Cyclotron motion in graphene

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**Abstract.** We investigate cyclotron motion in graphene monolayers considering both the full quantum dynamics and its semiclassical limit reached at high carrier energies. Effects of *zitterbewegung* due to the two dispersion branches of the spectrum dominate the irregular quantum motion at low energies and are obtained as a systematic correction to the semiclassical case. Recent experiments are shown to operate in the semiclassical regime.

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1. Introduction

The experimental discovery of graphene, i.e. single layers of graphite, has rapidly led to an extraordinary vast and still growing interest in this material, both experimental and theoretical [1]–[3]. Compared to conventional two-dimensional electronic systems, the peculiar properties of graphene mainly stem from its linear dispersion near the Fermi energy, and the chiral nature of electronic states entangling the momentum and sublattice degree of freedom [2, 3]. In particular, studies of carrier transport in perpendicular magnetic fields have revealed unusual features like a cyclotron mass being proportional to the square root of the particle density [4], and, most spectacular, a quantum Hall effect occurring at anomalous ('half-integer') filling factors [4]–[6]. Another partially related feature of graphene is its spectrum of Landau levels being non-equidistant in energy and proportional to the square root of the magnetic field, [4]–[9], properties also not shared by usual two-dimensional electron gases in semiconductor structures.

In this communication, we analyze the cyclotron motion in graphene considering both the full quantum dynamics as well as its semiclassical limit. The latter findings can directly be compared with the results of Shubnikov-de Haas measurements reported on in [4]. Most recently, cyclotron motion in graphene bilayers was also investigated experimentally [10]. We also comment on a recent preprint by Rusin and Zawadzki [11] studying cyclotron motion in graphene which appeared while the present work was reaching completion. These authors concentrate on the full quantum dynamics using a numerical approach analogous to very recent work [12] on two-dimensional electron gases in semiconductors, and they stress the role of zitterbewegung [13]–[26]. As we shall see below, signatures of zitterbewegung can also be seen in semiclassical corrections to the classical limit of the underlying quantum dynamics.

In the following section 2, we investigate the full quantum dynamics of the system using both a numerical and an analytical approach. The latter one is based on the analogy of the Hamiltonian to the Jaynes–Cummings model stemming from quantum optics. This analogy is the starting point for the analysis of the semiclassical limit to be discussed in section 3. There we also compare our results with the Shubnikov-de Haas experiments by Novoselov et al [4]. Section 4 contains our conclusions.

2. Quantum dynamics

For a graphene sheet in a perpendicular magnetic field, the single-particle states around one of the two inequivalent corners of the first Brillouin zone are described by [3]

\[ \mathcal{H} = v (\tau^i \pi_x \sigma^x + \pi_y \sigma^y), \]

with (using standard notation) \( \vec{\pi} = \vec{p} + e \vec{A} / c \) and \( v \approx 10^6 \text{ m s}^{-1} \). The Pauli matrices describe the sublattice or pseudospin degree of freedom, and the Zeeman coupling to the physical electron spin has been neglected. The label \( \tau^i = \pm 1 \) determines which corner of the Brillouin zone in considered; in what follows we shall concentrate on \( \tau^z = 1 \). The Heisenberg equations of motion read

\[ \frac{d}{dt} \vec{\pi}_H(t) = \frac{\hbar v}{\ell^2} \vec{\sigma}_H(t) \times \vec{e}_z, \]

\[ \frac{d}{dt} \vec{\sigma}_H(t) = \frac{2v}{\hbar} \vec{\pi}_H(t) \times \vec{\sigma}_H(t), \]
where $\ell = \sqrt{\hbar c / |eB|}$ and $(-e)B > 0$, is the magnetic length, and $\vec{e}_z$ is the unit vector along the $z$-direction. The magnetic field $\vec{B} = \nabla \times \vec{A} = B \vec{e}_z$ is assumed to point along the negative $z$-direction, $B < 0$. The position operator $\vec{r} = (x, y)$ can be given in terms of the kinetic momentum $\pi$ via the usual relations

$$x = x_0 + \frac{c}{eB} \pi_y, \quad (4)$$

$$y = y_0 - \frac{c}{eB} \pi_x, \quad (5)$$

where $\vec{r}_0 = (x_0, y_0)$ is conserved, $[H, \vec{r}_0] = 0$. For cyclotron motion in a usual non-interacting two-dimensional electron gas, the vector $\vec{r}_0$ describes the center of the classical circular orbits. As we shall see below, this is also the case for the classical limit of cyclotron motion in graphene.

