

Quantized Magnetic Susceptibility in (2 + 1)-Dimensional Gapless Semiconductors

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(Received 28 November 1990)

We argue that in a degenerate planar semiconductor, where the low-energy dynamics of electrons can be modeled by a relativistic Dirac theory, it is important to include the Zeeman interaction of the physical spin of the electron with magnetic fields. We show that including this interaction leads to a quantization of the high-field magnetic susceptibility.

PACS numbers: 72.15.Gd, 05.30.Fk, 11.30.Rd, 71.70.Ej

Level crossings of Dirac operators are responsible for axial anomalies¹ in gauge-field theories as well as several other phenomena. In this Letter we wish to point out a new effect due to level crossings of a particular Dirac operator which occur in strong external magnetic fields in 2+1 dimensions. We show that they lead to a steplike behavior of the high-field magnetic susceptibility and argue that they should be observable in the appropriate condensed-matter-physics systems.

We shall be concerned with gapless semiconductors in 2+1 dimensions. The distinct feature of gapless semiconductors is that the valence and conduction bands intersect in discrete points. When, as is often guaranteed by symmetry and charge neutrality, the chemical potential also lies at those energies, these materials have point Fermi surfaces.²

In general, near a degeneracy of two energy levels, the Hamiltonian describing the full theory may be approximated by an effective 2×2 Hamiltonian H_{eff} describing the states of the two-level subsystem. The spectrum of this Hamiltonian is linear. For example, for a gapless semiconductor the energy $\epsilon(k)$ of the electrons near a degeneracy is linear in the Bloch momentum \mathbf{k} :

$$\epsilon(k) = \hbar c_F |\mathbf{k}|, \quad (1)$$

with c_F the electron velocity describing the slope of the dispersion relation. A linear relation like (1) in the context of two-dimensional gapless semiconductors was first obtained in Ref. 3, where graphite, which is the prime example of such a system, was studied. The value of c_F in gapless semiconductors is typically of the order of 10^5 – 10^6 m/s, as in ordinary metals. The linear dispersion relation (1) has to be contrasted with the one in metals where the electron energy $\epsilon(k)$ depends quadratically on the Bloch momentum $\epsilon(k) \sim k^2$.

After appropriately shifting and rescaling the energy-momentum variables, the effective two-level Hamiltonian H_{eff} may be cast in the Dirac-like form

$$H_{\text{eff}} = i \hbar c_F \boldsymbol{\alpha} \cdot \nabla, \quad (2)$$

where $\boldsymbol{\alpha}$ are 2×2 Dirac matrices. (We note that the Dirac matrices here are not related to the physical spin

of the electron.)

There are several examples of two-dimensional tight-binding lattice systems where the low-energy electron spectrum is described by a massless Dirac Hamiltonian: the half-filled honeycomb (graphite) lattice^{3,4} and the half-filled square lattice with a background field of $\frac{1}{2}$ flux quantum per plaquette.⁵ The latter arises in, for example, the flux phase of the Heisenberg-Hubbard model.⁶ In these models it can be argued that at half filling and weak coupling the symmetries guarantee that the only relevant operators which contain the electron fields are precisely those which compose the massless Dirac Hamiltonian with an even number (2 or 4) of degenerate flavors of fermions.⁷ In these, as on all regular lattices, lattice doubling ensures that when the spectrum is relativistic there are an even number of degenerate species of fermions.⁸

Thus, in the general case there is more than one degeneracy point and the low-energy dynamics of a real gapless semiconductor is described by (2) with several degenerate species of electrons. A further potential source of degeneracy is the physical spin of the electron. We can imagine two scenarios. In the first, the spin degeneracy of the electron is split by interactions with the crystal lattice and (2) is an effective Hamiltonian for one of the spin degrees of freedom. In the second, the spin degeneracy is not split by such interactions, the spin operator commutes with the Hamiltonian, and there is a further doubling of the degrees of freedom in (2). It is the latter case which we shall consider in this Letter.

