Effective Model for Graphene

H. Falomir[1,5], J. Gamboa[2,3], F. Méndez[2,4] and M. Nieto[5]

[1] *IFLP - CONICET*
[2] *Facultad de Física, Pontificia Universidad Católica de Chile, Casilla 306, Santiago 22, Chile*
[3] *Departamento de Física, Universidad de Santiago de Chile, Casilla 307, Santiago, Chile*
[4] *Centre for Theoretical and Mathematical Physics, University of Cape Town, Rondebosch 770, South Africa*
[5] *Departamento de Física, Facultad de Ciencias Exactas, Universidad Nacional de La Plata, C.C. 67, (1900) La Plata, Argentina*

Abstract

We employ a simple nonrelativistic model, based on a deformation of the Heisenberg algebra, to describe the low energy excitation of graphene. This model (which reduces in a ceratin limit to the usual linear one employed to describe these excitations as massless Dirac fermions) reproduces the leading (isotropic) terms in the low energy expansion of the dispersion relation derived from the tight binding model for both nearest and next-to-nearest-neighbor interactions. We solve the Landau problem for the resulting Hamiltonian and, taking into account the contribution of both Dirac points, we evaluated the Hall conductivity within a ζ-function approach, showing that it is consistent with the anomalous integer quantum Hall effect *characteristic of graphene.*

Introduction

We consider a particle leaving on a plane whose dynamical variables satisfy the following deformed Heisenberg algebra:

$$[X_i, X_j] = 0\,, \quad [X_i, P_j] = \imath\delta_{ij}\,, \quad [P_i, P_j] = 2\imath\theta^2\epsilon_{ij3}\sigma_3\,, \quad [P_i, \sigma_j] = 2\imath\theta\epsilon_{ij3}\sigma_3\,, \quad i,j = 1,2\,, \tag{0.1}$$

where the momenta commutator is proportional to the *pseudospin* σ_3 and θ is a parameter with dimensions of momentum (we take $\hbar = 1$ and return to full units when necessary). This algebra can be realized in terms of ordinary coordinates and momenta by means of a *non-Abelian Bopp's shift* as $X_i \to x_i$, $P_i \to p_i + \theta\sigma_i$ (where σ_i are the Pauli matrices).

We consider the direct generalization of the (nonrelativistic) Hamiltonian of a particle of charge e and mass m, minimally coupled to an external electromagnetic field A_μ in the Coulomb gauge, $\boldsymbol{\nabla}\cdot\mathbf{A} = 0$. We also take $A_0 = 0$. Then,

$$H_0 = \frac{(\mathbf{p} - e\mathbf{A})^2}{2m} \quad \to \quad H_\theta = \frac{(\mathbf{p} - e\mathbf{A} + \theta\boldsymbol{\sigma})^2}{2m}\,. \tag{0.2}$$

which can also be written as

$$H = \frac{(\mathbf{p} - e\mathbf{A})^2}{2m} + v_F\,\boldsymbol{\sigma}\cdot(\mathbf{p} - e\mathbf{A})\,, \tag{0.3}$$

where we have defined the *Fermi velocity* $v_F := \frac{\theta}{m}$ and subtracted the constant θ^2/m.

In the $m \to \infty$ limit, with fixed $v_F > 0$, we get the linear Hamiltonian usually employed to describe the effective low energy excitations around the *Fermi points* of graphene [2, 6, 7], which justifies our proposal.

Our Model

- The *Free* Case

  First, we consider the $\mathbf{A} = 0$ case. There are two linearly independent constant solutions, $\begin{pmatrix}1\\0\end{pmatrix}$ and $\begin{pmatrix}0\\1\end{pmatrix}$, with vanishing eigenvalue.

  On the other hand, for $\mathbf{k} \neq \mathbf{0}$, if we write

$$\psi_{\mathbf{k}}(\mathbf{x}) = e^{\imath\mathbf{k}\cdot\mathbf{x}}\chi(\mathbf{k})\,, \tag{0.4}$$

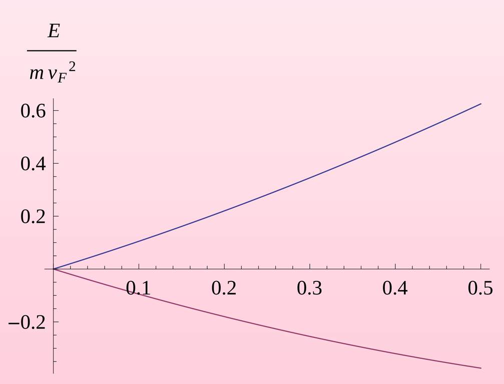
  with $\chi(\mathbf{k}) \in \mathbb{C}^2$, we get the dispersion relation (approximately linear for small $|\mathbf{k}|$, see Figure)

