Green’s function of electrons in monolayer and bilayer graphene in a magnetic field

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Received 14 November 2010, in final form 31 December 2010
Published 16 February 2011
Online at stacks.iop.org/JPhysA/44/105201

Abstract
Closed expressions for Green’s functions of the stationary two-dimensional two-component Schrödinger equation for an electron moving in monolayer and bilayer graphene, in the presence of a magnetic field, are obtained in terms of the Whittaker functions.

PACS numbers: 71.70.Di, 73.22.Pr

Sometime ago Dodonov et al [1] calculated the stationary Green’s function of a free 2D electron in a homogeneous magnetic field and obtained analytical results in terms of the Whittaker functions. Similar problems were recently investigated for low-dimensional systems [2–4], where Green’s functions were obtained as infinite sums of Laguerre polynomials. Recently, problems of propagators were analyzed theoretically for electrons in monolayer graphene [5, 6]. Horing and Liu [5] obtained a propagator as an infinite sum and, alternatively, as the second solution of the Bessel wave equation. A closed form of the propagator in monolayer graphene in terms of the confluent hypergeometric function was obtained by Piatkovskii and Gusynin [7]. To our knowledge, the expression for Green’s function in terms of the Whittaker functions has not been published in the literature. The problem of Green’s function for bilayer graphene in a magnetic field has not been analyzed earlier.

One should add here that a somewhat related problem was tackled many years ago by Schwinger [8] who considered Green’s function for a Dirac electron in a vacuum in external fields. However, the solution of this problem was found employing the proper-time formalism in which one can directly use the gauge-invariant fields rather than potentials. Also our problem is distinctly different since the Dirac electron is characterized by a rest mass \( m_0 \) and an energy gap \( 2m_0c^2 \), while the band structure of monolayer graphene has a vanishing ‘rest mass’ and a vanishing energy gap. In turn, in bilayer graphene there is no gap and the energy bands are parabolic.

The aim of this work is to derive an analytical closed form of the stationary electron Green’s function for electrons in monolayer and bilayer graphene in a uniform magnetic field.
The electron Green’s function is used in calculating the local density of states, scattering processes, transport and disorder properties of a material, as well as in many-body problems.

In the first step we consider the stationary Green’s function of a two-dimensional free electron in a magnetic field. The spin is omitted. The two-dimensional Hamiltonian is \( \hat{H}^e = \frac{\hat{p}^2}{2m} \), where \( \hat{p} = \hat{p} + eA \) and \( A \) is the vector potential. In the Landau gauge \( A = (-By, 0) \), the eigenstates of \( \hat{H}^e \) are \( \psi_{n\kappa,\mu}(\mathbf{r}) = e^{ik_x x} \phi_n(\xi)/\sqrt{2\pi} \), where \( \phi_n(\xi) = \sqrt{L} C_n H_n(\xi) e^{-\lambda/2\xi^2} \), \( H_n(\xi) \) are the Hermite polynomials, \( C_n = \sqrt{2n!\sqrt{\pi}} \), the magnetic radius is \( L = \sqrt{\hbar/eB} \) and \( \xi = y/L - k_xL \). The energy levels are \( E_n = \hbar\omega_c(n + 1/2) \) with \( \omega_c = eB/m \). Green’s function is by definition

\[
\tilde{G}_e(\rho, \rho', E) = \sum_n \int_{-\infty}^{\infty} \frac{e^{i\bar{\rho}(r_x-x')}\phi_n(\xi)\phi_n(\xi')^*}{2\pi|\hbar\omega_c(n + 1/2) - E|} \, dk_x,
\]

where \( \rho = (x, y) \). To integrate over \( k_x \) we use the identity [9]

\[
\int_{-\infty}^{\infty} e^{-x^2} H_0(x+y)H_0(x+z) \, dx = 2^\alpha \sqrt{\pi} m! z^n L_0^n(-2yz),
\]

where \( n' = n - m \) and \( m \leq n \). This gives

\[
\tilde{G}_e(\rho, \rho', E) = \frac{e^{-r^2/2|x'|}}{2\pi\hbar\omega_c L^2} \sum_{n=0}^{\infty} \frac{L^n_0(r^2)}{n + 1/2 - \tilde{E}},
\]

where \( \tilde{E} = E/\hbar\omega_c \), \( L^n_0(r^2) \) are the associated Laguerre polynomials, \( r^2 = (\rho - \rho')^2/(2L^2) \) and \( \chi = (x - x')(y + y')/2L^2 \) is the gauge-dependent phase factor. The summation over \( n \) in (3) can be performed with the use of formula (6.12.4) in [10]:

