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The quantum Hall effect in graphene samples and the relativistic Dirac effective action

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Abstract

We study the Euclidean effective action per unit area and the charge density for a Dirac field in a two-dimensional (2D) spatial region, in the presence of a uniform magnetic field perpendicular to the 2D plane, at finite temperature and density. In the limit of zero temperature we reproduce, after performing an adequate Lorentz boost, the Hall conductivity measured for different kinds of graphene samples, depending upon the phase choice in the fermionic determinant.

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Graphene is a bidimensional array of carbon atoms, packed in a honeycomb crystal structure. Actually, each layer of a graphene sample can be viewed as either an individual plane extracted from graphite or else an array of unrolled carbon nanotubes. Stable mono-, bi- and multi-layer samples of such a material have been, recently and independently, obtained by two groups [1, 2], and a surprising behaviour of the Hall conductivity and related density of states in mono-layer samples has been unravelled. Even more recently, an equally unexpected, though different, behaviour was reported [3] for bi-layer samples.

The most remarkable feature of graphene’s structure, from the theoretical point of view, is that its quanta or quasi-particles behave as two species (to account for the spin of the elementary non-relativistic constituents) of massless relativistic Dirac particles in the two non-equivalent representations of the Clifford algebra (which correspond to the two non-equivalent vertices in the first Brillouin zone [4, 5]) with an effective ‘speed of light’ about two orders of magnitude smaller than c.

To the best of our knowledge, the first approach to the quantum Hall effect in terms of a quantum relativistic Dirac field theory, at finite temperature and chemical potential, appeared
in [6], where a dimensional reduction argument was used. Later on, the relativistic Hall conductivity was obtained in [7, 8] using Green's function methods (for an entirely different calculation see, e.g., [9]). In [6–8], the divergent series were regularized through definitions which, as we will explain, are equivalent to neglecting the phase of the determinant. In the zero temperature limit, the results of [6–8] reproduce the unexpected behaviour of both the Hall conductivity and the density of states, as measured in mono-layer graphene [1, 2].

In a couple of papers [10, 11], two of the authors of the present paper developed a finite temperature field theory calculation based upon the ζ-function regularization of the Dirac determinant, and obtained the partition function and the related Hall current and density of states. There, the phase of the determinant was included, and its sign fixed according to the conventional wisdom [12], which lead to a Hall conductivity displaying a plateau around zero chemical potential.

It is the aim of this paper to show that, in turn, the inclusion of the phase of the determinant with the opposite sign leads to a Hall conductivity and to a zero-temperature density of states which coincide with those recently reported in the case of bi-layer graphene [3], while the behaviour of mono-layer graphene is reproduced when the phase is ignored, in coincidence with the results in [6–8].

In order to study the temperature-dependent effects for the system at hand, we will consider the three-dimensional (3D) Euclidean space, with metric (+, +, +) and coordinates \((x, y, \tau = -it)\), the \(\gamma\)-matrices \(\gamma_i = \sigma_i, i = 1, 2, 3\), and introduce the chemical potential as an imaginary component of the gauge potential [13]. Then, we will let the Euclidean imaginary time coordinate vary according to \(0 \leq \tau \leq \beta\), where \(\beta = 1/k_BT\), \(k_B\) is the Boltzmann constant, and impose antiperiodic boundary conditions on the Dirac field to reproduce Fermi–Dirac statistics. As is well known, another faithful non-equivalent representation of the Clifford algebra exists in odd dimensions, in which one of the gamma matrices changes sign (or, equivalently, all of them do so). We will comment about the consequences of such a change of representation, wherever adequate, throughout the rest of the paper.

Once some suitable regularization has been introduced, the partition function in the grand-canonical ensemble is given by

\[
\ln Z = \ln \det(D) = \ln \det(i\partial_t + eA),
\]

where \(-e\) is the electron charge. In order to evaluate the partition function in the zeta regularization approach [14], we must determine the spectral resolution of the Euclidean Dirac operator, in the presence of a gauge potential \(A_\mu = (0, Bx, i\mu/e)\), which corresponds to the selection of a non-symmetric gauge for the magnetic field orthogonal to the plane; in the following \(B > 0\). Here below we just report the main results; for a detailed calculation, see e.g. [10, 11]. The equation to be solved is (from here on, natural units are used, i.e. \(\hbar = c = 1\), unless explicitly stated)

\[
[\sigma_1 i\partial_x + \sigma_2 (i\partial_y + eBx) + \sigma_3 (i\partial_\tau + i\mu) - \omega] \Psi = 0.
\]

After writing

\[
\Psi_{k,l}(x, y, \tau) = (2\pi\beta)^{-1/2} \exp[iky + i\tau \lambda_l] \psi_{k,l}(x),
\]

where

\[
\psi_{k,l}(x) = \begin{pmatrix} \varphi_{k,l}(x) \\ \chi_{k,l}(x) \end{pmatrix}, \quad k \in \mathbb{R},
\]

and

\[
\lambda_l = (2l + 1)(\pi/\beta), \quad l \in \mathbb{Z},
\]
in order to satisfy the antiperiodic boundary conditions, one finds two types of eigenvalues and corresponding sets of eigenfunctions.