Defining the usual bosonic operators

$$a = \frac{1}{\sqrt{2}} \frac{\ell}{\hbar} (\pi_x + i\pi_y), \quad a^* = (a)^*, \quad (6)$$

fulfilling $[a, a^*] = 1$ the Hamiltonian reads

$$H = \frac{\hbar v}{\ell} \sqrt{2} (a \sigma^- + a^\dagger \sigma^+), \quad (7)$$

where $\sigma^\pm = (\sigma_x \pm i\sigma_y)/2$. The energy scale of this Hamiltonian is given as a function of the magnetic field by

$$\frac{\hbar v}{\ell} \approx 26 \text{meV} \sqrt{\frac{B}{\text{Tesla}}}, \quad (8)$$

while its length scale is the usual magnetic length, $\ell = 257 \text{Å}/\sqrt{B/\text{Tesla}}$. The well-known eigenstates [3] of the Hamiltonian (7) are given by $|0, \uparrow\rangle$ with energy $\varepsilon_0 = 0$ and, for $n > 0$,

$$|n, \pm\rangle = \frac{1}{\sqrt{2}} (|n, \uparrow\rangle \pm |n - 1, \downarrow\rangle), \quad (9)$$

with energy $\varepsilon_n^\pm = \pm (\hbar v / \ell) \sqrt{2n}$. Here, $n$ is the Landau level index, and the arrows are obvious standard notation for the sublattice spin states.

2.1. Numerical approach

The operator-valued equations of motion (2) and (3) do not seem to allow for a full explicit solution. However, it is straightforward though somewhat tedious to numerically evaluate the time evolution of momentum, position, and spin operators. A similar approach was performed recently in [12] investigating cyclotron motion in semiconductor quantum wells with spin–orbit coupling. In fact, the present case of graphene is technically clearly simpler than the previous one and was also studied very recently in [11]. For such numerical simulation it is convenient to work in the Landau gauge $\vec{A} = (0, Bx, 0)$ with the initial state $|\psi\rangle$ being a direct product of an orbital and a spin state,

$$|\psi\rangle = |\phi\rangle \begin{pmatrix} \kappa \\ \lambda \end{pmatrix}, \quad (10)$$
where the spin or components are related to the usual polar angles $\vartheta$ and $\varphi$ of the initial pseudospin direction via $\kappa = \exp(-i\varphi/2)\cos(\vartheta/2)$ and $\lambda = \exp(i\varphi/2)\sin(\vartheta/2)$. As a generic initial orbital state we consider
\[
\langle \mathbf{r} | \phi \rangle = \frac{1}{\sqrt{\pi d}} e^{-\left(\mathbf{r}^2/2d^2\right) + ik_0 y},
\]
i.e. a normalized Gaussian wave packet of spatial width $d$ and initial momentum $\hbar k_0$ along the $y$-axis, i.e. the direction of translational invariance of the Hamiltonian. The initial position of the particle is at the origin, $\langle \mathbf{r} | \psi \rangle = 0$, and its energy is given by
\[
E = \langle \psi | H | \psi \rangle = \hbar v k_0 \frac{1}{\ell} (\kappa \lambda - \kappa^* \lambda^*),
\]
with a quantum mechanical uncertainty of
\[
(\Delta H)^2 = \langle \psi | H^2 | \psi \rangle - \langle \psi | H | \psi \rangle^2 = \left( \frac{\hbar v}{\ell} \right)^2 \left( \frac{\ell^2}{d^2} + \frac{d^2}{2\ell^2} - (|\kappa|^2 - |\lambda|^2) + k_0^2 \ell^2 (1 + (\kappa \lambda - \kappa^* \lambda^*)^2) \right).
\]
Note that the initial state \((10)\) has in general non-vanishing overlap with single-particle eigenstates of the form \((9)\) of both positive and negative energies. As to be discussed below, this fact leads to additional oscillations in the time evolution that can be viewed as zitterbewegung [11, 13, 14].

We emphasize that, by the very construction of the Hamiltonian \((1)\), the wavenumber $k_0$ is to be interpreted relatively to the wavevector of the chosen corner of the first Brillouin zone \([3]\). The authors of \([11]\), however, consider a time evolution of an initial state of the form \((10)\) under the simultaneous action of the Hamiltonians of both inequivalent corners of the Brillouin zone, a theoretical modeling whose physical meaning remains rather unclear. Moreover, these two Hamiltonians are assumed to differ just in a global sign, i.e. one Hamiltonian is the negative of the other, which is at odds with the microscopic tight-binding description of graphene \([3]\).

