Berry M. V., *Proc. R. Soc. London, Ser. A*, **392** (1984) 45; Shapere A. and Wilczek F., *Geometric Phases in Physics* (World Scientific) 1989.

[13] Gosselin P., Bérard A., Mohrbach H. and Ghosh S., arXiv:0802.3565.

[14] Novoselov K. S. *et al.*, *Science*, **306** (2004) 666; Gusynin V. P., Sharapov S. G. and Carbotte J. P., *Int. J. Mod. Phys. B*, **21** (2007) 4611.