Green's functions for a graphene sheet and quantum dot in a normal magnetic field

2009 J. Phys. A: Math. Theor. 42 225301

(http://iopscience.iop.org/1751-8121/42/22/225301)

IOP PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **42** (2009) 225301 (9pp) doi:10.1088/1751-8113/42/22/225301

Green's functions for a graphene sheet and quantum dot in a normal magnetic field

Norman J Morgenstern Horing[1] **and S Y Liu**[2]

[1] Department of Physics and Engineering Physics, Stevens Institute of Technology, Hoboken, NJ 07030, USA
[2] Department of Physics, Shanghai Jiaotong University, 1954 Huashan Road, Shanghai 200030, People's Republic of China

Received 20 February 2009, in final form 7 April 2009
Published 8 May 2009
Online at stacks.iop.org/JPhysA/42/225301

Abstract
This paper is concerned with the derivation of the retarded Green's function for a two-dimensional graphene layer in a perpendicular magnetic field in two explicit, analytic forms, which we employ in obtaining a closed-form solution for the Green's function of a tightly confined magnetized graphene quantum dot. The dot is represented by a $\delta^{(2)}(\mathbf{r})$-potential well and the system is subject to Landau quantization in the normal magnetic field.

PACS numbers: 73.22.−f, 73.20.−r, 73.21.−b, 75.20.−g

1. Introduction

Over the past few years graphene, a single-atom-thick two-dimensional planar layer of carbon atoms in a hexagonal honeycomb lattice, has been found to have remarkable device-friendly properties [1, 2]. With mobility reaching 200 000 $\mathrm{cm}^2\,\mathrm{V}^{-1}\,\mathrm{s}^{-1}$, high electron density on the order of $10^{13}\,\mathrm{cm}^{-2}$, long mean free path $l \sim 400$ nm, stability up to 3000 K and a quantum hall effect at room temperature, it holds great promise for nanoelectronic applications. Such applications include sensors, field-effect transistors, spin valves, electromechanical resonators, quantum interference devices and others. Furthermore, as a planar layer of carbon atoms, it is amenable to highly developed top-down CMOS compatible process flows, a substantial advantage over carbon nanotubes.

The band structure of graphene gives rise to an electron/hole energy spectrum in the nature of a massless relativistic 'Dirac' dispersion law, with individual particle energies proportional to momentum, $\mathbf{p} = (p_x, p_y)$, at two inequivalent zero-gap points of the first Brillouin zone where the electron and hole bands touch ('Dirac' nodes, K and K'). The corresponding Hamiltonian is given by ($\hbar \to 1$ throughout)

$$H = \gamma \boldsymbol{\sigma}_v \cdot \mathbf{p}, \tag{1}$$

where $\boldsymbol{\sigma}_\nu = [\sigma_x, (\mathrm{sign}(\nu))\sigma_y]$ and σ_x, σ_y are Pauli spin matrices, associated with a 'pseudo-spin' in the two-dimensional space of the electron and hole bands; also $\mathrm{sign}(\nu) = 1$ or -1 for $\nu = K$ or K' and $\gamma = 3\alpha d/2$ (α is the hopping parameter in the tight binding approximation and d is the lattice spacing) plays the role of a constant Fermi velocity independent of density. The Green's function matrix of the infinite 2D graphene sheet, G, in this 2D pseudo-spin representation, is determined by the equation

$$\left(\mathrm{i}\frac{\partial}{\partial t} - H\right) G(\mathbf{r}, \mathbf{r}'; t, t') = I\delta^{(2)}(\mathbf{r} - \mathbf{r}')\delta(t - t') \tag{2}$$

(I is the 2×2 unit matrix).

To incorporate the magnetic field, $\mathbf{B}$, (taken normal to the graphene plane), we make the usual replacement $\mathbf{p} \to \mathbf{p} - e\mathbf{A}$, where $\mathbf{A} = \frac{1}{2}\mathbf{B} \times \mathbf{r}$ for a uniform, constant magnetic field. The requirement of gauge invariance (discussed in the appendix) leads to

$$G(\mathbf{r}, \mathbf{r}'; t, t') = C(\mathbf{r}, \mathbf{r}')G'(\mathbf{r} - \mathbf{r}'; t - t'), \tag{3}$$

where the factor $G'(\mathbf{r} - \mathbf{r}'; t - t')$ is spatially translationally invariant and gauge invariant, satisfying the equation ($\mathbf{R} = \mathbf{r} - \mathbf{r}'$, $T = t - t', \hbar \to 1$)