Type [I]. Asymmetric part of the spectrum

$$\omega_l = -(2l + 1)\pi/\beta + i\mu, \quad l = -\infty, \ldots, \infty.$$  

The corresponding eigenfunctions are quite particular, in that they are eigenfunctions of $\sigma_3$ with the eigenvalue $+1$, the ones in the orthogonal subspace being indeed eliminated by the square-integrability condition (for some related references, see, for instance, [15]). As a consequence, the corresponding eigenvalues $\omega_l$ are not the square roots of the eigenvalues of $D^\dagger D$. They will eventually lead to a spectral asymmetry and, thereby, to a phase of the determinant, which will be studied in detail below.

Type [II]. Symmetric part of the spectrum

$$\omega_{l,n}^\pm = \pm \sqrt{\lambda_l^2 + 2neB}, \quad n = 1, \ldots, \infty, \quad l = -\infty, \ldots, \infty.$$  

For both kinds of eigenfunctions, the degeneracy per unit area is given by the well-known Landau factor $L_\mu = eB/2\pi$. It is worthwhile to remark that, had we chosen the other non-equivalent representation of the $\gamma$-matrices, the eigenvalues of type [I] would have changed their sign, and the corresponding eigenfunctions would have been eigenfunctions of $\sigma_3$ with the eigenvalue $-1$. However, as will be discussed below, this fact will not lead to any modification in our physical predictions as long as $\mu$ is real. Thus, considering the contributions of both non-equivalent representations will amount to an overall factor of 2.

When parity is defined as, e.g., in [16], it is easy to check that, for a general Dirac operator, the effect on the spectrum is $\omega^P = -\omega$. This symmetry is obviously respected by the symmetric part [II] of our spectrum, while it actually produces a change in the sign of the asymmetric portion [I]. When acting on the latter, it is equivalent to $\mu \rightarrow -\mu$ and, thus, to charge conjugation ($\psi(x) \rightarrow \gamma_2 \psi^*(x), A_\nu(x) \rightarrow -A_\nu^*(x), \omega \rightarrow \omega^C = \omega^*$). So, parity is broken already at the classical level if only one representation of the gamma matrices is considered, due to the square-integrability condition.

If complex values of $\mu$ are allowed, the whole spectrum has an interesting symmetry: it turns out to be invariant under $\mu\beta \rightarrow \mu\beta + 2\pi ik, k \in \mathbb{Z}$, which is nothing but the symmetry under ‘large’ gauge transformations. The conflict between this last symmetry and parity invariance in different regularization schemes is well known [17], and it created some controversy in the past [16, 18, 19].

In this paper, we will concentrate on the case of a real chemical potential $\mu$. A discussion of both symmetries in the case of a complex chemical potential will be reported elsewhere [20].

Starting from the above-described spectrum, we shall evaluate, according to (1), the Euclidean effective action per unit area (in the statistical mechanics terminology, the latter coincides with the grand-potential per unit area in units of $k_B T$). From this effective action, the mean fermionic number per unit area, $N_F$, and, thus, the charge density can be retrieved as follows:

$$S_{\text{eff}} = \log Z \equiv \ln \det(D), \quad N_F = \beta^{-1} \frac{\partial S_{\text{eff}}}{\partial \mu}. \quad (2)$$

Here, the symbol $\equiv$ stands for the definition through an adequate regularization. For the reasons we have just explained (namely, all the eigenvalues are paired), it turns out that the contribution to the effective action coming from the symmetric part [II] of the spectrum does
not suffer from regularization ambiguities. For instance, after a proper definition in terms of the $\zeta$-regularization [10], it is given by

$$S^{I\!I}_{\text{eff}} = \Delta_L \left[ \beta \zeta_R (1/2) (2eB)^{1/2} + \sum_{n=1}^{\infty} \log \left[ (1 + z e^{-\beta \nu_n}) (1 + z^{-1} e^{-\beta \nu_n}) \right] \right]$$

with $z := \exp[\beta \mu]$, $\nu_n \equiv \sqrt{2neB}$.

