Universal conductivity and dimensional crossover in multi-layer graphene

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We show, by exact Renormalization Group methods, that in multi-layer graphene the dimensional crossover energy scale is decreased by the intra-layer interaction, and that for temperatures and frequencies greater than such scale the conductivity is close to the one of a stack of independent layers up to small corrections.

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Recent experiments [1] have found that the optical conductivity in multi-layer graphene is essentially constant in a wide range of frequencies and equal to $N\sigma_0$, with $N \leq 5$ the number of layers and $\sigma_0 = \frac{\pi e^2}{2h}$; remarkably, a value both independent from the intra-layer hopping $t \sim 3eV$ and inter-layer hopping $t^{\perp} \sim 0.3eV$ and depending only on the conductivity quantum h/e^2 and the number of layers N. In the absence of interaction, when N = 1 (monolayer graphene) this observation finds a nice explanation in the effective description of fermions on the honeycomb lattice in terms of massless Dirac fermions in 2+1 dimensions, whose conductivity in the limit of zero frequency is exactly σ_0 , as was shown in [2]. The band structure of multi-layer graphene is completely different and the description in terms of Dirac fermions breaks down at low energies; in the case of bilayer graphene, for instance, [3], a quadratic spectrum instead of a linear relativistic one is found for certain kind of hopping terms. However as pointed out in [1, 4] in multi-layer graphene there is a dimensional crossover scale t_\perp and at energy scales greater than t_{\perp} the conductivity of multilayer graphene is equal to the one of a stack of N independent layers up to small corrections.

The above reasoning neglects the role of the interactions among charge carriers, which are well known to be rather strong and producing observed important effects in several physical observables [5]. In the case of monolayer graphene there are several papers discussing the role of interactions on the conductivity [6–10], but in the case of multi-layer this problem is much less studied, even if interactions in multi-layer graphene are believed to radically alter the low energy properties and spontaneous symmetry breaking is expected [11, 12].

In the present paper we will consider a system of several layers in which the electrons can hop from a plane to another with coupling t^{\perp} , and $t^{\perp} \ll t$; each layer is described in terms of interacting fermions on the honeycomb lattice with an electromagnetic (e.m.) interaction [13, 14]. We will show that the interaction produces a renormalization of the dimensional crossover scale and the conductivity of multi-layer graphene is equal to the one of a stack of N independent layers up to small corrections at energy scales greater than

$$t^{*,\perp} \sim t^{\perp} \left(\frac{t^{\perp}}{t}\right)^{\frac{\eta}{1-\eta}} \tag{1}$$

where $\eta > 0$ is the exponent of the wave function renormalization. Note that the crossover scale is *decreased* by the intra-layer interaction, a phenomenon strongly resembling what happens in fermionic chains, see *e.g.* [15]. Even if our results are found for values of the parameters close to the infrared fixed point of monolayer graphene (that is, the Fermi velocity large enough), they provide an evidence that the many-body interaction preserves and even enforces the conductivity universal behavior, in qualitative agreement with experiments [1].

We consider the Hamiltonian for multi-layer graphene

$$H = \sum_{\alpha=1}^{N} H_{\alpha} + H_{\perp} \tag{2}$$

where H_{α} describe a single graphene layer; more exactly fermions hopping on the honeycomb lattice interacting through an e.m. field introduced via the Peierls substitution [14]

$$H_{\alpha} = -t \sum_{\substack{\vec{x} \in \Lambda_{A} \\ j=1,2,3}} a^{+}_{\vec{x},\alpha} b^{-}_{\vec{x}+\vec{\delta}_{j},\alpha} e^{ie \int_{0}^{1} \vec{\delta}_{j} \cdot \vec{A}_{\alpha}(\vec{x}+s\vec{\delta}_{j},0) \, ds} + c.c. + \frac{e^{2}}{2} \sum_{\vec{x},\vec{y} \in \Lambda_{A} \cup \Lambda_{B}} (n_{\vec{x}}-1)\varphi_{\alpha}(\vec{x}-\vec{y})(n_{\vec{y}}-1)$$
(3)

