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Corrigendum

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It has come to the attention of the authors that errors occured in equations (11) and (12) of the above paper. In equation (11), two α factors were missing in the matrix. The corrected equation is as follows:

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

Furthermore, in equation (12) there was a missing α^2 factor. The corrected equation is as follows:

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

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Energy spectrum and density of states for a graphene quantum dot in a magnetic field

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Abstract

In this paper, we determine the spectrum and density of states of a graphene quantum dot in a normal quantizing magnetic field. To accomplish this, we employ the retarded Green function for a magnetized, infinite-sheet graphene layer to describe the dynamics of a tightly confined graphene quantum dot subject to Landau quantization. Considering a $\delta^{(2)}(\mathbf{r})$ potential well that supports just one subband state in the well in the absence of a magnetic field, the effect of Landau quantization is to 'splinter' this single energy level into a proliferation of many Landau-quantized states within the well. Treating the graphene sheet and dot as a closed system subject to a fully Hermitian Hamiltonian (including boundary conditions), there is no indication of decay of the Landau-quantized graphene dot states into the quantized states of the host graphene sheet for 'tight' confinement by the $\delta^{(2)}(\mathbf{r})$ potential well, notwithstanding extension of the dot Green function (and eigenfunctions) outside the $\delta^{(2)}(\mathbf{r})$ potential well.

1. Introduction: the graphene quantum dot Green function

Our principal concern in this paper is with recent theoretical studies envisioning possible electronic devices based on transport in quantum dot systems *in which each dot by itself would support just one single energetically accessible energy level in the absence of a magnetic field*. Moreover, the role of the magnetic field is often represented merely in terms of a Peierls phase factor. In fact, the magnetic field also induces a 'splintering' of the single dot level into a proliferation of many Landau-quantized dot states which may also be energetically accessible, making the situation much more complicated. This also applies to graphene-based quantum dot systems, as shown in this paper. Moreover, we examine the Green function and Landau-quantized energy spectrum for a graphene quantum dot, and our closed-form analytic result is tractable and can facilitate accurate transport calculations involving graphene quantum-dot-based devices modified or probed by a magnetic field.

Graphene, as a 2D sheet of carbon atoms in a hexagonal honeycomb lattice, has special properties that arise from its band structure [1, 2], which gives rise to an electron/hole energy spectrum in the nature of a massless relativistic 'Dirac' dispersion law. These properties of graphene include a room temperature quantum Hall effect [3], Klein tunneling [4] and many other device-friendly features that mark it as an exceptionally promising material for the 'next generation' of electronics. The massless relativistic dispersion law occurs at two inequivalent zero-gap points of the first Brillouin zone where the electron and hole bands touch ('Dirac' nodes, K and K'), giving rise to low carrier energies that are proportional to momentum on the plane, $\mathbf{p} = (p_x, p_y)$, with the Hamiltonian given by ($\hbar \to 1$ throughout)

$$H = \gamma \boldsymbol{\sigma}_\nu \cdot \mathbf{p}. \tag{1}$$

Here, $\sigma_\nu = [\sigma_x, (\mathrm{sgn}(\nu))\sigma_y]$ 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 $\mathrm{sgn}(\nu) = 1$ or -1 for $\nu = K$ or K', and $\gamma = 3\tilde{\alpha}d/2$ (with $\tilde{\alpha}$ as 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. In this 2D pseudo-spin representation,

the 2×2 Green function matrix, G, obeys the equation

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

with I as the 2×2 unit matrix.

The magnetic field, $\mathbf{B}$, taken normal to the graphene plane, is incorporated through 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, which is sufficiently strong to induce Landau quantization. It is well known that the requirement of gauge invariance leads to a result of the form [5][3]

$$G(\mathbf{r}_1, \mathbf{r}_2; t_1, t_2) = C(\mathbf{r}_1, \mathbf{r}_2)G'(\mathbf{r}_1, \mathbf{r}_2; t_1 - t_2), \qquad (3)$$

where the factor $G'(\mathbf{r}_1, \mathbf{r}_2; t_1 - t_2)$ is gauge-invariant. For an infinite homogeneous sheet with planar translational invariance, it satisfies the equation ($\mathbf{R} = \mathbf{r}_1 - \mathbf{r}_2$, $T = t_1 - t_2$, $\hbar \to 1$):