For an infinite sheet of graphene it is natural to consider initial conditions where both sublattices have the same quantum mechanical weight, $|\kappa| = |\lambda|$, i.e. the sublattice or pseudospin lies initially in its $xy$-plane. Figure 1 shows several examples for numerically evaluated trajectories $\langle \mathbf{r}_H(t) \rangle := \langle \psi | \mathbf{r}_H(t) | \psi \rangle$ with this type of initial condition. For all further details of these conceptually straightforward but technically somewhat involved numerical simulations we refer to \([11, 12]\). In the two top panels of figure 1 the sublattice spin is initially collinear with the momentum. These simulations can be compared with figure 5 of \([11]\) where the authors consider a time evolution under a single Hamiltonian (not two of them) given by equation \((1)\). Indeed, all results given in that figure are essentially reproduced by our own simulations underlying the present work.

The remaining panels of figure 1 contain simulations where the sublattice spin is in the initial state not collinear with the momentum. Note that the initial velocity $\langle \mathbf{\dot{r}}_H \rangle = \langle \mathbf{\dot{r}}_H \rangle$ is determined by the initial direction of the sublattice spin via
\[
\mathbf{\dot{v}} = \frac{i}{\hbar} \left[ \mathcal{H}, \mathbf{r} \right] = v \mathbf{\dot{\sigma}}.
\]
Moreover, further simulations show that there is no dynamics in the initial direction of the momentum, i.e. $\langle y_H(t) \rangle = 0$, if the sublattice spin is initially perpendicular to it, i.e. in the $xz$-plane. In such a case also no sublattice spin component collinear with the initial momentum...
Figure 1. Orbital dynamics of a wave packet of initial width $d = 1.0\ell$ and group wavenumber $k_0 = 1.0/\ell$. In all cases, the sublattice spin lies initially in the $xy$-plane, i.e. $\vartheta = \pi/2$ leading to $|\kappa| = |\lambda|$, and the total simulation time is always $50\ell/v$. In the left and right top panel, the sublattice spin is initially collinear with the momentum with $\varphi = \pi/2$ and $\varphi = 3\pi/2$, respectively. In the middle panels, we have $\varphi = \pi/4$ (left) and $\varphi = 5\pi/4$ (right) as initial conditions, while in the bottom panels $\varphi = 3\pi/4$ and $\varphi = 7\pi/4$ were used.

develops in the time evolution, $\langle \sigma^y_H(t) \rangle = 0$. These observations were partially already made in [11] and can be understood from the equations of motion (2), (3). In general, the trajectories seen in figure 1 are rather irregular which is a consequence of the many different excitation frequencies being present in the spectrum at low energies. In [11], contributions to the time evolution involving transition frequencies between states of positive and negative energy have been regarded as an effect of $zitterbewegung$. Indeed, as to be shown below, such type of $zitterbewegung$ also occurs as a correction to the classical limit.

As already mentioned in [11, 12] the numerical approach discussed above is technically limited to initial states having significant overlap with rather low Landau levels only, i.e. the
method is restricted to the regime dominated by quantum effects. In the following, we shall therefore explore the semiclassical limit using an analytical approach.

2.2. Analogy to the Jaynes–Cummings model

Further analytical progress regarding the full quantum dynamics can be made by exploiting the fact that the Hamiltonian (7) is formally equivalent to the Jaynes–Cummings model for atomic transitions in a radiation field. A similar observation has been made recently in [24] for the two-dimensional electron gas in semiconductor quantum wells with Rashba spin–orbit coupling. The Jaynes–Cummings model has been studied very intensively in theoretical quantum optics, and the time evolution of orbital and spin operators has been obtained in terms of analytical but rather implicit expressions [27, 28]. Using the method described in [27, 28] one can solve for the time-dependent position operators in the Heisenberg picture as

\[
x_H(t) + i y_H(t) = x_0 + i y_0 + \frac{i \ell e^{-i \kappa_0 t}}{\omega_- - \omega_+} \left( \omega_-(\kappa_x + i \kappa_y) \ell - 2 \frac{v}{\ell} \sigma^+ \right)
- \frac{i \ell e^{-i \kappa_0 t}}{\omega_- - \omega_+} \left( \omega_+(\kappa_x + i \kappa_y) \ell - 2 \frac{v}{\ell} \sigma^+ \right),
\]

with \(\vec{\kappa} = \vec{\pi}/\hbar\), and the operator-valued frequencies \(\omega_{\pm}\) are given by

\[
\hbar \omega_{\pm} = -\mathcal{H} \pm \sqrt{\mathcal{H}^2 + 2 \left( \frac{\hbar v}{\ell} \right)^2}.
\]

All operators on the rhs of equation (15) are in the Schrödinger picture, i.e. at time \(t = 0\). As in the case of the two-dimensional electron gas with Rashba spin–orbit coupling investigated previously [12, 24], the result (15) is still rather implicit and difficult to evaluate for a given initial state, mainly due to the operator character of the frequencies \(\omega_{\pm}\). However, as we shall see in next section, the above result provides a very natural access to the classical limit of the dynamics including semiclassical corrections.