In actuality, this scenario can only be approximately true because spin degeneracy is always broken by electromagnetic interactions through the Zeeman coupling to magnetic photons. This is most evident in the situation where there is an external (three-dimensional) magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$. The effective Hamiltonian will, to a first approximation, simply be minimally coupled to the vector potential by the replacement $i \hbar \nabla \rightarrow i \hbar \nabla - (e/c_F) \mathbf{A}$, for both physical spin states. The next correction will involve a Zeeman term that describes the interaction of the electron's physical spin with the magnetic field. That is, the effective Hamiltonian describing a gapless

semiconductor becomes

$$H_{\text{eff},\sigma\tau,ab} = \delta_{\sigma\tau} \alpha_{ab} \cdot (i\hbar c_F \nabla - e\mathbf{A}) - 2g\mu_B s_{\sigma\tau} \cdot \mathbf{B} \delta_{ab}, \quad (3)$$

where the last term is the Zeeman interaction, with $2s_{\sigma\tau}$ the Pauli matrices describing the physical spin of the electrons; $\mu_B = e\hbar/2m$, with m the free-electron mass, is Bohr's magneton (in SI units), and g is the effective g factor which determines the strength of the Zeeman interaction. To our knowledge, no conclusive experimental value of this g factor near a degeneracy point of a two-dimensional gapless semiconductor is known. For narrow-gap semiconductors this factor is given by the ratio m/m^* , with m^* the effective electron mass; it is typically of the order 100 since the effective mass is usually small, $m^* \sim 0.01m$. We shall assume in the following that the g factor near a degeneracy is of this order. The essential results of this Letter are not sensitive to this particular choice of the g factor. In (3) σ, τ ($=\uparrow, \downarrow$) are spin indices and we also made explicit the Dirac indices a, b ($=1, 2$). If, as usual, there is further degeneracy, the Hamiltonian (2) should be multiplied by the unit matrix in the degenerate degrees of freedom. We stress that (3) describes the situation without doping, since we did not include a chemical potential to account for a finite density of electrons. Because of the special role played by the Zeeman term, this case will, nevertheless, prove to be nontrivial.

We note that the Zeeman interaction in (3) should not be confused with the interaction inherent in the 2×2 Hamiltonian (2) of the electron with external magnetic fields. The latter can be seen by considering the square of (2) in an external field, $H_{\text{eff}}^2 = -(\hbar c_F \nabla + ie\mathbf{A})^2 - ie\hbar c_F \alpha^1 \alpha^2 B_3$, where the last term resembles a Zeeman coupling and, if the Dirac Hamiltonian had a mass term, would yield an apparent Zeeman interaction in the low-energy "nonrelativistic" limit. Since the Dirac matrices here are not related to spin, it does not describe the interaction of the electron's physical spin with the external field.

The spacing between energy levels of the massless Dirac Hamiltonian in a magnetic field is proportional to $B^{1/2}$. Since the Zeeman term is linear in the field, this term in the Hamiltonian (3) will be enhanced for large fields. Consequently, when the magnetic field is increased, an increasing number of spin-up states cross from a positive-energy eigenvalue to a negative value, and vice versa for spin-down states. One, therefore, expects the magnetization to increase as a function of the magnetic field. In this Letter we point out that this is indeed the case. Moreover, we show that the magnetization makes discontinuous jumps at the values of B for which an energy level crosses zero, and that the high-field magnetic susceptibility is quantized.

The method we use to calculate the magnetization differs from the one usually employed in the context of

condensed-matter physics. For this reason, before considering the effect of the Zeeman interaction, let us illustrate the method for the standard (massless) Dirac Hamiltonian. The energy eigenvalues of this Hamiltonian in a magnetic field are the well-known Landau levels

$$\lambda_0 = 0, \quad (4)$$

$$\lambda_{\pm n} = \pm (2|eB|n\hbar c_F^2)^{1/2} \quad (n=1, 2, \dots).$$

In terms of these Landau levels, the ground-state energy E per unit (two-dimensional) volume and spin degree of freedom reads

$$E = -\frac{|eB|}{2\pi\hbar} \frac{1}{2} \sum_n |\lambda_n|, \quad (5)$$

where $|eB|/2\pi\hbar$ is the degeneracy per Landau level per unit volume. The sum in (5) may be evaluated by introducing the "proper-time" representation of the square root,^{9,10}

$$\sqrt{a} = -\int_0^\infty \frac{ds}{(\pi s)^{1/2}} \frac{d}{ds} \exp(-as). \quad (6)$$

After a partial integration and after subtracting the B -independent part, i.e., the free-particle contribution, one thus obtains for the ground-state energy

$$E = \frac{1}{8\pi^{3/2}} \int_0^\infty \frac{ds}{s^{3/2}} \left[\frac{|eB|}{\hbar} \coth(|eB|\hbar c_F^2 s) - \frac{1}{(\hbar c_F)^2 s} \right], \quad (7)$$

which should be compared with Schwinger's result in $3+1$ dimensions.¹¹ Using the expansion

$$\coth(x) - \frac{1}{x} = \sum_{n=1}^\infty \frac{2x}{(\pi n)^2 + x^2}, \quad (8)$$

and carrying out the proper-time integration, the ground-state energy (7) reduces to the well-known form¹² that can also be obtained by other methods,

$$E = \frac{1}{2\pi^2} \zeta\left(\frac{3}{2}\right) \frac{c_F}{\hbar^{1/2}} \left[\frac{|eB|}{2} \right]^{3/2}, \quad (9)$$

with $\zeta(z)$ the Riemann zeta function

$$\zeta(z) = \sum_{n=1}^\infty n^{-z}. \quad (10)$$

From (9) one easily derives the magnetization and the magnetic susceptibility.