 $\psi_{\vec{x},\alpha}^{\pm} = (a_{\vec{x},\alpha}^{\pm}, b_{\vec{x}+\vec{\delta}_1,\alpha}^{\pm}) = |\mathcal{B}|^{-1} \int_{\vec{k}\in\mathcal{B}} d\vec{k} \,\psi_{\vec{k},i,\alpha}^{\pm} e^{\pm i\vec{k}\vec{x}}$ for electrons with plane index $\alpha = 1, 2$ and sitting at the sites of the two triangular sublattices Λ_A and Λ_B of a honeycomb lattice. We assume that Λ_A has basis vectors $\vec{l}_{1,2} = \frac{1}{2}(3, \pm\sqrt{3})$ and that $\Lambda_B = \Lambda_A + \vec{\delta}_j$, with $\vec{\delta}_1 = (1,0)$ and $\vec{\delta}_{2,3} = \frac{1}{2}(-1, \pm\sqrt{3})$ the nearest neighbor vectors; \mathcal{B} is the first Brillouin zone and \vec{A}_{α} and ϕ_{α} are the respectively the vector field and the coulomb potential on the plane α .

Finally H_{\perp} describes the hopping between graphene layers and is assumed of the form

$$H_{\perp} = t^{\perp} \sum_{\alpha=1}^{N-1} \sum_{\vec{x}} j_{\alpha,\vec{x}}^{\perp}$$

$$\tag{4}$$

where $j_{\alpha,\vec{x}}^{\perp}$ is a bilinear operator describing the hopping from layer α to layer $\alpha + 1$, see *e.g.* [3]. The *planar paramagnetic current* is defined as

$$\vec{J}_{\vec{p}} = iet \sum_{\alpha=i}^{N} \sum_{\vec{x} \in \Lambda_A, j} e^{-i\vec{p}\vec{x}} \vec{\delta}_j \eta_{\vec{p}}^j \left(a_{\vec{x},\alpha}^+ b_{\vec{x}+\vec{\delta}_j,\alpha}^- - b_{\vec{x}+\vec{\delta}_j,\alpha}^+ a_{\vec{x},\alpha}^-\right)$$

where $\eta_{\vec{p}}^{j} = \frac{1-e^{-i\vec{p}\vec{\delta}_{j}}}{i\vec{p}\vec{\delta}_{j}}$. The two components of the paramagnetic current $\vec{J}_{\vec{p}}$ will be seen as the spatial components of a "space-time" three-components vector $\hat{J}_{\vec{p},\mu}$, $\mu = 0, 1, 2$, with $\hat{J}_{\vec{p},0} = e\hat{\rho}_{\vec{p}}$ and $\hat{\rho}_{\vec{p}}$ the density operator. If $O_{\mathbf{x}} = e^{x_0 H_{\Lambda}} O_{\vec{x}_i} e^{-x_0 H_{\Lambda}}$, with $\mathbf{x} = (x_0, \vec{x})$, we denote by $\langle O_{\mathbf{x}_1}^{(1)} \cdots O_{\mathbf{x}_n}^{(n)} \rangle$ the thermodynamic limit of $\Xi^{-1} \text{Tr}\{e^{-\beta H} \mathbf{T}(O_{\mathbf{x}_1}^{(1)} \cdots O_{\mathbf{x}_n}^{(n)})\}$, where $\Xi = \text{Tr}\{e^{-\beta H}\}$ and \mathbf{T} is the operator of fermionic time ordering. The current-current functions $\hat{K}_{\mu\nu}(\mathbf{p})$ is defined as the 2D Fourier transforms of $\langle J_{\mathbf{x},\mu}; J_{\mathbf{y},\nu} \rangle_{\beta}$ and the conductivity is [4] (here l, m = 1, 2):

$$\sigma_{lm}(\omega) = -\frac{2}{3\sqrt{3}} \frac{1}{\omega} [\hat{K}_{l,m}(\omega,0) - \hat{K}_{l,m}(0,0)] \qquad (5)$$

where $3\sqrt{3}/2$ is the area of the hexagonal cell of the honeycomb lattice. In our notations, $\mathbf{p} = (\omega, \vec{p})$, with $\omega \in \frac{2\pi}{\beta}\mathbb{Z}$ the Matsubara frequency.