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

whereas the Peierls factor $C(\mathbf{r}, \mathbf{r}')$ embodies all non-spatially invariant structure due to the magnetic field and all gauge dependence as

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

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

The potential for a 'tightly' confined quantum dot at the origin (which induces further spatial inhomogeneity) is taken as ($\hbar \to 1$)

$$U(\mathbf{r}) = \alpha\delta^{(2)}(\mathbf{r}), \qquad (\alpha < 0) \qquad (6)$$

where $\alpha = \int \mathrm{d}^2\mathbf{r}\, U(\mathbf{r}) < 0$ is essentially the product of the confining potential well depth, U_0, and the area of the dot. This representation of a quantum dot with just a single accessible energy level in the absence of a magnetic field in terms of the $\delta^{(2)}(\mathbf{r})$ potential is a perfectly good vehicle to use in exploring the effects of Landau quantization on a small graphene quantum dot. It provides insight into qualitative (as well as quantitative) features that pervade the phenomenology induced by the magnetic field. Notwithstanding the fact that this formulation is relatively easy to solve in closed form, its results are very informative about the fundamental physics involved and it provides clear predictions relating to experiment; namely the role of the magnetic field in splintering the single dot level into a proliferation of levels by Landau quantization.

The graphene Green function for electron propagation over the entire sheet, *including the dot region*, obeys the integral equation (frequency representation; for either K or K')

$$G'_{\mathrm{dot}}(\mathbf{r}_1, \mathbf{r}_2; \omega) = G'(\mathbf{r}_1, \mathbf{r}_2; \omega) + \alpha \int \mathrm{d}^2\mathbf{r}_3 G'(\mathbf{r}_1, \mathbf{r}_3; \omega)\delta^{(2)}(\mathbf{r}_3)G'_{\mathrm{dot}}(\mathbf{r}_3, \mathbf{r}_2; \omega), \qquad (7)$$

[3] (Use equation (10) with no Fermi averaging and execute the $\mathbf{p} \to \mathbf{R}$ Fourier transform.)

where G' is the Landau-quantized electron Green function of equation (4) for the full 2D magnetized sheet, with *no* quantum well. This equation may be rewritten as (bear in mind that the Green function is a 2×2 matrix in pseudo-spin space, and that the matrices involved are not commutative, in general)

$$G'_{\mathrm{dot}}(\mathbf{r}_1, \mathbf{r}_2; \omega) = G'(\mathbf{r}_1, \mathbf{r}_2; \omega) + \alpha G'(\mathbf{r}_1, 0; \omega)G'_{\mathrm{dot}}(0, \mathbf{r}_2; \omega), \qquad (8)$$

and setting $\mathbf{r}_1 \to 0$ throughout, we can solve for $G'(0, \mathbf{r}_2; \omega)$, which facilitates the full solution of the matrix Green function:

$$G'_{\mathrm{dot}}(\mathbf{r}_1, \mathbf{r}_2; \omega) = \begin{bmatrix} G'_{\mathrm{dot}}(\mathbf{r}_1, \mathbf{r}_2; \omega)_{11} & G'_{\mathrm{dot}}(\mathbf{r}_1, \mathbf{r}_2; \omega)_{12} \\ G'_{\mathrm{dot}}(\mathbf{r}_1, \mathbf{r}_2; \omega)_{21} & G'_{\mathrm{dot}}(\mathbf{r}_1, \mathbf{r}_2; \omega)_{22} \end{bmatrix}, \qquad (9)$$

in the form

$$G'_{\mathrm{dot}}(\mathbf{r}_1, \mathbf{r}_2; \omega) = G'(\mathbf{r}_1, \mathbf{r}_2; \omega) + \alpha G'(\mathbf{r}_1, 0; \omega)[I - \alpha G'(0, 0; \omega)]^{-1}G'(0, \mathbf{r}_2; \omega). \qquad (10)$$

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

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

where all G'-arguments are $(0, 0)$ with ω suppressed and

$$\Delta = \left[\left(1 - \alpha G'_{11}\right)\left(1 - \alpha G'_{22}\right) - G'_{12}G'_{21}\right]. \qquad (12)$$

In regard to the issue of confinement, it should be noted that equations (10) and (3) clearly indicate that the dot Green function has spatial extension outside the dot (notwithstanding the $\delta^{(2)}(\mathbf{r})$ potential well). This means that tunneling is quite possible under appropriate external conditions, including a potential difference that can drive the system out of equilibrium. (This applies both for null and finite magnetic fields.)