In the theory described by the Hamiltonian (3) with \mathbf{B} chosen to point in some arbitrary direction, there are basically two separate subsystems. This is because to a first approximation the spins of the electrons align or antialign themselves with the magnetic field, so that besides the Dirac Hamiltonian also the Zeeman interaction term is diagonal in spin space. The states with spin up are, therefore, independent of the states with spin down, and

the ground-state energy E splits into two parts.

To facilitate the evaluation of E we note that the Zeeman term effectively acts as a chemical potential in the two subsystems. For the spin-up and -down states this chemical potential is respectively given by

$$\mu_{\uparrow} = g\mu_B B, \quad \mu_{\downarrow} = -g\mu_B B. \quad (11)$$

Without loss of generality, we take $g\mu_B B > 0$. At zero temperature, all states with energy less than the chemical potential are occupied. Since μ_{\uparrow} increases with increasing external field, it follows that at higher fields more and more spin-up states become occupied. For spin-down states, on the other hand, the number of occupied states decreases at higher fields, since μ_{\downarrow} decreases with increasing field. At this stage we also note the dual role played by the magnetic field in the present problem. It not only determines the degeneracy per Landau level, but it also determines which levels are occupied.

The first term in (3) couples only to the perpendicular component of the magnetic field $B \cos\theta$, where θ is the angle between the applied field and the normal of the plane in which the electrons are confined to move. On the other hand, the Zeeman term (at least in the isotropic approximation that we use here) couples to the full magnitude of the three-dimensional magnetic field.

The effect of introducing a chemical potential μ in general is simply to shift the energy eigenvalues $\lambda_n \rightarrow \lambda_n - \mu$. Consequently, in the presence of a chemical potential, expression (5) for the ground-state energy generalizes to

$$E = - \frac{|eB \cos\theta|}{2\pi\hbar} \frac{1}{2} \sum_n |\lambda_n - \mu|. \quad (12)$$

For the eigenvalues λ_n given by (4) with the substitution $B \rightarrow B \cos\theta$, the ground-state energy of the system under consideration is easily calculated to be

$$\begin{aligned} E &= - \frac{eB \cos\theta}{2\pi\hbar} \frac{1}{2} \left(|-\mu_{\uparrow}| + \sum_{|n|=1}^{\infty} |\lambda_n - \mu_{\uparrow}| + |-\mu_{\downarrow}| + \sum_{|n|=1}^{\infty} |\lambda_n - \mu_{\downarrow}| \right) \\ &= - \frac{eB \cos\theta}{\pi\hbar} \left[\sum_{n=n_0+1}^{\infty} (2ne\hbar c_F^2 \cos\theta B)^{1/2} + (n_0 + \frac{1}{2})g\mu_B B \right], \end{aligned} \quad (13)$$

with n_0 the integer

$$n_0 = (g\mu_B/e)^2 eB/2\hbar c_F^2 \cos\theta, \quad (14)$$

and where we have chosen $eB \cos\theta > 0$. The integer n_0 counts the number of Landau levels with spin up that become filled as the magnetic field increases from zero. For a given magnetic-field strength the value of n_0 can be varied by simply tilting the magnetic field relative to the plane. Because the chemical potentials μ_{\uparrow} and μ_{\downarrow} differ only by a minus sign, it follows that whenever a Landau level with spin up is filled, a level with opposite spin is emptied.

In the proper-time representation the ground-state energy (13) reads

$$E = \frac{eB \cos\theta}{\pi\hbar} \int_0^{\infty} \frac{ds}{(\pi s)^{1/2}} \frac{d}{ds} \left[\frac{\exp[-2(n_0+1)e\hbar c_F^2 \cos\theta Bs]}{1 - \exp(-2e\hbar c_F^2 \cos\theta Bs)} - \frac{1}{2e\hbar c_F^2 \cos\theta Bs} \right] - (n_0 + \frac{1}{2}) \frac{g\mu_B e B^2 \cos\theta}{\pi\hbar}, \quad (15)$$

where we again subtracted the free-particle contribution. Apart from a factor of 2 due to the spin degeneracy, the standard case without the Zeeman interaction is recovered by letting the coupling constant g go to zero, so that $n_0 = 0$. In spite of the complicated form of (15), one can see from (13) that the ground-state energy changes continuously whenever a Landau level is filled or emptied. Moreover, (15) shows that the n_0 levels that have been filled (spin-up states) and emptied (spin-down states) in the process of turning on the external field have a contribution which is proportional to B^2 , rather than $B^{3/2}$. This makes the magnetization discontinuous.