$$\left(\mathrm{i}\frac{\partial}{\partial T} - \gamma\boldsymbol{\sigma}_\nu \cdot \left[\frac{1}{i}\frac{\boldsymbol{\partial}}{\partial \mathbf{R}} - \frac{e}{2}\mathbf{B} \times \mathbf{R}\right]\right) G'(\mathbf{R}, T) = I\delta^{(2)}(\mathbf{R})\delta(T), \tag{4}$$

while the factor $C(\mathbf{r}, \mathbf{r}')$ embodies all non-spatially-translationally-invariant structure and all gauge dependence as

$$C(\mathbf{r}, \mathbf{r}') = \exp\left[\frac{\mathrm{i}e}{2\hbar c}\mathbf{r} \cdot \mathbf{B} \times \mathbf{r}' - \phi(\mathbf{r}) + \phi(\mathbf{r}')\right] \tag{5}$$

($\phi(\mathbf{r})$ is an arbitrary gauge function).

2. Landau quantization and the graphene Green's function

2.1. Expansion in Laguerre polynomials

The role of Landau quantization in graphene electron dynamics is embedded in the solution of equation (4) for $G'(\mathbf{R}, T)$, which may be written in ω-frequency representation as (define $\gamma_\nu = \gamma\,\mathrm{sign}(\nu)$; also $\hbar \to 1$ and $c \to 1$)

$$[\omega - \gamma\sigma_x\Pi_{XY} - \gamma_\nu\sigma_y\Pi_{YX}]G'(\mathbf{R}, \omega) = I\delta(X)\delta(Y), \tag{6}$$

where we have defined

$$\Pi_{XY} \equiv \frac{1}{i}\frac{\partial}{\partial X} + \frac{eB}{2}Y \qquad \text{and} \qquad \Pi_{YX} \equiv \frac{1}{i}\frac{\partial}{\partial Y} - \frac{eB}{2}X. \tag{7}$$

The elements of the matrix equation, equation (6), are given by

$$\omega G'_{11} - [\gamma\Pi_{XY} - \mathrm{i}\gamma_\nu\Pi_{YX}]G'_{21} = \delta(X)\delta(Y), \tag{8}$$

$$\omega G'_{21} = [\gamma\Pi_{XY} + \mathrm{i}\gamma_\nu\Pi_{YX}]G'_{11} \tag{9}$$

and

$$\omega G'_{22} - [\gamma\Pi_{XY} + \mathrm{i}\gamma_\nu\Pi_{YX}]G'_{12} = \delta(X)\delta(Y), \tag{10}$$

$$\omega G'_{12} = [\gamma\Pi_{XY} - \mathrm{i}\gamma_\nu\Pi_{YX}]G'_{22}. \tag{11}$$

Equations (8) and (9) yield

$$\left[\omega - \frac{1}{\omega}\left\{\gamma^2\left(\Pi_{XY}^2 + \Pi_{YX}^2\right) + \mathrm{i}\gamma\gamma_v(\Pi_{XY}\Pi_{YX} - \Pi_{YX}\Pi_{XY})\right\}\right] G'_{11}(X, Y; \omega) = \delta(X)\delta(Y). \tag{12}$$

It is readily verified that

$$\Pi_{XY}\Pi_{YX} - \Pi_{YX}\Pi_{XY} \equiv -\frac{1}{i}eB, \tag{13}$$

whence, using equation (7) to evaluate Π_{XY}^2 and Π_{YX}^2, we obtain

$$\begin{aligned}\left[\omega + \frac{\gamma\gamma_v}{\omega}(eB)\right] G'_{11}(X, Y; \omega) + \frac{\gamma^2}{\omega}\Bigg\{&\frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial Y^2} \\ &- \left(\frac{eB}{2}\right)^2 [X^2 + Y^2] + \frac{eB}{i}\left(X\frac{\partial}{\partial Y} - Y\frac{\partial}{\partial X}\right)\Bigg\} G'_{11}(X, Y; \omega) \\ &= \delta(X)\delta(Y).\end{aligned} \tag{14}$$

Defining the operator

$$L_Z = \frac{1}{i}\left(X\frac{\partial}{\partial Y} - Y\frac{\partial}{\partial X}\right) = L_z + L_{z'} \tag{15}$$