It is convenient to introduce the following *Grassman* integral

$$e^{W(J)} = \int P(d\Psi) \int P(dA) e^{\mathcal{V}(A+J,\psi)}$$
(6)

where: $\psi_{\mathbf{k}}^{\pm}$ are Grassman variables ($\mathbf{k} = (k_0, \vec{k})$) and $P(d\psi)$ is the fermionic gaussian integration with inverse propagator

$$g^{-1}(\mathbf{k}) = -\begin{pmatrix} ik_0 & v\Omega^*(\vec{k}) \\ v\Omega(\vec{k}) & ik_0 \end{pmatrix}$$
(7)

with $v = \frac{3}{2}t \ \Omega(\vec{k}) = \frac{2}{3}\sum_{j=1,2,3}e^{i\vec{k}(\vec{\delta}_j-\vec{\delta}_1)}$ (note that $g(\mathbf{k})$ is singular only at the Fermi points $\mathbf{k} = \mathbf{k}_F^{\pm} = (0, \frac{2\pi}{3}, \pm \frac{2\pi}{3\sqrt{3}})$); if $\mu = 0, 1, 2, A_{\mu}^{\alpha}(\mathbf{p})$ are gaussian variables with propagator $\delta_{\alpha,\beta}\delta_{\mu\nu}\frac{\chi(\mathbf{p})}{|\mathbf{p}|}$ where χ act an an ultraviolet cut-off; finally \mathcal{V} is the interaction whose explicit form can be easily inherited from H. By suitable derivatives with respect to J the current-current correlation can be obtained; note that we have exploited gauge invariance to write the photon propagator in the Feynman gauge. The generating function (6) can be computed by exact Renormalization Group methods. After the integration of the fields $\psi^{(1)}, A^{(1)}, ..., \psi^{(h+1)}, A^{(h+1)}$ we get

$$e^{\mathcal{W}(J)} = \int P(d\psi^{(\leq h)}) P(dA^{(\leq h)}) e^{\mathcal{V}^{(h)}(\sqrt{Z_h}\Psi^{(\leq h)}, A^{(\leq h)} + J)},$$
(8)

where $P(d\psi^{(\leq h)})$ is the fermionic integration with propagator, if $r = \pm$ is the valley index

$$\begin{split} \hat{g}_r^{(\leq h)}(\mathbf{k}') &= \\ -\frac{\chi_h(\mathbf{k}')}{Z_h} \begin{pmatrix} ik_0 & v_h \Omega^*(\vec{k}' + \vec{p}_F^r) \\ v_h \Omega(\vec{k}' + \vec{p}_F^r) & ik_0 \end{pmatrix}^{-1} \end{split}$$

where Z_h is effective wave renormalization and v_h the effective Fermi velocity, $P(dA^{(\leq h)})$ is the gauge field integration with propagator $\delta_{\alpha,\beta}\delta_{\mu,\nu}\frac{\chi_h(\mathbf{p})}{2|\mathbf{p}|}$, with $\chi_h(\mathbf{k}'), \chi_h(\mathbf{p})$ smooth cut-off functions with support smaller than $t2^h$; moreover $\mathcal{V}^{(h)}$ is the effective potential which has the form

$$\mathcal{V}^{(h)}(\psi, A) = \int d\mathbf{\underline{x}} d\mathbf{\underline{y}} W_{n,m}^{(h)} \prod_{i=1}^{n} \psi_{\mathbf{x}_{i}, r_{i}, \alpha_{i}}^{\varepsilon_{i}} \prod_{i=1}^{m} A_{\mu_{i}, \mathbf{y}_{i}} \quad (9)$$