The contribution to the effective action arising from the asymmetric part [I] of the spectrum is given by the formal expression

$$S^I_{\text{eff}} = \Delta_L \sum_{l=0}^{\infty} \log \left[ (1 - 1)(2l + 1) \pi / \beta - i\mu \right] \times [(2l + 1) \pi / \beta + i\mu] .$$

Choosing a symmetric regularization, as done in [6-8], is equivalent to ignoring the infinite term $\sum_{l=0}^{\infty} \log(-1)$, which reduces the previous expression to

$$S^I_{\text{eff}} = \Delta_L \sum_{l=0}^{\infty} \log \left[ [(2l + 1) \pi / \beta]^2 + \mu^2 \right] ,$$

i.e. one evaluates the logarithm of the ‘absolute value’ of the Euclidean Dirac operator which, once regularized, leads to

$$S^I_{\text{eff}} = \Delta_L \log [2 \cosh(\mu \beta/2)].$$

However, a first-principle $\zeta$-function regularization of the determinant unavoidably drives to a careful definition of the phase of the determinant, which is equivalent to the selection of a cut in the complex plane of the eigenvalues [21], when the asymmetric part of the spectrum is treated. Going back to the formal relation (4), we define it in a proper mathematical sense in terms of the $\zeta$-function regularization, namely,

$$S^I_{\text{eff}} := - \Delta_L \frac{d}{ds} \left. \left\{ \sum_{l=0}^{\infty} \left[(2l + 1) \frac{\pi}{\beta} + i\mu \right]^{-s} + \sum_{l=0}^{\infty} \left[e^{i\pi}(2l + 1) \frac{\pi}{\beta} + i\mu \right]^{-s} \right\} \right|_{s=0} ,$$

the phase of the determinant being fixed by the cut in the complex plane of the eigenvalues [22]. More explicitly, we can write

$$S^I_{\text{eff}} := - \Delta_L \frac{d}{ds} \left. \left\{ \sum_{l=0}^{\infty} \left[(2l + 1) \frac{\pi}{\beta} + i\mu \right]^{-s} + \sum_{l=0}^{\infty} \left[e^{-i\theta}(2l + 1) \frac{\pi}{\beta} + i\mu e^{-i\theta} \right]^{-s} \right\} \right|_{s=0} ,$$

where $-\pi \leq \theta \leq \pi$. The prescription usually adopted [12] amounts to choosing the cut in such a way that the expression in the last square bracket never vanishes, as one goes continuously from the eigenvalues with a positive real part to the eigenvalues with a negative real part, i.e. $(2l + 1) \pi / \beta + \mu \sin \theta$ and $\mu \cos \theta$ do not simultaneously vanish (which could happen if $\mu = (2l + 1) \pi / \beta$ and $\theta = -\pi/2$ or $\mu = -(2l + 1) \pi / \beta$ and $\theta = \pi/2$). This requires that the cut is chosen below (above) the real axis when $\mu$ is positive (negative), which gives for the final value $\theta = \pi \text{sign} \mu$. With this choice, the contribution of the asymmetric part of the spectrum—see [10] for more details—to the effective action is given by

$$S^I_{\text{eff}} = \Delta_L \left[ - \frac{1}{2} \beta |\mu| + \log \left( 2 \cosh \frac{\mu \beta}{2} \right) \right] .$$

The opposite, and less popular, definition of the phase would lead to

$$S^I_{\text{eff}} = \Delta_L \left[ - \frac{1}{2} \beta |\mu| + \log \left( 2 \cosh \frac{\mu \beta}{2} \right) \right] .$$
At this point, it is important to stress (always in the case of a real chemical potential) that exactly the same results are obtained, provided the same criteria are applied, if the other non-equivalent representation for the $\gamma$-matrices is chosen. Thus, the inclusion of both contributions amounts to an overall factor of 2 if the phase is consistently chosen in both representations. In this sense, the exclusion of the phase is equivalent to the adoption of opposite criteria for the phase selection in both representations.

Putting together the contributions from the symmetric part (3) and the asymmetric part of the spectrum (5), (6) or (7), depending on the phase definition adopted, we come to the following expression for the $\zeta$-function definition of the Euclidean effective action:

$$S_{\text{eff}} = \Delta_L \left\{ \log \left( 2 \cosh \frac{\mu B}{2} \right) + \frac{1}{2} \kappa \beta |\mu| + \beta \zeta_R \left(-1/2\right) \sqrt{2eB} ight.$$ \n
$$+ \sum_{n=1}^{\infty} \log \left[(1 + z e^{-\beta \epsilon_n})(1 + z^{-1} e^{-\beta \epsilon_n})\right] \right\},$$

$\kappa = 0, \pm 1$, \quad $z = \exp[\beta \mu]$, \quad $\epsilon_n = \sqrt{2neB}$.