(L_z is the angular momentum operator) a considerable simplification may be achieved by noting that $L_Z G'(\mathbf{R}, T) = 0$. This may be shown most easily by choosing the gauge $\phi = 0$, for then $L_Z G'(\mathbf{R}, T) = C^{-1}(\mathbf{x}, \mathbf{x}')L_Z G(\mathbf{x}, t; \mathbf{x}', t')$ by virtue of the fact that $L_Z C(\mathbf{x}, \mathbf{x}') = 0$. The vanishing of

$$L_Z G(\mathbf{x}, t; \mathbf{x}', t') = (L_z + L_{z'})G(\mathbf{x}, t; \mathbf{x}', t')$$

may be argued from the bilinear dependence of $G(\mathbf{x}, t; \mathbf{x}', t')$ on the field operators, $\psi(\mathbf{x}, t)$, $\psi^+(\mathbf{x}', t')$, and the concomitant interpretation of $G(\mathbf{x}, t; \mathbf{x}', t')$ in terms of the creation of a particle at $(\mathbf{x}, t)$ which is subsequently annihilated at $(\mathbf{x}', t')$. The action of L_z on $G(\mathbf{x}, t; \mathbf{x}', t')$ may be regarded as measuring the component of orbital angular momentum in the direction of the magnetic field associated with the particle at the point of creation, while the action of $L_{z'}$ must be regarded as measuring the negative of it at the point of annihilation because $L_{z'}$ is acting on the adjoint operator. Therefore $L_Z = L_z + L_{z'}$ measures the loss of orbital angular momentum in the direction of the magnetic field suffered by the particle during its propagation from $(\mathbf{x}, t)$ to $(\mathbf{x}', t')$, and this must vanish because we are dealing with a conserved quantity. This argument that $L_Z G(\mathbf{x}, t; \mathbf{x}', t') = 0$ (and consequently $L_Z G'(\mathbf{R}, T) = 0$) is readily verified by expanding the field operators in a series of angular momentum eigenfunctions, and applying the operator $L_Z = L_z + L_{z'}$. (One can readily show that similar considerations apply when $\phi \neq 0$.) Correspondingly, we have

$$L_Z G'_{11}(X, Y; \omega) = 0, \tag{16}$$

and equation (14) may be rewritten as

$$\begin{aligned}\left[\omega + \frac{\gamma\gamma_v}{\omega}eB\right] G'_{11}(X, Y; \omega) + \frac{\gamma^2}{\omega}\left\{\frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial Y^2} - \left(\frac{eB}{2}\right)^2 [X^2 + Y^2]\right\} G'_{11}(X, Y; \omega) \\ = \delta(X)\delta(Y).\end{aligned} \tag{17}$$

Writing equation (17) in the form

$$\Omega G'_{11}(\mathbf{R}, \Omega) + \left[\frac{1}{2\mathcal{M}}\nabla_{\mathbf{R}}^2 - \mathcal{M}\frac{\Omega_c^2}{8}\mathbf{R}^2\right] G'_{11}(\mathbf{R}, \Omega) = \delta^{(2)}(\mathbf{R}), \tag{18}$$

it is readily recognizable as the Green's function equation for an isotropic two-dimensional harmonic oscillator (with the impulsive Dirac-δ-function driving term having its source point at the origin) in position–frequency representation. Its retarded solution in position–time (τ) representation may be written as [3]

$$G'_{11}(\mathbf{R};\tau) = -\eta_+(\tau)\frac{\mathcal{M}\Omega_c}{4\pi\sin(\Omega_c\tau/2)}\exp\left\{\frac{\mathrm{i}\mathcal{M}\Omega_c[X^2+Y^2]}{4\tan(\Omega_c\tau/2)}\right\}. \tag{19}$$

($\eta_+(\tau)$ is the Heaviside unit step function.) Consequently,

$$G'_{11}(\mathbf{R};\Omega) = \frac{-\mathcal{M}\Omega_c}{4\pi}\int_0^\infty \mathrm{d}\tau\,\frac{\mathrm{e}^{\mathrm{i}\Omega\tau}}{\sin(\Omega_c\tau/2)}\exp\left\{\frac{\mathrm{i}\mathcal{M}\Omega_c[X^2+Y^2]}{4\tan(\Omega_c\tau/2)}\right\}, \tag{20}$$

with the identifications for $\nu = K$

$$\Omega = \omega + \frac{\gamma\gamma_\nu}{\omega}eB = \omega + \frac{\gamma^2}{\omega}eB, \qquad \mathcal{M} = \frac{\omega}{2\gamma^2}, \qquad \Omega_c = \frac{2\gamma^2}{\omega}eB \tag{21}$$

leading to

$$G'_{11}(\mathbf{R};\omega)_K = -\frac{eB}{4\pi}\int_0^\infty \mathrm{d}\tau\,\frac{\exp[\mathrm{i}(\omega+\gamma^2eB/\omega)\tau]}{\sin(\gamma^2eB\tau/\omega)}\exp\left\{\frac{\mathrm{i}eB[X^2+Y^2]}{4\tan(\gamma^2eB\tau/\omega)}\right\}. \tag{22}$$