The vanishing of all the positional arguments of the elements of $G'(0, 0; \omega)$ leads to divergences. However, such divergences are an artifact of the $\delta^{(2)}(\mathbf{R})$ confinement of the potential well to a single point at the origin. Realistically, the well has a small but finite radius, a, and the original integral equation should be reformulated and solved more carefully with $U(\mathbf{R})$ occupying a small, finite region. Considering this, it is reasonable to view the formal solution as being 'smeared' over the radius a and make the replacement

$$G(0, 0; \omega) \Rightarrow G(a; \omega), \qquad (13)$$

which relieves the divergence problem. On this level of approximation, we have shown 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.

2. The magnetic field Green function of a graphene quantum dot

It is apparent from equations (10) and (11) that the determination of the magnetic field Green function for the

graphene quantum dot requires knowledge of its full sheet counterpart. We have found that the latter solution of equation (4) in frequency representation is given in terms of a closed-form integral representation involving only elementary functions (which generate Landau eigenfunctions) as[4]

$$G'_{11}(\mathbf{R};\Omega) = \frac{-\mathcal{M}\Omega_c}{4\pi}\int_0^\infty \mathrm{d}\tau \frac{\mathrm{e}^{\mathrm{i}\Omega\tau}}{\sin(\Omega_c\tau/2)} \times \exp\left\{\frac{\mathrm{i}\mathcal{M}\Omega_c[X^2+Y^2]}{4\tan(\Omega_c\tau/2)}\right\}. \quad (14)$$

Equivalently, we find that

$$G'_{11}(\mathbf{R};\Omega) = \frac{\mathcal{M}}{\pi} Z_2(\mathrm{i}\mathcal{M}\Omega_c/2, \sqrt{2\mathcal{M}\Omega}, R), \quad (15)$$

where Z_2 is the second solution of the Bessel wave equation [6].

For the case $\boldsymbol{\nu} = \boldsymbol{K}$, we have the identifications

$$\Omega = \omega + \frac{\gamma\gamma_\nu}{\omega}eB = \omega + \frac{\gamma^2}{\omega}eB; \qquad \mathcal{M} = \frac{\omega}{2\gamma^2}; \qquad \Omega_c = \frac{2\gamma^2}{\omega}eB, \quad (16)$$

whence (for $\nu = K$)

$$G'_{11}(\mathbf{R};\omega)_K = G'_{22}(\mathbf{R};\omega)_K = -\frac{eB}{4\pi} \times \int_0^\infty \mathrm{d}\tau \frac{\exp[\mathrm{i}(\omega+\gamma^2eB/\omega)\tau]}{\sin(\gamma^2eB\tau/\omega)} \times \exp\left\{\frac{\mathrm{i}eB[X^2+Y^2]}{4\tan(\gamma^2eB\tau/\omega)}\right\}. \quad (17)$$

Defining $\tilde{T} \equiv \tau/\omega$, the τ integral is

$$\int_0^\infty \mathrm{d}\tau \cdots = \omega\int_0^\infty \mathrm{d}\tilde{T}\ \exp[\mathrm{i}\tilde{T}(\omega^2+\gamma^2eB)] \times \frac{1}{\sin(\gamma^2eB\tilde{T})}\exp\left\{\frac{\mathrm{i}eB[X^2+Y^2]}{4\tan(\gamma^2eB\tilde{T})}\right\}, \quad (18)$$

and expanding the integrand as a generator of Laguerre polynomials, L_n, we obtain [7]

$$\int_0^\infty \mathrm{d}\tau \cdots = 2\mathrm{i}\omega\exp\left(-\frac{eB}{4}[X^2+Y^2]\right) \times \int_0^\infty \mathrm{d}\tilde{T}\ \exp[\mathrm{i}\tilde{T}(\omega^2+\gamma^2eB)] \times \sum_{n=0}^\infty L_n\left(\frac{eB}{2}[X^2+Y^2]\right)\mathrm{e}^{-\mathrm{i}(n+\frac{1}{2})2\gamma^2eB\tilde{T}}, \quad (19)$$

with the result

$$G'_{11}(\mathbf{R};\omega)_K = \frac{eB}{2\pi}\omega\exp\left(-\frac{eB}{4}[X^2+Y^2]\right) \times \sum_{n=0}^\infty \frac{L_n\left(\frac{eB}{2}[X^2+Y^2]\right)}{\omega^2-2n\gamma^2eB}. \quad (20)$$