$$\mathcal{E}(\mathbf{k}) = \frac{\mathbf{k}^2}{2m} \pm v_F\,|\mathbf{k}|\,, \tag{0.5}$$

  which can be compared with the isotropic terms in the dispersion relation obtained from the tight binding model for graphene around one Fermi point $\mathbf{K}$,

$$E_s(\mathbf{k}) = s\,t\left[\frac{3}{2}a|\mathbf{k}| - \frac{3}{8}a^2\mathbf{k}^2\sin(3\theta)\right] + t'\left[-\frac{9}{4}a^2\mathbf{k}^2 + 3\right] + O\left(|\mathbf{k}|^3\right)\,, \tag{0.6}$$

  where $a \approx 1.42\mathring{A}$, $\tan(\theta) = k_2/k_1$ and $s = \pm 1$. This leads to the identification $v_F \equiv \frac{3}{2}at$ and $m = -2/\left(9t'a^2\right) < 0$ (a negative mass parameter).



- Constant Magnetic Field Perpendicular to the Plane

  We now consider the Landau problem, with

$$\mathbf{A} = Bx_1\hat{\mathbf{e}}_2 \quad \Rightarrow \quad \partial_1 A_2 - \partial_2 A_1 = B \quad \text{and} \quad \boldsymbol{\nabla}\cdot\mathbf{A} = 0\,. \tag{0.7}$$

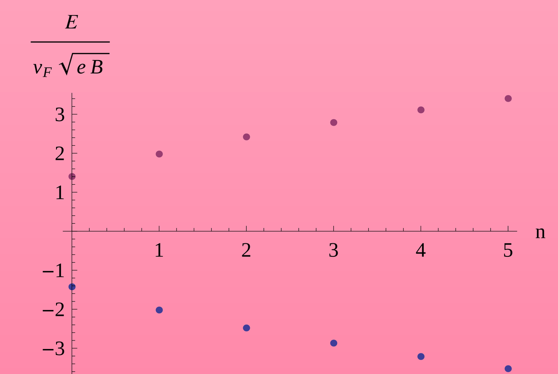
  The eigenvalue problem can be solved to get the non-degenerate spectrum

$$\mathcal{E}_{n,s} = \frac{\lambda_{n,s}}{2m} = -\left(v_F\sqrt{eB}\right)\frac{1}{w}\left[n + 1 + \frac{s}{2}\sqrt{1 + 8w^2(n+1)}\right]\,, \quad n \in \mathbb{N}\,, \tag{0.8}$$

  with $s = \pm 1$ and $w := -\frac{mv_F}{\sqrt{eB}} > 0$, and a linearly independent solution with $\mathcal{E}_0 = eB/2m = -eB/2|m| < 0$ (a ***hole*** with small energy).

  Since we are only interested in the low energy excitations and $w \sim 10^3$ for $B \approx 10$ Tesla, it is sufficient to retain (See Figure 2)

$$\mathcal{E}_{n,s} = \left(v_F\sqrt{eB}\right)\left\{-s\sqrt{2(n+1)} - \frac{n+1}{w} + O\left(w^{-2}\right)\right\}\,. \tag{0.9}$$



In the linear model for graphene, the Hamiltonians of excitations around both Fermi points are related by

$$H_{\mathbf{K}'} = -\sigma_2 H_{\mathbf{K}}\sigma_2\,. \tag{0.10}$$

So, we incorporate the second Fermi point $\mathbf{K}'$ in our model assuming the same relation to hold. This unitary transformations leads to the same spectrum but reflected around the origin. In particular, we get a *quasi-particle* state with small energy, $\mathcal{E}'_0 = -eB/2m \approx 2.43 \times 10^{-5}\,\text{eV}$ for $B \approx 10$ Tesla.

In this way, we get an almost doubly degenerate spectrum (the gap between contiguous states is $\triangle\mathcal{E}_n \sim \left\{\frac{n+1}{w} + O\left(w^{-2}\right)\right\}$), except for one state of quasi-particle and one state of hole with energies near zero.

The Hall conductivity

The Hall conductivity has a topological character and can be calculated from the weak field and gradient expansion of the effective action of the system. In our case, we know the exact energy eigenvalues of our model (a discrete spectrum with no accumulation points) and so, we can employ a more direct evaluation method (a ζ-function approach), based on the relation between the external electromagnetic field and the conserved current, whose density is given by

$$j^0 = e\,\psi^\dagger\psi\,. \tag{0.11}$$

It is known that, in 2+1 dimensions, this relation is dominated by a Chern-Simons term which gives the Hall conductivity in terms of the density mean value,

$$\langle j_0 \rangle = J_0 = \sigma_{xy}B\,. \tag{0.12}$$

If we consider the partition function (in the Grand Canonical ensamble) for fluctuations around $\mathbf{K}$ at inverse temperature β and chemical potential μ, the mean number of particles is given by

$$\frac{\partial \log\mathcal{Z}}{\partial\mu}(\beta,\mu,B) = \beta\int d^2x\,\frac{\sigma_{xy}}{e}\,B\,. \tag{0.13}$$