Setting $\tilde{T} \equiv \tau/\omega$, we have

$$\int_0^\infty \mathrm{d}\tau\cdots = \omega\int_0^\infty \mathrm{d}\tilde{T}\exp[\mathrm{i}\tilde{T}(\omega^2+\gamma^2eB)]\frac{1}{\sin(\gamma^2eB\tilde{T})}\exp\left\{\frac{\mathrm{i}eB[X^2+Y^2]}{4\tan(\gamma^2eB\tilde{T})}\right\}, \tag{23}$$

and expanding the integrand as a generator [4] of Laguerre polynomials, L_n, we obtain

$$\begin{aligned}\int_0^\infty \mathrm{d}\tau\cdots &= 2\mathrm{i}\omega\exp\left(-\frac{eB}{4}[X^2+Y^2]\right)\int_0^\infty \mathrm{d}\tilde{T}\exp[\mathrm{i}\tilde{T}(\omega^2+\gamma^2eB)]\\ &\quad\times\sum_{n=0}^\infty L_n\left(\frac{eB}{2}[X^2+Y^2]\right)\mathrm{e}^{-\mathrm{i}(n+\frac{1}{2})2\gamma^2eB\tilde{T}},\end{aligned} \tag{24}$$

with the result

$$G'_{11}(\mathbf{R};\omega)_K = \frac{eB}{2\pi}\omega\exp\left(-\frac{eB}{4}[X^2+Y^2]\right)\sum_{n=0}^\infty\frac{L_n\left(\frac{eB}{2}[X^2+Y^2]\right)}{\omega^2-2n\gamma^2eB}. \tag{25}$$

Similar treatment of equations (10) and (11) yields an equation for $G'_{22}(X,Y;\omega)_K$ as

$$\begin{aligned}&\left[\omega - \frac{1}{\omega}\left\{\gamma^2\left(\Pi^2_{XY}+\Pi^2_{YX}\right)+i\gamma\gamma_\nu(\Pi_{YX}\Pi_{XY}-\Pi_{XY}\Pi_{YX})\right\}\right]G'_{22}(X,Y;\omega)_K\\ &\qquad = \delta(X)\delta(Y).\end{aligned} \tag{26}$$

Noting the hermiticity of the operators Π_{XY} and Π_{YX}, comparison of equation (26) with equation (12) immediately shows that

$$G'_{22}(\mathbf{R};\omega)_K = G'^*_{11}(\mathbf{R};\omega)_K = \frac{eB}{2\pi}\omega\exp\left(-\frac{eB}{4}[X^2+Y^2]\right)\sum_{n=0}^\infty\frac{L_n\left(\frac{eB}{2}[X^2+Y^2]\right)}{\omega^2-2n\gamma^2eB}, \tag{27}$$

due to the reality of $G'_{11}(\mathbf{R};\omega)_K$.

The energy spectrum of the infinite graphene sheet, obtained from the frequency poles of equation (27) is given by

$$\omega' = \pm\sqrt{2n\gamma^2eB}, \tag{28}$$

as was found earlier by Ando [5]. Moreover, G'_{21} and G'_{12} are readily obtained from G'_{11} and G'_{22} using equations (9) and (11), respectively.

In the case $\nu = K'$, we have identifications in equation (20) as

$$\Omega = \omega + \frac{\gamma\gamma_v}{\omega}eB = \omega - \frac{\gamma^2}{\omega}eB, \qquad \mathcal{M} = \frac{\omega}{2\gamma^2}, \qquad \Omega_c = \frac{2\gamma^2}{\omega}eB \tag{29}$$

and, proceeding as above, we obtain

$$G_{11}^{'}(\mathbf{R},\omega)_{K'} = G_{22}^{'}(\mathbf{R},\omega)_{K'} = \frac{eB}{2\pi}\omega\exp\left(-\frac{eB}{4}[X^2+Y^2]\right)\sum_{n=0}^{\infty}\frac{L_n\left(\frac{eB}{2}[X^2+Y^2]\right)}{\omega^2 - 2(n+1)\gamma^2 eB}. \tag{30}$$

This has energy pole positions for the infinite graphene sheet at

$$\omega = \pm\sqrt{2(n+1)\gamma^2 eB}, \tag{31}$$

but the residues representing the relative strengths of the modes differ from those obtained above by a unit shift of the index of the $L_n\left(\frac{eB}{2}[X^2+Y^2]\right)$ amplitude.