\[
t^{-\alpha} \sum_{n=0}^{\infty} \frac{L^n_0(t)}{n + a - \alpha} = \Gamma(a - \alpha)\Psi(a, a + 1; t),
\]

where \( \Psi(a, c; t) \) is the second solution of the confluent hypergeometric equation [10]. The series in (4) converges for \( t > 0 \) and \( \alpha > -1/2 \). There is (see formula (6.9.4) in [10])

\[
\Psi(a, c; t) = e^{t/2} t^{-1/2 - \mu} W_{a,\mu}(t),
\]

where \( W_{a,\mu}(t) \) is the Whittaker function, \( \kappa = c/2 - a \) and \( \mu = c/2 - 1/2 \). On combining equations (3), (4) and (5), setting \( a = 0, t = r^2 \) and \( \alpha = 1/2 - \tilde{E} \) we obtain: \( c = 1, \mu = 0 \) and \( \kappa = \tilde{E} \), so that the free electron Green’s function is

\[
\tilde{G}_e(\rho, \rho', E) = \frac{e^{ix}}{2\pi\hbar\omega_c L^2} \Gamma(1/2 - \tilde{E}) W_{1,0}(r^2).
\]

The same result was obtained by Dodonov et al [1] using the Laplace transform of the time-dependent electron Green’s function \( \tilde{G}_e(\rho, \rho'; \beta) \). Comparing (3) and (6) we have an important auxiliary result for free electrons employed in the following calculations:

\[
e^{-r^2/2} \sum_{n=0}^{\infty} \frac{L^n_0(r^2)}{n + 1/2 - \tilde{E}} = \frac{1}{|r|} \Gamma(1/2 - \tilde{E}) W_{1,0}(r^2).
\]

Now we turn to the main subject of our work. The Hamiltonian for electrons at the \( K \) point of the Brillouin zone in monolayer graphene in a magnetic field \( B \) is \( \hat{H}^M = u\hat{\sigma}_x\hat{\sigma}_z + u\hat{\sigma}_y \), where \( u \simeq 1 \times 10^8 \) cm s\(^{-1} \) is the band electron velocity and \( \hat{\sigma}_x, \hat{\sigma}_y \) are the Pauli matrices [11, 12]. In the Landau gauge, the eigenstates of \( \hat{H}^M \) are

\[
\psi_{nk,\mu}(\rho) = \frac{e^{ik_x x}}{\sqrt{2\pi(2 - \delta_{n,0})}} \left( -s\phi_{n-1}(\xi) \phi_n(\xi) \right),
\]
where \( s = \pm 1 \) and \( \phi_n(\xi) \) are defined above. The energy levels are \( E_{ns} = \hbar \omega \sqrt{n} \) with \( \omega = \sqrt{2} \hbar / L \).

The stationary Green’s function of the Hamiltonian \( \hat{H}^M \) is a 2 \times 2 matrix
\[
\hat{G}^M = \begin{pmatrix} \hat{G}_{00}^M & \hat{G}_{01}^M \\ \hat{G}_{10}^M & \hat{G}_{11}^M \end{pmatrix}
\]
where
\[
\hat{G}_{\sigma,\sigma}'(\rho, \rho', E) = \sum_{n,s} \int_{-\infty}^{\infty} \frac{e^{i k_0 (x-x') \rho} \phi_{n,-\sigma}(\xi) \phi_{n,\sigma}(\xi')^*}{2 \pi (2 - \delta_{\rho,0})(\hbar \omega \sqrt{n} - E)} \, dk_x,
\]
\[
\hat{G}_{\sigma,\sigma}^M(\rho, \rho', E) = \sum_{n,s} \int_{-\infty}^{\infty} \frac{e^{i k_0 (x-x') \rho} \phi_{n,-\sigma}(\xi) \phi_{n,\sigma}(\xi')^*}{4\pi (\hbar \omega \sqrt{n} - E)} \, dk_x,
\]
in which \( \sigma, \sigma' = 0, 1 \) and \( \sigma \neq \sigma' \). Performing the summation over \( s \) and integration over \( k_0 \) with the use of identity (2) we obtain
\[
\hat{G}_{00}^M(\rho, \rho', E) = \frac{\hbar \omega L^2}{2 \pi} \sum_{n=0}^{\infty} \frac{L_0^n(r^2)}{n + \sigma - E^2},
\]
\[
\hat{G}_{01}^M(\rho, \rho', E) = \frac{\hbar \omega L^2}{2 \pi} \sum_{n=1}^{\infty} \frac{L_1^n(r^2)}{n - E^2},
\]
where \( E = \hbar / (2 \hbar \omega), r_{10} = [(y-y') - i(x-x')]/(L \sqrt{2}) \) and \( r_{01} = [(y-y') - i(x-x')]/(L \sqrt{2}) \).