[4] This will be discussed in greater detail elsewhere.

For the case $\boldsymbol{\nu} = \boldsymbol{K}'$, we have identifications in equation (14) as

$$\Omega = \omega + \frac{\gamma\gamma_\nu}{\omega}eB = \omega - \frac{\gamma^2}{\omega}eB; \qquad \mathcal{M} = \frac{\omega}{2\gamma^2}; \qquad \Omega_c = \frac{2\gamma^2}{\omega}eB \quad (21)$$

with the result

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

The off-diagonal terms, G'_{12} and G'_{21}, are not of immediate interest, and will not be presented here.

Consequently, the dispersion relation for the Landau-quantized 'tightly' bound graphene dot energy levels, $\Delta = 0$ (equation (12)), takes the form for $\nu = K$ with $\omega \to \omega_K$:

$$\Delta \cong [1 - \alpha G'_{11}(a;\omega_K)]^2 = 0, \quad (23)$$

or

$$1 = \alpha\frac{eB}{2\pi}\omega_K\mathrm{e}^{-\frac{eBa^2}{4}}\sum_{n=0}^\infty \frac{L_n\left(\frac{eBa^2}{2}\right)}{\omega_K^2-2n\gamma^2eB}. \quad (24)$$

This series converges slowly since [7] $L_n(x) \to \frac{\mathrm{e}^{\frac{x}{2}}}{\sqrt{\pi}}\frac{\cos(2\sqrt{nx}-\frac{\pi}{4})}{(nx)^{\frac{1}{4}}}$ as $n \to \infty$, with the denominator on the right of equation (24) contributing a factor $\frac{1}{n}$. It is instructive to install typical graphene parameters in equation (24), with $\frac{eBa^2}{2} \cong 3.8\times10^{-3}$; $\exp(-\frac{eBa^2}{4}) \cong 1$; $\gamma^2eB \cong 3.5\times10^{-4}$ meV $\frac{\alpha eB}{2\pi} \cong 3.4\times10^{-7}$ meV, yielding

$$\frac{10^7}{3.4\omega_K} = \sum_{n=0}^\infty \frac{L_n(3.8\times10^{-3})}{\omega_K^2 - 7\times10^{-4}n}.$$

The left-hand side is large and rises steadily as a function of ω_K^{-1}, while the numerators of the terms on the right are relatively small and diminish as n increases. Correspondingly, as n increases, the roots involve ω_K^2 in the denominators on the right side having to closely approach the frequency poles at $\pm(7\times10^{-4}n)^{1/2}$ in order to establish equality with the large left-hand side; in which case the pole for that particular n value *alone* determines the position of the energy level root. In this situation, as n increases, the graphene dot energy levels are close to the frequency poles of the individual terms of the series. Accordingly, we write, approximately:

$$\omega_K^2 - \omega_K\frac{\alpha eB}{4\pi}\mathrm{e}^{-eBa^2/4}L_n\left(\frac{eBa^2}{2}\right) - 2n\gamma^2eB = 0, \quad (25)$$

with the solutions

$$\omega_K = \frac{\alpha eB}{4\pi}\mathrm{e}^{-eBa^2/4}L_n\left(\frac{eBa^2}{2}\right) \pm \frac{1}{2}\sqrt{\left(\frac{\alpha eB}{2\pi}\right)^2\mathrm{e}^{-eBa^2/2}\left(L_n\left(\frac{eBa^2}{2}\right)\right)^2 + 8n\gamma^2eB}. \quad (26)$$