2.2. An alternative representation: Bessel wavefunction

Yet another interesting representation of the graphene Green's function can be derived by rewriting equation (18) in circular coordinates as (for either K or K')

$$\left[\frac{\partial^2}{\partial R^2} + \frac{1}{R}\frac{\partial}{\partial R} - \frac{\mathcal{M}^2\Omega_c^2 R^2}{4} + 2\mathcal{M}\Omega\right]G'_{11}(R;\Omega) = \frac{2\mathcal{M}}{\pi}\frac{\delta(R)}{R}, \tag{32}$$

since there is no angular dependence. For $R > 0$, equation (32) has the form of the '*Bessel wave equation*' [6],

$$\left[\frac{\partial^2}{\partial R^2} + \frac{1}{R}\frac{\partial}{\partial R} + \alpha^2 R^2 + q^2 - \frac{p^2}{R^2}\right]Z(R) = 0, \tag{33}$$

with $p = 0$; $\alpha^2 = -\mathcal{M}^2\Omega_c^2/4$ and $q^2 = 2m\Omega$. The '*Bessel wavefunction*' solutions [6] of equation (33) for the case at hand, $p = 0$, are denoted by $Z_1 = \mathcal{J}_0(\alpha, q, R)$ having small R behavior as $Z_1 \cong 1 + 0(R^2)$; and the second solution is $Z_2 = Z_1\ln(R) + 0(R^2)$ for small R. Thus, the solution of the homogeneous equation may be written as a linear combination of Z_1 and Z_2

$$G'_{11}(R;\Omega) = AZ_1(\mathrm{i}\mathcal{M}\Omega_c/2, \sqrt{2\mathcal{M}\Omega}, R) + BZ_2(\mathrm{i}\mathcal{M}\Omega_c/2, \sqrt{2\mathcal{M}\Omega}, R), \tag{34}$$

subject to the condition at small $R \to \varepsilon \to 0^+$ arising from the Dirac-$\delta(R)$-function of equation (32):

$$\frac{\partial}{\partial\varepsilon}G'_{11}(\varepsilon,\Omega) \cong \frac{\mathcal{M}}{\pi\varepsilon} \qquad \text{or} \qquad G'_{11}(\varepsilon,\omega) \cong \frac{\mathcal{M}}{\pi}\ln(\varepsilon). \tag{35}$$

From this, it is clear that the coefficient B in equation (35) must be $B = \mathcal{M}/2$. The coefficient A must be chosen to prevent singular behavior as $R \to \infty$. To examine the solutions further for large R, we note that the term $\Omega G'_{11}$ is negligible compared to $\left(\mathcal{M}\Omega_c^2 R/8\right)G'_{11}$ in this limit, and equation (32) then becomes

$$\left[\frac{\partial^2}{\partial R^2} + \frac{1}{R}\frac{\partial}{\partial R} - \frac{\mathcal{M}^2\Omega_c^2 R^2}{4}\right]G'_{11}(\mathbf{R},\Omega) = 0. \tag{36}$$

Carrying out an inverse Lommel transform [7] on equation (36), we obtain a modified Bessel equation of order 0, yielding the large-R solution for G'_{11} as

$$G'_{11}(\mathbf{R},\Omega) \Rightarrow \tilde{A}I_0\left(\frac{\mathcal{M}\Omega_c}{4}R^2\right) + \tilde{B}K_0\left(\frac{\mathcal{M}\Omega_c}{4}R^2\right). \tag{37}$$

Here, I_0 and K_0 are modified Bessel functions [8] of the first and third kinds, respectively, with the latter embodying a typical second solution log-singularity for finite R but falling off for large R as $K_0(z) \to \sqrt{\frac{\pi}{2z}}\,\mathrm{e}^{-z}$, whereas the former solution of the first kind diverges as $I_0(z) \to \sqrt{\frac{\pi}{2z}}\,\mathrm{e}^{z}$. On the basis of these considerations jointly with the log-requirement of equation (35) we conclude that

$$G_{11}(\mathbf{R};\Omega) = \frac{\mathcal{M}}{\pi} Z_2(\mathrm{i}\mathcal{M}\Omega_c/2, \sqrt{2\mathcal{M}\Omega}, R), \tag{38}$$

with Z_2 as the second solution of the Bessel wave equation. Clearly, $G'_{22}(\mathbf{R};\Omega)$ can be written similarly by virtue of its equality with $G'_{11}(\mathbf{R};\Omega)$, equation (27), and G_{21} and G'_{12} can be determined as indicated above.