3. Semiclassical limit

Cyclotron motion of massful electrons is in the simplest case just described as a kinetic (effective-)mass term, and the quantum mechanical and the classical equations of motion coincide, the latter ones being the obvious and well-defined classical limit of the former. However, the classical limit of the Hamiltonian (1) describing massless fermions appears prima vista not as obvious. In general, the classical limit of a quantum system is approached in the limit of high energies. For our problem here this means that the energy \(E = \langle \mathcal{H} \rangle\) of electron must be large compared to the characteristic energy scale \(\hbar v/\ell\) of the Hamiltonian, which is equivalent to the condition \(\langle \vec{\kappa} \cdot \vec{\sigma} \rangle \ell \gg 1\). In what follows, we shall assume an initial state of the form (10) with momentum and sublattice spin being parallel to each other. This leads to the condition

\[
k_0 \ell \gg 1.
\]

This very natural classical limit of the graphene model in a perpendicular magnetic field corresponds to the ‘strong-coupling scenario’ discussed in [26]. We note that a similar limit
is reached for negative energies of large modulus. Here, momentum and sublattice spin are initially antiparallel.

In the limit of large energies \( E \), the operator-valued frequencies \( \omega_{\pm} \) can be replaced with classical variables,

\[
\hbar \omega_{\pm} \mapsto -E \pm \sqrt{E^2 + 2 \left( \frac{\hbar v}{\ell} \right)^2}.
\]

Then, treating also the quantities \( \vec{r} \) and \( \vec{r}_0 \) as well as \( \vec{\kappa} \) and \( \vec{\sigma} \) as classical variables (not as operators) one derives from the full quantum result (15) in the above classical limit

\[
x(t) - x_0 = \frac{\ell}{\omega_- - \omega_+} \left[ \omega_-(\kappa_x \ell \sin(\omega_0 t) - \kappa_y \ell \cos(\omega_0 t)) \right.
\]
\[+ \frac{v}{\ell} (\sigma^x \sin(\omega_0 t) + \sigma^y \cos(\omega_0 t)) - \omega_+(\kappa_x \ell \sin(\omega_0 t) - \kappa_y \ell \cos(\omega_0 t)) \]
\[ - \frac{v}{\ell} (\sigma^x \sin(\omega_0 t) + \sigma^y \cos(\omega_0 t)) \biggr],
\]

\[
y(t) - y_0 = \frac{\ell}{\omega_- - \omega_+} \left[ \omega_-(\kappa_x \ell \cos(\omega_0 t) + \kappa_y \ell \sin(\omega_0 t)) \right.
\]
\[+ \frac{v}{\ell} (\sigma^x \cos(\omega_0 t) + \sigma^y \sin(\omega_0 t)) - \omega_+(\kappa_x \ell \cos(\omega_0 t) + \kappa_y \ell \sin(\omega_0 t)) \]
\[ + \frac{v}{\ell} (\sigma^x \cos(\omega_0 t) + \sigma^y \sin(\omega_0 t)) \biggr].
\]

Again the quantities \( \vec{\kappa} \) and \( \vec{\sigma} \) in the rectangular brackets on the rhs are at time \( t = 0 \). Moreover, in the classical limit \( E \gg \hbar v / \ell \) we have \( \hbar \omega_- \approx -2E \) and \( \hbar \omega_+ \approx (\hbar v / \ell)^2 / E \). It is instructive to rewrite the latter expression in the usual form of a cyclotron frequency \( \hbar \omega_+ =: \omega_c = |eB| / m_c c \).