where the kernels $W_{n,m}^{(h)}$ depends on the effective charge at scale $h \ e_{\mu,h}$ and the effective hopping t_h^{\perp} . We have now to describe the integration of the field $\psi^{(h)}, A^{(h)}$ and in this way we will iteratively define the effective constants $Z_h, v_h, e_{\mu,h}, t_h^{\perp}$. In order to do that we have to decompose $\mathcal{V}^{(h)}$ as $\mathcal{V}^{(h)} = \mathcal{L}\mathcal{V}^{(h)} + \mathcal{R}\mathcal{V}^{(h)}$ with $\mathcal{R} = 1 - \mathcal{L}; \ \mathcal{L}\mathcal{V}^{(h)}$ is the *relevant* or *marginal* part of the effective interaction while $\mathcal{R}\mathcal{V}^{(h)}$ is the *irrelevant* part. Generally this decomposition is dictated by the naive scaling dimension which in the present case is given by

$$D = 3 - n - m \tag{10}$$

 \mathcal{L} should select the terms with positive or vanishing dimension D. However, if h_{β} is the temperature scale $\beta t = 2^{-h_{\beta}}$ and if the temperature verifies the condition

$$t2^{h_{\beta}} > t_{h_{\beta}}^{\perp} \tag{11}$$

where t_h^{\perp} is the hopping at scale h, there is an improvement with respect to naive power counting, and certain terms which are dimensionally relevant or marginal are indeed irrelevant. In order to verify this fact, we can split the kernels as

$$W_{n,m}^{(h)} = W_{n,m}^{(a)(h)} + W_{n,m}^{(b)(h)}$$
(12)

where $W_{n,m}^{(a)(h)}$ is obtained from $W_{n,m}^{(h)}$ setting $t^{\perp} = 0$. Note that $W_{n,m}^{(a)(h)}$ in correspondence of external fields with different plane index are vanishing.

We define the \mathcal{L} operator as

$$\mathcal{L}\hat{W}_{2,1}^{(h)}(\mathbf{k}') = \hat{W}_{2,1}^{(a)(h)}(0)$$
(13)

so that

$$\mathcal{R}\hat{W}_{2,1}^{(h)}(\underline{\mathbf{k}}') = [\hat{W}_{2,1}^{(a)(h)}(\mathbf{k}') - \hat{W}_{2,1}^{(a)(h)}(\underline{\mathbf{0}})] + \hat{W}_{2,1}^{(b)(h)}(\mathbf{k}')$$
(14)

The first term in the r.h.s. of (14) can be rewritten as $\underline{\mathbf{k}}' \cdot \underline{\partial} W_{n,m}^{(a)(h)}$, and this produces an improvement $\sim 2^{h'-h}$

in the bound of the kernel, if h' is the scale of the momentum, which is sufficient to make it irrelevant. Similarly the second term in (14), namely $\hat{W}_{2,1}^{(b)(h)}(\hat{\mathbf{k}}')$, has an extra $t_h^{\perp} 2^{-h} \leq 2^{(h_\beta - h)(1-\eta)}$, $\eta = O(e^2)$ (see below) with respect to the bound for $W_{2,1}^{(h)}$, which again is enough to make it irrelevant; therefore, the true marginal contribution is given by the r.h.s. of (13). Regarding the terms quadratic in the gauge fields,

$$\mathcal{L}\hat{W}_{0,2}^{(h)}(\mathbf{p}) = \hat{W}_{0,2}^{(a)(h)}(0) + \mathbf{p}\partial\hat{W}_{0,2}^{(a)(h)}(0)$$
(15)

where we have used that $\hat{W}_{0,2}^{(b)(h)}(0)$ has an extra $(2^{-h}t_h^{\perp})^2$ with respect to the naive dimension. Finally the terms quadratic in the fermionic variables, if they have the same plane index then

$$\mathcal{L}\hat{W}_{2,0}^{(h)}(\mathbf{k}') = \hat{W}_{2,0}^{(a)(h)}(0) + \mathbf{k}'\partial\hat{W}_{2,0}^{(a)(h)}(\mathbf{k}')$$
(16)

where we have used that in $\hat{W}_{2,0}^{(b)(h)}$ there is an extra gain $O((t_h^{\perp}2^{-h})^2)$, due to the conservation of the plane index α . On the other hand for the quadratic terms with external fields corresponding to j^{\perp} we define $\mathcal{L}\hat{W}_{2,0}^{(h)}(\mathbf{k}') = \hat{W}_{2,0}^{(h)}(\mathbf{0})$, while for the other terms with different layer index $\mathcal{L}\hat{W}_{2,0}^{(h)}(\mathbf{k}') = 0$.