Moreover,

$$\log\mathcal{Z}(\beta,\mu,B) = \log\mathrm{Det}\,(D) := -\frac{d}{du}\mathrm{Tr}\left\{\left(\frac{D}{\Lambda}\right)^{-u}\right\}\Bigg|_{u\to 0}\,, \tag{0.14}$$

where Λ is an arbitrary mass scale and $D = -\frac{\partial}{\partial\tau} + \mu - H$ is a differential operator defined on a domain of anti-periodic functions of $\tau \in [0,\beta]$.

Then,

$$\log\mathcal{Z}(\beta,\mu,B) = -\frac{d}{du}\left\{\sum_{l,n,s}\left(\frac{\lambda_{l,n,s}}{\Lambda}\right)^{-u} + \sum_{l}\left(\frac{\lambda_{l,0}}{\Lambda}\right)^{-u}\right\}\Bigg|_{u\to 0}\,. \tag{0.15}$$

with

$$\lambda_{l,n,s} = \imath\omega_l + \mu - \mathcal{E}_{n,s}\,, \qquad \lambda_{l,0} = \imath\omega_l + \mu - \mathcal{E}_0\,, \tag{0.16}$$

where $\mathcal{E}_{n,s}$ y $\mathcal{E}_0$ are the eigenvalues of our Hamiltonian and ω_l are the Matsubara frequencies.

Let us first consider the contribution of the lowest level. We can write

$$\sum_{l=-\infty}^{\infty}\left(\frac{\lambda_{l,0}}{\Lambda}\right)^{-u} = \left(\frac{2\pi}{\beta\Lambda}\right)^{-u}\left\{e^{-\imath\frac{\pi}{2}u}\zeta\left(u, \frac{1}{2} + e^{-\imath\frac{\pi}{2}\mathrm{sign}\,(\mu - \mathcal{E}_0)}\frac{\beta}{2\pi}|\mu - \mathcal{E}_0|\right) + e^{\imath\frac{\pi}{2}u}\zeta\left(u, \frac{1}{2} + e^{\imath\frac{\pi}{2}\mathrm{sign}\,(\mu - \mathcal{E}_0)}\frac{\beta}{2\pi}|\mu - \mathcal{E}_0|\right)\right\}\,. \tag{0.17}$$

Taking into account that we are interested in the mean particle number with respect to the neutral material ($\mu = 0$), we get for the contribution of the Landau level with energy $\mathcal{E}_0$ to the Hall conductivity at zero temperature

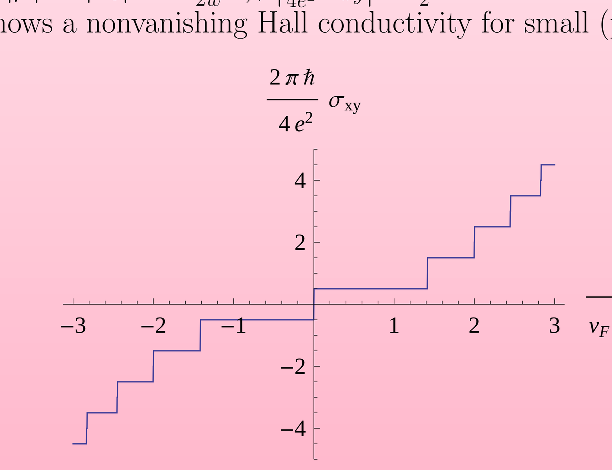
$$\frac{B}{e}\sigma_{xy}\Big|_{\mathcal{E}_0} = \frac{Be}{2\pi}\left\{\frac{\partial}{\partial\mu}\left[(\mathcal{E}_0 - \mu)\,\Theta\,(\mathcal{E}_0 - \mu)\right] - \frac{\partial}{\partial\mu}\left[(\mathcal{E}_0 - \mu)\,\Theta\,(\mathcal{E}_0 - \mu)\right]\Big|_{\mu=0}\right\} = \frac{Be}{2\pi}\left\{\Theta(\mathcal{E}_0)\Theta\,(\mu - \mathcal{E}_0) - \Theta\,(-\mathcal{E}_0)\,\Theta\,(\mathcal{E}_0 - \mu)\,\right\} \tag{0.18}$$