A similar treatment for $\nu = K'$ yields the dispersion relation

$$1 = \alpha \frac{eB}{2\pi} \omega_{K'} \mathrm{e}^{\frac{-eBa^2}{4}} \sum_{n=0}^{\infty} \frac{L_n(\frac{eBa^2}{2})}{\omega_{K'}^2 - 2(n+1)\gamma^2 eB}, \tag{27}$$

with approximate solutions:

$$\omega_{K'} = \frac{\alpha eB}{4\pi} \mathrm{e}^{\frac{-eBa^2}{4}} L_n\left(\frac{eBa^2}{2}\right) \pm \frac{1}{2}\sqrt{\left(\frac{\alpha eB}{2\pi}\right)^2 \mathrm{e}^{\frac{-eBa^2}{4}} \left(L_n\left(\frac{eBa^2}{2}\right)\right)^2 + 8(n+1)\gamma^2 eB}. \tag{28}$$

3. Conclusions: graphene dot density of states in a quantizing magnetic field

Of course, the splintering of the electron and hole spectra into discrete states by Landau quantization is embodied in the discrete integer values of n. This is reflected in the many roots of the $\nu = K, K'$ dispersion relations for graphene dots in equations (24)–(28), as well as for an infinite graphene sheet. To explore this more carefully we have determined the density of dot states, $D(\omega)$, from the retarded Green function of the magnetized graphene quantum dots:

$$D(\omega) = -\frac{1}{\pi} Tr\ \mathrm{Im}\, G(\omega). \tag{29}$$

The calculated results, exhibited in figure 1, are in reasonably good agreement with the analytic approximations of equations (26) and (28) for $n > 1$, as discussed above (but certainly not so for $n = 0$). The lines are very sharp, except for a small artificial width introduced to facilitate computation. Actually, the lines have zero width, corresponding to the fact that the graphene dot and sheet together are treated as a closed system subject to a fully Hermitian Hamiltonian (including boundary conditions), and are fully quantized by the magnetic field, with discrete spectra that have no matching states. Therefore, electrons in the dot can *not* decay into the sheet, although that would change if the thickness of the sheet should be sufficient to induce a continuum of states along the magnetic field direction having a constituent energy value matching the energy of an electron in one of the Landau-quantized dot states. Moreover, other recent considerations addressing the system under consideration as open (rather than closed) have yielded information about tunneling-induced linewidth of the dot states [8, 9]. The formulation presented here can, in due course, be applied to graphene magnetotunneling studies without introducing the usual transfer-matrix assumption, or further assumptions about non-Hermitian boundary conditions. Insofar as boundary conditions are concerned, our $\delta^{(2)}(\mathbf{r})$ well potential builds them in implicitly for a small dot within the framework of the massless Dirac spectrum. We expect that the results for differing boundary shapes will exhibit qualitatively similar features of Landau quantization, and be quantitatively close to our analytic results as those wells shrink in size. Despite the simplicity of the $\delta^{(2)}(\mathbf{r})$ well model employed here, the Green function analyzed in this paper can facilitate rigorously detailed magnetotunneling/transport studies through small graphene quantum dot systems (including 'relativistic' phenomenology) when appropriate couplings are introduced.