Now we make use of (7). Making the substitutions \( \hat{\xi} \to \hat{\xi} + 1/2 \) for \( \sigma = 0 \) and \( \hat{\xi} \to \hat{\xi} - 1/2 \) for \( \sigma = 1 \), the sum over \( n \) in (11) can be converted into the sum appearing in (7). Thus, the diagonal terms of \( \hat{G}^M(\rho, \rho', E) \) are
\[
\hat{G}_{00}^M(\rho, \rho', E) = \frac{\hbar \omega L^2}{2 \pi} \Gamma(-\hat{E}^2) W_{E^2 + \hat{E}^2}(r^2),
\]
\[
\hat{G}_{11}^M(\rho, \rho', E) = \frac{\hbar \omega L^2}{2 \pi} \Gamma(1 - \hat{E}^2) W_{E^2 - \hat{E}^2}(r^2).
\]

To calculate the off-diagonal elements of \( \hat{G}^M(\rho, \rho', E) \) we use the identity \( L_{n-1}^1(r^2) = n \left( L_n^0(r^2) - L_{n-1}^0(r^2) \right) / r^2 \). Putting it into (12) we obtain after simple calculation
\[
\hat{G}_{01,1-0}^M(\rho, \rho', E) = \frac{\hbar \omega L^2}{2 \pi} \frac{E^2}{r^2} \left( \hat{G}_{11}^M - \hat{G}_{00}^M \right).
\]

Equations (13)–(15) are the final results for the stationary Green’s function of an electron in monolayer graphene in the presence of a homogenous magnetic field. The poles of \( \hat{G}^M(\rho, \rho', E) \) occur for \( \hat{E}_{ns} = 0, \pm 1, \pm \sqrt{2}, \pm \sqrt{3}, \ldots, \pm \sqrt{n} \), which is a direct consequence of the above given Landau energies in monolayer graphene. The residues of \( \hat{G}^M(E_{ns}) \) can be obtained from (11) and (12).

In figure 1 we plot the gauge-independent part of the dimensionless Green’s function \( \hbar \omega L^2 \hat{G}^M_{0,0}(\rho, 0, E) \) for electrons in monolayer graphene in a magnetic field for three values of \( \hat{E} \). It is seen that for large \( \hat{E} \) Green’s function \( \hbar \omega L^2 \hat{G}^M(\rho, 0, E) \) decays exponentially. For large values of energy \( \hat{E} \) the decay has an oscillating character. As follows from (15), the off-diagonal components are given by the difference of \( \hat{G}_{11}^M \) and \( \hat{G}_{00}^M \).

Expressing Green’s function in terms of the Whittaker functions is useful because the latter can be either calculated using, for example, procedures given in Mathematica or conveniently computed from the formula
\[
W_{s,0}(z) = \sqrt{\frac{z}{2}} e^{-z/2} \Gamma(1/2 - \lambda) \sum_{k=0}^{\infty} \frac{\Gamma(k - \lambda + 1/2)}{(k!)^2} z^k [2 \psi(k + 1) - \psi(k - \lambda + 1/2) - \ln(z)],
\]
where \( \lambda = \frac{1}{2}(s + 1) \) and \( \psi(x) \) is the digamma function.
Figure 1. Diagonal elements of the gauge-independent part of the dimensionless Green’s function \[ \bar{h}\omega L^2 \hat{G}_{00}(\rho, 0, E) \] for monolayer graphene, as given in (13) and (14) for three values of \[ \bar{E} = E/(\bar{h}\omega) \]. Distance is measured in \[ r = \sqrt{x^2 + y^2}/(\sqrt{2}L) \]. All curves are calculated with the use of expansion (16).

where \( \psi(z) = d \ln[\Gamma(z)]/dz \), see [9]. This expansion can be obtained from the Barnes integral representation of the Whittaker function \( W_{\bar{E},0}(z) \) through the calculation of residues. In this formula, the index \( k \) labels the residues. The details of the expansion can be found e.g. in [14]. Other convenient ways to calculate the Whittaker functions are: expansion of \( W_{\bar{E},0}(x) \) in terms of the Bessel functions [15], combinations of power-series expansions for small-\( x \) and large-\( x \) approximations (see [1, 9]), or numerical solutions of the Whittaker equation.