3. Graphene quantum dot: magnetic field Green's function

We consider a two-dimensional delta-function potential to represent a 'tightly' confined quantum dot at the origin as ($\hbar \to 1$)

$$U(\mathbf{r}) = \alpha\delta^{(2)}(\mathbf{r}) \qquad (\alpha < 0). \tag{39}$$

Here, $\alpha = \int \mathrm{d}^3\mathbf{r}\, U(\mathbf{r}) < 0$ is essentially the product of the confining potential well depth and the area of the dot. Such Dirac delta function model potentials have long been employed in quantum-mechanical scattering theory, providing useful information [9]; as does the present model δ-potential when the dot radius is the smallest length of the system under consideration. The Green's function for electron/hole propagation everywhere on the graphene sheet, including the dot region, G'_{dot}, obeys the integral equation (frequency representation; for either K or K')

$$G'_{\mathrm{dot}}(\mathbf{r}_1,\mathbf{r}_2;\omega) = G'(\mathbf{r}_1,\mathbf{r}_2;\omega) + \alpha\int \mathrm{d}^2\mathbf{r}_3\, G'(\mathbf{r}_1,\mathbf{r}_3;\omega)\delta^{(2)}(\mathbf{r}_3)G'_{\mathrm{dot}}(\mathbf{r}_3,\mathbf{r}_2;\omega), \tag{40}$$

with G' as the bulk Landau-quantized electron Green's function for the infinite 2D graphene sheet, in the *absence* of the quantum well. Equation (40) may be rewritten as

$$G'_{\mathrm{dot}}(\mathbf{r}_1,\mathbf{r}_2;\omega) = G'(\mathbf{r}_1,\mathbf{r}_2;\omega) + \alpha G'(\mathbf{r}_1,0;\omega)G'_{\mathrm{dot}}(0,\mathbf{r}_2;\omega), \tag{41}$$

and setting $\mathbf{r}_1 \to 0$ throughout equation (41) we can solve algebraically for $G'_{\mathrm{dot}}(0,\mathbf{r}_2;\omega)$, which yields the full solution for G'_{dot} as (suppress ω)

$$G'_{\mathrm{dot}}(\mathbf{r}_1,\mathbf{r}_2;\omega) = G'(\mathbf{r}_1,\mathbf{r}_2;\omega) + \alpha G'(\mathbf{r}_1,0;\omega)[I-\alpha G'(0,0;\omega)]^{-1}G'(0,\mathbf{r}_2;\omega), \tag{42}$$

where I is the 2×2 unit matrix. The first term on the right describes propagation of Landau-quantized graphene carriers on the infinite 2D host sheet with no quantum well, and the second term introduces the effects of the quantum well 'dot'. The 2×2 matrix inversion of $[I-\alpha G'(0,0;\omega)]$ yields

$$[I-\alpha G'(0,0;\omega)]^{-1} = \triangle^{-1}\begin{pmatrix} 1-\alpha G'_{22} & -\alpha G'_{12} \\ -\alpha G'_{21} & 1-\alpha G'_{11}\end{pmatrix}, \tag{43}$$

where

$$\triangle = [(1-\alpha G'_{11})(1-\alpha G'_{22}) - \alpha^2 G'_{12}G'_{21}]. \tag{44}$$

In equations (43) and (44) all of the positional arguments of the elements of $G'(0,0;\omega)$ vanish. It is clear from equation (23) that for $X = Y = 0$, this leads to divergencies at the lower limit of the $\tilde{T}$-integral. Such divergence arises from the artificiality of representing particle confinement by the $\delta^{(2)}(\mathbf{r})$-potential well to a *single* point at the origin. In reality,

the well has a small but finite radius a and the integral equation, equation (40), should be re-examined and solved more carefully with $U(\mathbf{r})$ occupying a small, finite region. In view of this, it is reasonable to view the formal solution of equation (42) as being 'smeared' over the radius a and make the replacement

$$G(0,0;\omega) \Rightarrow G(a;\omega), \tag{45}$$

which eliminates the divergence problem. In this approximation, which takes the radius a to be the smallest length parameter of the system, it may be noted that $G'_{12} \sim G'_{21} \sim (\gamma eBa/\omega)G'_{11} = (\gamma eBa/\omega)G'_{22}$, so that G'_{12} and G'_{21} can be neglected in comparison with $G'_{11} = G'_{22}$ due to the smallness of a.

4. Summary

We have derived graphene Green's functions in a quantizing magnetic field perpendicular to the 2D graphene sheet. For the infinite 2D sheet, we determined the Green's function elements $G'_{11} = G'_{22}$ explicitly, in closed form *in terms of elementary functions* in direct time representation in equation (19) for both Dirac nodes, K and K'. The off-diagonal terms are readily obtained using equations (9) and (11), but are quite small in applications of interest for a quantum dot. We have also Fourier transformed the Green's function into frequency representation and expanded it in terms of Languerre polynomials (equations (24) and (30)). Separate from this, we also developed an alternative expression for the infinite-sheet 2D graphene Green's function in frequency representation in terms of the second solution of the Bessel wave equation.