Here, $\kappa = 0$ corresponds to a vanishing phase, $\kappa = -1$ to the usual phase choice and $\kappa = +1$ to the opposite and unusual phase choice. Note that $\epsilon_n$ is the absolute value of the $n$th non-vanishing Landau level. In all cases, the Euclidean effective action is an even function of $\mu$.

Thus, it is invariant under charge conjugation and parity.

Also in all the cases, the mean fermionic number per unit area turns out to change sign under $\mu \to -\mu$. In fact, from its very definition in (2), we get

$$N(\kappa; \beta, \mu) = \Delta_L \left\{ \frac{1}{2} \tanh \frac{\mu B}{2} + \frac{1}{2} \kappa \sgn(\mu) \right.$$ \n
$$+ \sum_{n=1}^{\infty} \left[ 1 + e^{\beta \sqrt{2neB} - \mu B} \right]^{-1} - \sum_{n=1}^{\infty} \left[ 1 + e^{\beta \sqrt{2neB} + \mu B} \right]^{-1} \right\}.$$ 

Note that the first two terms are those coming from the asymmetric part of the spectrum. So no matter how one defines the phase of the determinant, at any finite temperature there is a kind of parity breaking charge, which is the sum of a $\mu$-analytic contribution (the first term) and a non-analytic one (the phase of the determinant). In the zero temperature limit, for $n < \mu^2/2eB < n+1$, we finally obtain

$$\lim_{\beta \to \infty} N(\kappa; \beta, \mu) = \left( n + \frac{1 + \kappa}{2} \right) \sgn(\mu) \Delta_L. \quad (8)$$

In this limit, the contribution of the asymmetric part of the spectrum is that corresponding to $n = 0$, and is non-analytic in all cases. It only vanishes so that parity and charge conjugation symmetries are indeed fulfilled, for the most commonly accepted selection of the phase $\kappa = -1$.

Moreover, it is easy to check that Nernst’s theorem holds true for any $\kappa$. Actually, it turns out that the entropy can be obtained from the well-known Boltzmann–von Neumann formula

$$S(\beta, \mu; B, \kappa) = k_B \left( 1 - \beta \frac{\partial}{\partial \beta} \right) S_{\text{eff}},$$

whence, one can verify by direct inspection that, indeed,

$$\lim_{\beta \to \infty} S(\beta, \mu; B, \kappa) = 0, \quad \forall \kappa = 0, \pm 1,$$

in agreement with Nernst’s theorem.
From (8), the mean value of the charge density in the zero temperature limit can be immediately obtained for one representation and one fermion species. Turning back to physical units, and recalling that the particle charge is $-e$, we find

$$ J_\tau (\kappa; \beta, \mu) = -\frac{eN_F(\kappa; \beta, \mu)}{\beta \to \infty} \frac{\text{sgn}(\mu)}{\beta} \mu_n + 1 + \kappa^2 \cdot \frac{e^2B}{hc} , $$

for $n < (\mu^2/2eBhc^2) < n + 1, n \in \mathbb{N}$,

the spatial components of the current density being equal to zero in the absence of electric fields.

Now, the zero temperature limit of the same vector in the presence of crossed homogeneous electric $E'$ and magnetic $B'$ fields can retrieved, for $E' < B'$, by performing a Lorentz boost with an absolute value of the velocity $v = cE'/B'$. Suppose, for definiteness, that the homogeneous electric field points towards the positive $Oy$-axis. Then the speed of the Lorentz boost must point towards the negative $Oy$-axis and the transformation law gives, as a result,

$$ J_0 (\kappa; \mu) = -\frac{e^2B'}{hc} \left( n + \frac{1 + \kappa}{2} \right) \text{sgn}(\mu), $$

$$ J_0 (\kappa; \mu) = -\frac{eE'}{h} \left( n + \frac{1 + \kappa}{2} \right) \text{sgn}(\mu), $$

$$ J_0 (\kappa; \mu) = 0, $$

for $n < (\mu^2/2eBhc^2) < n + 1, n \in \mathbb{N}$. As a consequence, the contribution to the quantized Hall conductivity at zero temperature becomes, for each representation and each fermion species,

$$ \sigma_{xy} = -\frac{e^2}{h} \left( n + \frac{1 + \kappa}{2} \right) \text{sign}(\mu), n \in \mathbb{N}. $$