We have compared numerically (13), (14) and (15) with (11) and (12) for many random values of \( 0 < \bar{E} < 3 \) and \( 0 < r < 3 \), in which \( W_{\lambda,0}(z) \) was calculated using expansion (16). In addition, numerical values of \( W_{\lambda,0}(z) \) were calculated using the procedures given in Mathematica. After truncating the summations in (11) and (12) at \( n = 1 \times 10^6 \) terms (!) we obtained only four to six significant digits of the exact results given in terms of the Whittaker functions. We conclude that expansion (7) of Green’s function in terms of the Laguerre polynomials converges quite slowly.

Next, we consider electrons in bilayer graphene. At the \( K \) point of the Brillouin zone, they are described by the Hamiltonian \[ \hat{H}^B = -1/(2m^*)(0 0 \hat{\pi}_x \hat{\pi}_y (\hat{\pi}_x^2 \hat{\pi}_y^2)), \] with \( m^* = 0.054 m_e \) and \( \hat{\pi}_x = \hat{\pi}_x \pm i\hat{\pi}_y \) [13]. This Hamiltonian is applicable within the energy range \( |E| < 100 \text{ meV} \).

To find Green’s function in this case we proceed in a way similar to that described above for monolayer graphene. In the Landau gauge, the eigenstates of \( \hat{H}^B \) are

\[
\psi^B_{nk,s}(\rho) = \frac{e^{ik_s x}}{\sqrt{4\pi}} \left( -s \phi_{n-2}(\xi) \phi_0(\xi) \right),
\]

where \( s = \pm 1 \) and \( \phi_0(\xi) \) are defined above. The energy levels are \( E_n = \hbar\omega_c \sqrt{n(n-1)} \) with \( \omega_c = eB/m^* \). The above expressions are valid for \( n \geq 2 \). For \( n = 0, 1 \), the eigenstates of \( \hat{H}^B \) are \( \psi^B_{nk,0}(\rho) = e^{ik_s x}/\sqrt{2\pi} (\phi_0(\xi)) \) and the corresponding energies are \( E_n = 0 \).
The stationary Green’s function of the Hamiltonian $\hat{H}^B$ is again a $2 \times 2$ matrix

\[ \hat{G}^B = \begin{pmatrix} \hat{G}^B_{00} & \hat{G}^B_{01} \\ \hat{G}^B_{10} & \hat{G}^B_{11} \end{pmatrix} \]

with

\[ G^B_{\sigma\sigma}(p, p', E) = \sum_{n,s} \int_{-\infty}^{\infty} \frac{e^{ik_x(x-x')} \phi_{n-\sigma}(\xi) \phi_{n-\sigma}(\xi')^*}{4\pi(\hbar\omega_c \sqrt{n(n+1)} - E)} \, dk_x, \]

\[ G^B_{\sigma',\sigma}(p, p', E) = \sum_{n,s} \int_{-\infty}^{\infty} \frac{\sum_{\sigma} \phi_{n-\sigma}(\xi) \phi_{n-\sigma}(\xi')^*}{4\pi(\hbar\omega_c \sqrt{n(n+1)} - E)} \, dk_x, \]

where $\sigma, \sigma' = 0, 2$ and $\sigma \neq \sigma'$. Performing the summation over $s$ and integration over $k_x$ with the use of identity (2) we obtain

\[ \hat{G}^B_{\sigma\sigma}(p, p', E) = \frac{\hat{E}e^{-r^2/4\hat{E}}}{2\pi\hbar\omega_c L^2} \sum_{n=0}^{\infty} \frac{L_n^0(r^2)}{(n+\sigma)(n+\sigma-1) - \hat{E}}, \]

\[ \hat{G}^B_{\sigma,\sigma'}(p, p', E) = r_{\sigma,\sigma'} \frac{e^{-r^2/4\hat{E}}}{2\pi\hbar\omega_c L^2} \sum_{n=2}^{\infty} \frac{L_n^2(r^2)}{n(n-1) - \hat{E}}, \]

where $\hat{E} = E/(\hbar\omega_c)$, $r_{2,0} = [(y' - y) - i(x - x')]^2/(2L^2)$ and $r_{0,2} = [(y - y') - i(x - x')]^2/(2L^2)$. To calculate $\hat{G}^B_{\sigma\sigma}$, we use the combination of simple fractions $\sum_{i} a_i/(n-n_i)$ with suitably chosen parameters $\{a_i\}$ and $\{n_i\}$. Thus we have

\[ \frac{1}{(n+\sigma)(n+\sigma-1) - \hat{E}} = \frac{n^+_{\sigma}}{n^+_{\sigma} - n^-_{\sigma}} \left( \frac{1}{n+1/2-n^+_{\sigma}} - \frac{1}{n+1/2-n^-_{\sigma}} \right), \]

with

\[ n^\pm_{\sigma} = 1 - \sigma \pm (1/2)\sqrt{1+4\hat{E}^2}. \]