Furthermore, we have determined the Green's function for a graphene quantum dot in a normal magnetic field using a potential modeled by $U(\mathbf{r}) = \alpha\delta^{(2D)}(\mathbf{r})$ for a 'tightly' bound graphene quantum dot. An exact closed form solution for this Green's function is exhibited in equations (42) and (43) in terms of the infinite 2D sheet graphene Green's functions discussed in the preceding paragraph. A divergence problem encountered was 'regularized' using an approximation which is valid for a dot whose radius is the smallest length parameter of the system, which is, in fact, the case of interest. The result obtained here for the graphene quantum dot Green's function in a quantizing magnetic field has been employed in an examination of the spectrum of energy states of this system by analyzing the frequency poles of equations (42)–(45), as given by

$$\det(I - \alpha G'(a;\omega)) = 0, \tag{46}$$

and the dot spectrum was found to be 'splintered' by Landau quantization into infinitely many eigenstates [10]. Of course, all the Green's functions determined here can be used extensively in analyzing the dynamics and interactions of graphene sheets and dots in a normal magnetic field in a plethora of applications.

Appendix. Gauge considerations

In the presence of a magnetic field, $\mathbf{B}(\mathbf{x})$, even a uniform one, the momentum direction is not conserved and the Green's function depends on $(\mathbf{x} + \mathbf{x}')$ as well as $(\mathbf{x} - \mathbf{x}')$. To examine this dependence we start by considering a gauge transformation of the vector potential, $\mathbf{A}(\mathbf{x},t) \rightarrow \mathbf{A}(\mathbf{x},t) + \nabla\lambda(\mathbf{x},t)$ and $\phi(\mathbf{x},t) \rightarrow \phi(\mathbf{x},t) - \frac{1}{c}\partial\lambda(\mathbf{x},t)/\partial t$. Corresponding to this, invariance of the Hamiltonian then requires that $\psi(\mathbf{x},t) \rightarrow \mathrm{e}^{\frac{ie\lambda(\mathbf{x},t)}{\hbar c}}\psi(\mathbf{x},t)$, and in view of the bilinear structure of the Green's function, it must change in accordance with

$$G(\mathbf{x},t;\mathbf{x}',t') \rightarrow G'(\mathbf{x},t;\mathbf{x}',t') = \exp\left(\frac{ie}{\hbar c}[\lambda(\mathbf{x},t) - \lambda(\mathbf{x}',t')]\right)G(\mathbf{x},t;\mathbf{x}',t'). \tag{A.1}$$

Writing the Schrödinger operator as $\Lambda = \mathrm{i}\frac{\partial}{\partial t} - H$, we have the Green's function equation for an electron in a constant magnetic field in the form,

$$\Lambda(\nabla, \mathbf{A}(\mathbf{x}), \mathbf{B}(\mathbf{x}))G(\mathbf{x}, t; \mathbf{x}', t') = \delta^{(3)}(\mathbf{x} - \mathbf{x}')\delta(t - t'), \tag{A.2}$$

or, equivalently,

$$\Lambda(\nabla, \mathbf{A}(\mathbf{x}) + \nabla\lambda(\mathbf{x}), \mathbf{B}(\mathbf{x}))G_1'(\mathbf{x}, t; \mathbf{x}', t') = \delta^{(3)}(\mathbf{x} - \mathbf{x}')\delta(t - t'). \tag{A.3}$$

Anticipating application to a uniform **B**-field (as well as constant in time), we choose λ to depend on *both* $\mathbf{x}$ *and* $\mathbf{x}'$, such that

$$\mathbf{A}(\mathbf{x}) + \nabla\lambda(\mathbf{x}, \mathbf{x}') = \tfrac{1}{2}\mathbf{B}(\mathbf{x}) \times (\mathbf{x} - \mathbf{x}'). \tag{A.4}$$

The advantage of this choice is that equation (A.3) becomes

$$\Lambda\left(\nabla, \tfrac{1}{2}\mathbf{B}(\mathbf{x}) \times (\mathbf{x} - \mathbf{x}')\right) G'(\mathbf{x}, t; \mathbf{x}', t') = \delta^{(3)}(\mathbf{x} - \mathbf{x}')\delta(t - t'), \tag{A.5}$$

and if $\mathbf{B}(\mathbf{x}) \to \mathbf{B}$ is a constant vector, in both space and time, then the structure of this equation mandates that G' depends on $(\mathbf{x} - \mathbf{x}')$ to the exclusion of $(\mathbf{x} + \mathbf{x}')$, and also on $(t - t')$ to the exclusion of $(t + t')$:

$$G'(\mathbf{x}, t; \mathbf{x}', t') = G'(\mathbf{x} - \mathbf{x}'; t - t') = \exp\left(\frac{\mathrm{i}e}{\hbar c}[\lambda(\mathbf{x}, \mathbf{x}') - \lambda(\mathbf{x}', \mathbf{x}')]\right) G(\mathbf{x}, t; \mathbf{x}', t'). \tag{A.6}$$