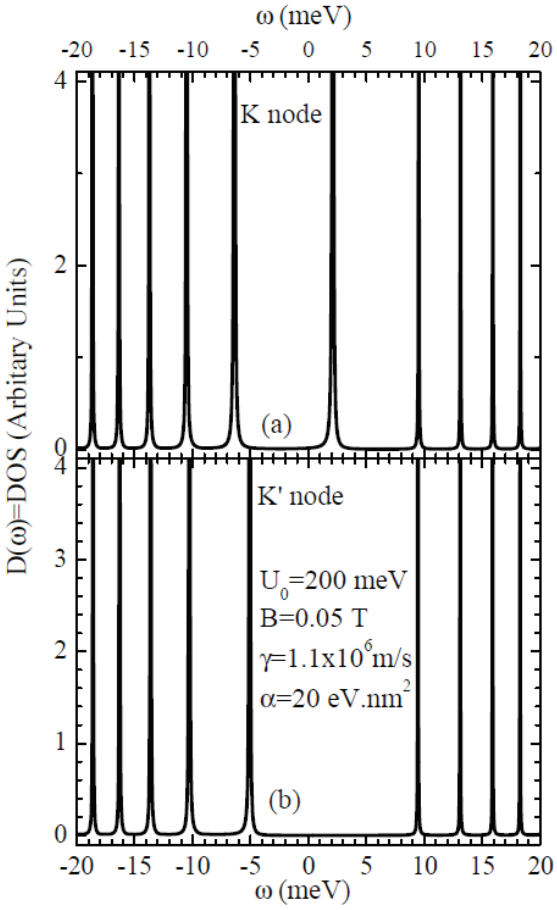

Figure 1. Density of states for the K, K' nodes of a graphene quantum dot subject to Landau quantization as a function of frequency/energy.

It should be noted that the graphene dot K and K' spectra (DOS) are generally closely aligned (but slightly displaced from each other), except for the almost-central mode of the K node, which has no K' counterpart. In figures 2 and 3 we also exhibit the K, K' eigenenergies as functions of the square root of the magnetic field.

To put this work into proper perspective, we note that the energy spectrum of a graphene quantum dot in a perpendicular magnetic field has already been studied experimentally [10, 11] and theoretically [12–15]. The theoretical analysis that we have presented here differs from that of [12–15] as follows: in regard to [12], we feel that the magnetic field should not be limited to the region of the dot, vanishing elsewhere; in regard to [13], we consider the gapless case; in regard to [14], we avoid the employment of an 'infinite mass' boundary condition; while, in regard to [15], we do not assume a parabolic model for quantum dots, nor do we treat a bilayer.

In summary, we have analyzed the retarded Green function for a graphene quantum dot in terms of the infinite-sheet

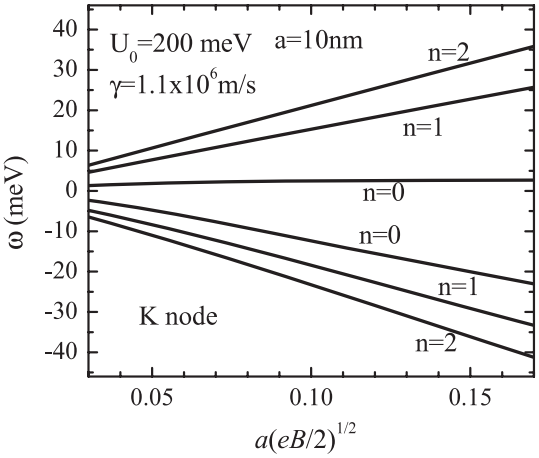

Figure 2. Energy/frequency levels of a graphene quantum dot subject to Landau quantization for the K node as a function of the square root of the magnetic field.

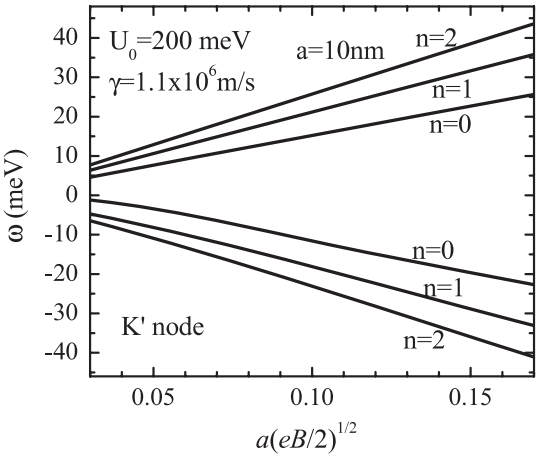

Figure 3. Same as figure 2, for the K' node (instead of the K node).

graphene Green function in a quantizing magnetic field, and have employed it in obtaining the spectrum and density of states of a graphene quantum dot subject to a high magnetic field. In this regard, we have found that the single-dot energy level supported by the $\delta^{(2)}(\mathbf{r})$ potential in the absence of a magnetic field is splintered into a proliferation of many discrete Landau-quantized dot states within the well by a magnetic field normal to the graphene sheet. Consequently, the validity of recent theoretical studies envisioning possible electronic devices based on transport in quantum dot systems (possibly including graphene) in which each dot would support just one single energetically accessible energy level in the absence of a magnetic field, and representing the role of the magnetic field merely in terms of a Peierls phase factor, needs to be carefully reconsidered.

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