Using (7) and (22) and making the substitution $\hat{E} \rightarrow n^\pm_{\sigma}$ we obtain

\[ \hat{G}^B_{\sigma\sigma}(p, p', E) = \frac{\hat{E}e^{i\hat{E}}}{2\pi\hbar\omega_c L^2}\sqrt{1+4\hat{E}^2} \times \left( \Gamma(1/2-n^+_{\sigma})W_{n^+_{\sigma},0}(r^2) - \Gamma(1/2-n^-_{\sigma})W_{n^-_{\sigma},0}(r^2) \right). \]

For the off-diagonal elements of $\hat{G}^B$ we express the associated Laguerre polynomials $L_n^2(r^2)$ by the linear combinations of $L_n^0(r^2)$ using the identity $sL_n^{s+1}(x) = (n + a + 1)L_n^a(x) - (n + 1)L_{n+1}^a(x)$. This gives, in analogy to (15),

\[ \hat{G}^B_{\sigma,\sigma'}(p, p', E) = \frac{r_{\sigma,\sigma'} \hat{E}}{r^4} (\hat{G}^B_{00} + \hat{G}^B_{01} - 2\hat{G}^B_{11}). \]

Equations (24) and (25) are the final results for the stationary Green’s function of an electron in bilayer graphene in the presence of a magnetic field. The poles of $\hat{G}^B(p, p', E)$ occur for $E_{ns} = 0, \pm\sqrt{2}, \pm\sqrt{6}, \ldots, \pm\sqrt{n(n-1)}$. The residues of $\hat{G}^B(E_{ns})$ can be obtained from (20) and (21).

In figure 2 we plot the gauge-independent part of the dimensionless Green’s function $\hbar\omega_c L^2 \hat{G}_{\sigma\sigma}(p, 0, E)$, calculated for three values of $\hat{E}$. Similarly to electrons in monolayer graphene, the components of Green’s function $\hbar\omega_c L^2 \hat{G}^B(p, 0, E)$ decay exponentially for large $r$. For higher values of $\hat{E} = E/(\hbar\omega_c)$ they exhibit an oscillatory behavior.
Finally, we write Green’s functions of monolayer and bilayer graphene taking into account contributions from the inequivalent $K'$ point of the Brillouin zone. For monolayer graphene the Hamiltonian at the $K'$ point is $\hat{H}^M = (-\hat{H}^M)^T$ and its eigenstates are $\psi^M_{nk}(\rho) = e^{ik_x x} [\phi_n(\xi), s\phi_n^{-1}(\xi)]/\sqrt{4\pi}$ [16]. In the basis $\{-s\phi_{n-1}^K, \phi_n^K, \phi_{n'}^K, s\phi_{n-1}^{K'}\}$, where the superscripts indicate the Brillouin zone point, Green’s function is

$$\hat{G}^M = \begin{pmatrix} \hat{G}^M_{11} & -\hat{G}^M_{10} & 0 & 0 \\ -\hat{G}^M_{01} & \hat{G}^M_{00} & 0 & 0 \\ 0 & 0 & \hat{G}^M_{00} & \hat{G}^M_{01} \\ 0 & 0 & \hat{G}^M_{10} & \hat{G}^M_{11} \end{pmatrix}. \quad (26)$$

For bilayer graphene at the $K'$ point the wavefunction is $\psi^B_{nk}(\rho) = e^{ik_x x} [\phi_n(\xi), -s\phi_{n-1}(\xi)]/\sqrt{4\pi}$ [13]. Thus, Green’s function of bilayer graphene in the basis $\{-s\phi_{n-2}^K, \phi_n^K, \phi_{n'}^K, -s\phi_{n-2}^{K'}\}$ is

$$\hat{G}^B = \begin{pmatrix} \hat{G}^B_{22} & -\hat{G}^B_{20} & 0 & 0 \\ -\hat{G}^B_{02} & \hat{G}^B_{00} & 0 & 0 \\ 0 & 0 & \hat{G}^B_{00} & -\hat{G}^B_{02} \\ 0 & 0 & -\hat{G}^B_{20} & \hat{G}^B_{22} \end{pmatrix}. \quad (27)$$

To summarize, we calculated Green’s functions for electrons in monolayer and bilayer graphene in the presence of a magnetic field and expressed them in terms of the Whittaker functions. The obtained formulas allow one to compute Green’s functions using quickly converging expansions of the Whittaker functions. This is a good starting point in more complicated calculations for monolayer and bilayer graphene.
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