Apart from the introduction of the source point $\mathbf{x}'$, equation (A.4) reflects the fact that for a uniform magnetic field, $\mathbf{A}(\mathbf{x})$ can differ from $\frac{1}{2}\mathbf{B} \times \mathbf{x}$ by at most a gauge transformation,

$$\mathbf{A}(\mathbf{x}) + \nabla\phi(\mathbf{x}) = \tfrac{1}{2}\mathbf{B} \times \mathbf{x}, \tag{A.7}$$

$\phi(\mathbf{x})$ being the gauge function. An equation for $\lambda(\mathbf{x}, \mathbf{x}')$ may be obtained by subtracting equation (A.7) from equation (A.4), with the result,

$$\nabla[\lambda(\mathbf{x}, \mathbf{x}') - \phi(\mathbf{x})] = -\tfrac{1}{2}\mathbf{B} \times \mathbf{x}', \tag{A.8}$$

which is readily line-integrated as

$$\lambda(\mathbf{x}, \mathbf{x}') = -\frac{1}{2}\int \mathrm{d}\mathbf{x} \cdot \mathbf{B} \times \mathbf{x}' + \phi(\mathbf{x}) = -\frac{1}{2}\mathbf{x} \cdot \mathbf{B} \times \mathbf{x}' + \phi(\mathbf{x}). \tag{A.9}$$

Thus, both the $(\mathbf{x} + \mathbf{x}')$ and gauge dependences of G are explicitly given in the factor $C(\mathbf{x}, \mathbf{x}')$,

$$G(\mathbf{x}, t; \mathbf{x}', t') = C(\mathbf{x}, \mathbf{x}')G'(\mathbf{x} - \mathbf{x}'; t - t'), \tag{A.10}$$

where

$$C(\mathbf{x}, \mathbf{x}') = \exp\left[\mathrm{i}\frac{e}{2\hbar c}\mathbf{x} \cdot \mathbf{B} \times \mathbf{x}' - \phi(\mathbf{x}) + \phi(\mathbf{x}')\right] \tag{A.11}$$

is the factor accounting for the changing direction of the momentum vector (circularity of the path) in a magnetic field, with the magnitude of momentum conserved.

As noted in equation (A.6), the Green's function factor G' is spatially translationally invariant since in place of $\mathbf{A}$ we have $\frac{1}{2}\mathbf{B} \times (\mathbf{x} - \mathbf{x}')$. It is also independent of gauge.

References

[1] Castro Neto A H, Guinea F, Peres N M R, Novoselov K S and Geim A K 2007 The electronic properties of graphene 7 arXiv:0709.1163v1 [cond-mat.other]

[2] Novoselov K S, Geim A K, Morozov S V, Jiang D, Zhang Y, Dubonos S V, Grigorieva I V and Firsov A A 2004 *Science* **306** 666

Novoselov K S, Geim A K, Morozov S V, Jiang D, Zhang Y, Dubonos S V, Grigorieva I V and Firsov A A 2005 *Nature* **384** 197

[3] Horing N J M 1965 *Ann. Phys., NY* **31** 1

Horing N J M and Yildiz M M 1976 *Ann. Phys., NY* **97** 216 (use equation (10) with no Fermi averaging, and execute the $\mathbf{p} \to \mathbf{R}$ Fourier transform)
[4] Erdelyi A *et al* 1953 *Higher Transcendental Functions (Bateman Manuscript Project* vol 2*)* (New York: McGraw-Hill) p 189
[5] Ando T 2005 *J. Phys. Soc. Japan* **74** 777
[6] Moon P and Spencer E 1971 *Field Theory Handbook* 2nd edn (Berlin: Springer) p 171ff (see also bottom of p 154)
[7] Erdelyi A *et al* 1953 *Higher Transcendental Functions (Bateman Manuscript Project* vol 2*)* (New York: McGraw-Hill) p 13
[8] Erdelyi A *et al* 1953 *Higher Transcendental Functions (Bateman Manuscript Project* vol 2*)* (New York: McGraw-Hill) chapter VII
[9] Southerland B 2004 *Beautiful Models* (Singapore: World Scientific) p 44 (section 2.4)
[10] Horing N J M and Liu S Y unpublished