As explained throughout the paper, this result must be multiplied by an overall factor of 4, in order to make contact with the relativistic effective theory associated with graphene [4, 5]. It is interesting to remark that the three values of the phase correspond to three different vacuum polarization (Casimir-type) effects due to the interaction with the magnetic field at zero temperature. More precisely, the quantum (in the field-theory sense) filling factor is given, in each of the three cases, by

$$ \nu_Q = -\frac{J_0 \cdot hc}{e^2B'} = \left( n + \frac{1 + \kappa}{2} \right). $$

(9)

The (rescaled) Hall conductivity is presented in figure 1, for the three values of $\kappa$, as a function of $\nu_c = \text{sgn}(\mu)\mu^2/2eBhc^2$, which is nothing but the classical density of carriers in the relativistic theory, divided by the total degeneracy of each Landau level.

It is well known that any regularization procedure is acceptable, unless either it manifestly violates some of the symmetries of the system or it is ruled out by the experimental data. So, the measured Hall conductivities of graphene as reported, for instance, in [3], should shed light on the relevance (or lack thereof) of the different phases of the determinant.

On these grounds, the first and clearer conclusion of this paper is that the behaviour of monolayer graphene, as presented not only in [3] but also in [1, 2], corresponds to $\kappa = 0$, i.e. to not including the phase of the determinant, as done in [6–8]. In fact, in this case the (rescaled) Hall conductivity shows a jump of height 1 for $\nu_c = 0$ and further jumps of the same magnitude for $\nu_c = \pm 1, \pm 2, \ldots$.

Let us now compare our predictions with the contents of [3], which is devoted to bilayer graphene. In this case, the (rescaled) Hall conductivity presents a jump of height 2 for $\nu_c = 0$ and further jumps of height 1. The main point here concerns the positions of these subsequent jumps. As a matter of fact, according to figure 1.b in the same reference, these
subsequent jumps appear for \( \nu_C = \pm 1, \pm 2, \ldots \), which is exactly the behaviour predicted, in our calculation, for \( \kappa = +1 \) (the less popular selection of phase in the Dirac determinant). However, the same reference interprets the Hall behaviour of bilayer graphene through a theoretical prediction first made in [23], where the theory is ‘almost’ non-relativistic, with a Landau spectrum given by \( E_n = \pm \frac{\varepsilon_B}{m} \sqrt{n(n - 1)} \). This last model does, indeed, predict a double jump for \( \nu_C = 0 \), due to the existence of two zero modes in each representation. But, for the very same reason, the next jump should appear, in this theoretical scenario, at \( \nu_C = \pm \sqrt{2} \sim \pm \frac{3}{2} \) (for a related discussion see, for instance, [24]). As stressed by the authors, figure 1.b in [3] is only schematic. However, the experimental results corresponding to \( B = 12T \) in figures 2.b and 2.c of the same reference also tend to confirm the prediction of our relativistic quantum field calculation, with \( \kappa = 1 \) (unusual phase), where the next jumps occurs at \( \nu_C = \pm 1 \). The text in the same reference also seems to confirm our prediction, since the distance between jumps is said to be, always for \( B = 12T \), \( \Delta n \sim 1.2 \times 10^{12} \text{ cm}^{-2} \), which corresponds to \( \Delta \nu_C = \Delta n \frac{h}{eB} \sim 1 \), the same for all jumps. However, the experimental results corresponding to \( B = 20T \) seem to agree with the width of the first plateau being approximately 1.3 times the width of the subsequent ones. Thus, a further experimental study of bilayer graphene is crucial in distinguishing both theoretical scenarios.

At this point, one can naturally wonder whether there is place at all for the usual selection of phase (\( \kappa = -1 \)) in the description of graphene samples. It is quite interesting to gather that the three non-equivalent phase selections correspond to the three non-equivalent unitary representations of the cyclic group \( C_3 \), which is precisely the relevant symmetry group for graphene. Even though the study of the Hall conductivity in graphene samples with three layers [25] is certainly far from being conclusive, they seem to indicate that a quantum Hall effect does occur in such devices, with a plateau at \( \nu_C = 0 \). Does the usual phase selection correspond to the behaviour of three-layered graphene?
In any case, from a theoretical point of view, further experiments on graphene samples can give an answer to a long-standing question in the field of the $\zeta$-function regularization, i.e. which phase must be selected in the definition of Dirac determinants, in order to evaluate effective actions?

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