When $(g\mu_B/e)^2 eB/2\hbar c_F^2 \cos\theta$ is an integer, the magnetization M ,

$$M = - \frac{\partial E}{\partial B}, \quad (16)$$

is discontinuous. Away from these points it is given by

$$M = - \frac{3}{4} \frac{ec_F \cos\theta}{\pi} \left(\frac{eB \cos\theta}{\pi\hbar} \right)^{1/2} \int_0^{\infty} \frac{dx}{x^{1/2}} \frac{d}{dx} \left[e^{-2n_0 x} [\coth(x) - 1] - \frac{1}{x} \right] + 2(n_0 + \frac{1}{2}) \frac{g\mu_B B \cos\theta}{\pi\hbar}. \quad (17)$$

In Fig. 1 the magnetization is depicted as a function of the magnetic field for the case $\theta = \pi/4$, $g = 200$, $c_F = 10^5$ m/s. As already alluded to above, M increases as a function of B , due to the fact that for higher fields there is an excess of filled spin-up states over spin-down states. The discrete jumps in the magnetization arise from the presence of the integer n_0 (14) in the last term of expression (17) for the magnetization. They indicate the filling of the next Landau level.

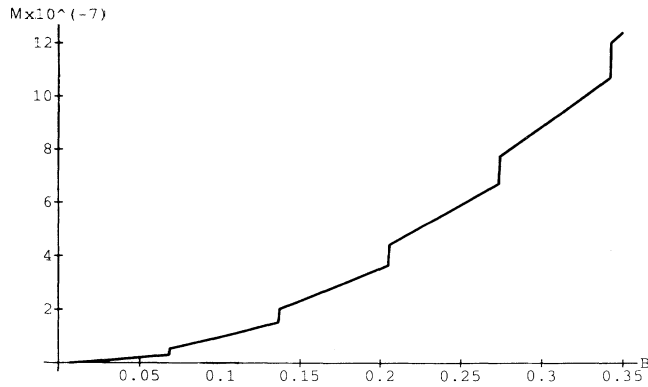


FIG. 1. Plot of the magnetization M (in A, remembering that we have two spatial dimensions) as a function of the magnetic field B (in T). The effective g factor is given the value $g=200$; for the electron velocity c_F at the degeneracy we took $c_F=10^5$ m/s, while the angle θ between the normal of the plane and the applied field is chosen to be $\theta=\pi/4$.

el with spin up and the emptying of the corresponding level with spin down.

The value of the magnetic field at which the first Landau levels with spin up (down) are filled (emptied) can be obtained from expression (14) for the integer n_0 . It follows that for n_0 to be of the order 1–10, a magnetic field of order

$$B \sim 10^{-6} (c_F/g)^2 \cos\theta \text{ T} \quad (18)$$

is needed. So, for $c_F \sim 10^5$ – 10^6 m/s and $g \sim 10^2$, we predict the first discrete jumps in the magnetization to occur at magnetic fields of the order of (1–100) $\cos\theta$ T. Hence, by tilting the magnetic field away from the normal of the plane, one easily brings these predictions into the realm of present-day laboratory conditions.

For large fields, the magnetic susceptibility

$$\chi = \frac{\partial M}{\partial B} \quad (19)$$

that follows from the magnetization (17) is given by

$$\chi = 2(n_0 + \frac{1}{2})(g\mu_B e/\pi\hbar)\cos\theta, \quad (20)$$

implying that the high-field magnetic susceptibility has a

steplike behavior (with singularities between the steps).

In closing we remark that in the undoped system under consideration there is no ordinary quantized Hall effect. The reason is that the Hall current in a massless Dirac theory is proportional to the sign of the chemical potential.¹³ Since the chemical potentials μ_\uparrow and μ_\downarrow differ by a minus sign, the contributions of the spin-up states cancel the contributions of the spin-down states, and the Hall current is zero. Whether an integer quantum Hall effect can be induced by doping and the electron-electron interaction is the subject of ongoing research.

This research was financially supported by the Natural Sciences and Engineering Research Council (NSERC) of Canada.

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