Here, the cyclotron mass is given by the well-known semiclassical expression \([4, 29] m_c = (\hbar^2 / 2\pi) \partial S / \partial E = E / v^2 \), where \( S = \pi h k_0 \) is the area enclosed by a cyclotron orbit, and \( E = \hbar v k_0 \). Now, expanding the above expressions in first-order in \((\hbar v / \ell) / E \) one finds

\[
x(t) - x_0 = \kappa_x \ell^2 \sin(\omega_c t) - \kappa_y \ell^2 \cos(\omega_c t) + \frac{\hbar v}{E} (-\sigma^x \sin(\omega_c t) + \sigma^y \cos(\omega_c t))
\]
\[- \sigma^x \sin(2Et / \hbar) - \sigma^y \cos(2Et / \hbar)),
\]

\[
y(t) - y_0 = \kappa_x \ell^2 \cos(\omega_c t) + \kappa_y \ell^2 \sin(\omega_c t) - \frac{\hbar v}{E} (\sigma^x \cos(\omega_c t) + \sigma^y \sin(\omega_c t))
\]
\[- \sigma^x \cos(2Et / \hbar) + \sigma^y \sin(2Et / \hbar)).
\]

The first lines of the above rhs describe the classical cyclotron motion \([12, 29] \) with an energy-dependent cyclotron mass \([4] \). The other contribution are lowest-order semiclassical corrections to this classical limit. In particular, the terms in the last lines oscillate with the large frequency \( 2E / \hbar \gg \omega_c \) which equals the energy separation \( 2E = 2\hbar v k_0 \) between states of positive and negative energies at given wavevector in the absence of a magnetic field \([3] \). Therefore, these semiclassical correction can be viewed as an effect of zitterbewegung \([11, 13, 14] \). We note that
in connection with graphene the term ‘zitterbewegung’ was also used recently to express the fact that the velocity operator (14) fails to commute with the Hamiltonian (1) [30].

So far, we have concentrated on semiclassical dynamics at large positive energies $E \gg \hbar v/\ell$. In the analogous case of negative energies of large modulus one obtains a similar result with the frequencies $\omega_{\pm}$ being interchanged, $\omega_+ \approx 2|E|$ and $\omega_- \approx -\omega_c$.

Finally, we note the equivalence of the following three conditions:

$$E \gg \hbar \omega_c = \frac{(\hbar v/\ell)^2}{E},$$  \hspace{1cm} (23)

$$\Leftrightarrow E^2 = (\hbar v k_0)^2 \gg \left(\frac{\hbar v}{\ell}\right)^2,$$  \hspace{1cm} (24)

$$\Leftrightarrow (k_0 \ell)^2 \gg 1.$$  \hspace{1cm} (25)

Thus, the condition (23) is fulfilled whenever (17) is valid. On the other hand, the condition (17) can be rewritten as $r_c \gg \ell$ with $r_c = k_0 \ell^2$ being the classical cyclotron radius. This is indeed the usual textbook criterion for the validity of semiclassical approximations to cyclotron dynamics in solids [29] and confirms again our above strategy of obtaining the semiclassical limit.

Let us now compare our results with the Shubnikov-de Haas measurements by Novoselov et al [4]. The data presented in figure 2(a) of [4] were obtained at an electron density of $n \approx 4.3 \cdot 10^{12}$ cm$^{-2}$ and magnetic fields of up to about $B = 10$ T, corresponding to a Fermi wavevector of $k_f = \sqrt{\pi n} \approx 3.7 \cdot 10^6$ cm$^{-1}$ and a magnetic length of $\ell \gtrsim 81$ Å. Thus, $k_f \ell \gtrsim 3$, and the criterion (17) is still reasonably fulfilled even for the highest fields used in those measurements. Correspondingly, we have $(\hbar v/\ell)/E \lesssim 0.33$ with $E = \hbar v k_f$, showing that the semiclassical correction obtained in equations (21) and (22) are sufficiently suppressed which allows for an interpretation of the experimental data in purely classical terms. At higher magnetic fields, quantum effects dominate, and quantized Hall transport is observed [4]–[6].

4. Conclusions

We have investigated cyclotron motion in graphene monolayers considering both the full quantum dynamics and its semiclassical limit obtained for high carrier energies. At low energies, the quantum dynamics leads to rather irregular particle trajectories dominated by effects of zitterbewegung due to the two dispersion branches of the spectrum. The semiclassical limit of the system is obtained using the analogy of the Hamiltonian with the Jaynes–Cummings model [12, 24]. A similar analysis of the classical limit can be done for cyclotron motion in semiconductor quantum wells with spin–orbit interaction [12, 24]. The semiclassical limit of cyclotron dynamics in graphene is described by the usual cyclotron frequency and the characteristic frequency of zitterbewegung which occurs as a semiclassical correction. Recent experiments are shown to operate in the semiclassical regime.

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