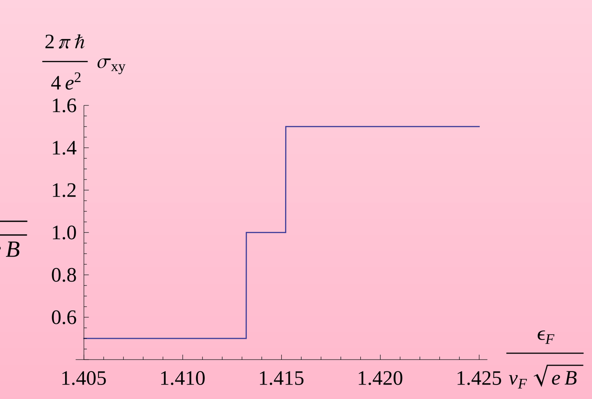
Therefore, for positive $\mathcal{E}_0$, we get a contribution $(+\frac{e^2}{2\pi})$ to σ_{xy} if $\mu > \mathcal{E}_0$ and zero otherwise. On the other hand, for negative $\mathcal{E}_0$ we get a contribution $(-\frac{e^2}{2\pi})$ if $\mu < \mathcal{E}_0$ and zero otherwise.

Similar results are obtained for other Landau levels. Then, taking into account that the complete spectrum is the union of the spectra of both Dirac points, and considering the additional degeneracy corresponding to the two polarizations of the electron spin we get, in full units and for a given chemical potential μ, the Hall conductivity

$$\sigma_{xy} = \frac{2e^2}{h}\left\{\Theta(\mu)\left(\sum_{0<\mathcal{E}<\mu}1\right) - \Theta(-\mu)\left(\sum_{\mu<\mathcal{E}<0}1\right)\right\}\,. \tag{0.19}$$

For small $|\mu|$ (but $|\mu| > |\mathcal{E}_0| = \frac{v_F\sqrt{eB}}{2w}$), $\left|\frac{h}{4e^2}\sigma_{xy}\right| = \frac{1}{2}$. This is the characteristic behavior of the *anomalous integer quantum Hall effect* of graphene, which shows a nonvanishing Hall conductivity for small (positive or negative) values of the Fermi level.





Conclusions

We have studied a simple non-relativistic model, obtained through the introduction of a ***non-Abelian magnetic field*** proportional to the pseudo-spin, to describe the low energy excitations of graphene. The parameters of the model can be identified with those in the tight binding model employed to describe the low energy expansion of the dispersion relation around a Dirac point, $\mathbf{K}$, when the leading order terms for both nearest and next-to-nearest-neighbor interactions are retained.

We have obtained an ***almost*** doubly degenerate spectrum, where the degeneracy is broken by $O\left(w^{-1}\right)$ terms, with $w = \frac{|m|v_F}{\sqrt{eB}} \simeq 10^3$ for realistic values of the parameters. Moreover, there is one quasi-particle state of energy $\mathcal{E}'_0 = eB/2|m|$ and one hole state of energy $\mathcal{E}_0 = -eB/2|m|$.

The Hall conductivity of the model has been obtained from the partition function, employing the ζ-function approach to evaluate the associated functional determinant in the zero temperature limit. This led us to a rather general expression, valid for the Landau problem of a system with a discrete spectrum without accumulation points. In the case under study, the result is consistent with the anomalous integer quantum Hall effect found in graphene, in which the (reduced) Hall conductivity as a function of the Fermi energy takes half-integer values. In particular, $\frac{h}{4e^2}\sigma_{xy} = \pm\frac{1}{2}$ for small (but $|\epsilon_F| > \frac{v_F\sqrt{eB}}{2w}$) positive or negative Fermi level, respectively.

Acknowledgements

This work was supported in part by grants from CONICET (PIP 0681), ANPCyT (PICT 00909) and UNLP (Proy. 11/X615), Argentina, and from FONDECYT (grants 1095217 and 1095106) and Proyecto Anillos ACT119, Chile. M.N. also acknowledge support from Universidad Nacional de La Plata, Argentina. We acknowledge E.M. Santangelo and C.G. Beneventano for useful discussions.

References

[1] H. Falomir, j. Gamboa, M. Loewe and M. Nieto, *J. Phys. A: Math Theor.*, **45**, 135308, (2012).

[2] G.W. Semenoff, Phys. Rev. Lett. 53, (1984) 2449.

[3] Novoselov, K. S., A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Gregorieva, and A. A. Firsov, 2004, Science 306, 666.

[4] Novoselov, K. S., A. K. Geim, S. V. Morozov, D. Jiang, M. I. Katsnelson, I. V. Grigorieva, S. V. Dubonos, and A. A. Firsov, 2005, Nature 438, 197.

[5] Zhang, Y., Y.-W. Tan, H. L. Stormer, and P. Kim, 2005, Nature 438, 201.

[6] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov and A. K. Geim, Rev. Mod. Phys. Vol. 81, (2009) 109.

[7] M.A.H. Vozmediano, M.I. Katsnelson and F. Guinea, Physics Reports **496**, 109, (2010).