The terms in $\partial_0 \hat{W}_{2,0}^{(a)(h)}$ and $\partial_1 \hat{W}_{2,0}^{(a)(h)}$ with both fields with the same plane index are included in the free fermionic intergration and produces the new effective wave function renormalization Z_{h-1} and Fermi velocity v_{h-1} ; therefore we get after rescaling

$$e^{\mathcal{W}(J)} = \int P_{Z_{h-1}, v_{h-1}}(d\psi^{(\leq h-1)}) P(dA^{(\leq h-1)})$$
$$e^{\tilde{\mathcal{V}}^{(h)}(\sqrt{Z_{h-1}}\psi^{(\leq h)}, A^{(\leq h)} + J))}, \qquad (17)$$

with

$$\mathcal{L}\tilde{\mathcal{V}}^{(h)}(\psi^{(\leq h)}, A^{(\leq h)}) = \frac{1}{\beta |\mathcal{S}_L|} \sum_{\mu, \mathbf{p}} Z_h^{(\mu)} e \hat{j}_{\mu, \mathbf{p}}^{(\leq h)} \hat{A}_{\mu, \mathbf{p}}^{(\leq h)} + \sum_{\alpha} 2^h \nu_{\mu, h} \hat{A}_{\mu, \alpha, -\mathbf{p}}^{(\leq h)} \hat{A}_{\mu, \alpha, \mathbf{p}}^{(\leq h)} \right] + t_h^{\perp} \int d\mathbf{x} \sum_{\alpha = 1}^{N-1} j_{\mathbf{x}, \alpha}^{(\leq h)\perp}$$
(18)

where $\hat{j}_{\mu,\mathbf{p}}^{(\leq h)}$ is the intra-layer current and $j_{\mathbf{x},\alpha}^{(\leq h)\perp}$ the inter-layer current. Note that by construction the effective Fermi velocity v_h , effective wave function renormalization Z_h and effective charge $e \frac{Z_h^{\mu}}{Z_h} \equiv e_{\mu,h}$ are the same as in the $t^{\perp} = 0$ case and by exploiting Ward Identities we get, see [14] $\nu_h = O(e^2)$ and

$$\frac{Z_h^{(0)}}{Z_h} = 1 + O(e) \qquad \frac{Z_h^{(i)}}{Z_h v_h} = 1 + O(e)$$
(19)

Moreover, see [14], the wave function renormalization diverges with a power law with a critical exponent and the effective Fermi velocity increases up to the light velocity with a power law

$$Z_h \sim 2^{\eta h} \qquad 1 - v_h \sim 2^{\tilde{h}h} \tag{20}$$

with $\eta = \frac{e_{-\infty}^2}{12\pi^2} + O(e_{-\infty}^3)$ and $\tilde{\eta} = \frac{2e_{-\infty}^2}{5\pi^2} + O(e_{-\infty}^3)$. Regarding the flow of t_h^{\perp} we obtain

$${}^{\perp}_{h-1} = \frac{Z_h}{Z_{h-1}} (t_h^{\perp} + \beta_t^{(h)})$$
(21)

with $|\beta_t^{(h)}| \leq C_1 t_h^{\perp} e^6 (t_h^{\perp} 2^{-h})^2$. It is easy to see by induction that $|Z_h t_h^{\perp} - t^{\perp}| \leq C_2 t^{\perp} e^6$. Assume indeed that it is true for $k \geq h$; therefore

$$|t_{h-1}^{\perp} Z_{h-1} - t^{\perp}| \le 2t^{\perp} C e^{6} \sum_{k=h}^{0} (t_{k}^{\perp} 2^{-k})^{2} \qquad (22)$$

from which the inductive assumption follows. Note that the effective hopping, even if *relevant* in the RG sense according to naive power counting, remains small in this region of temperatures. Moreover, from (11) we obtain the condition between the temperature and the hopping

$$\beta^{-1} \ge t^{\perp} \left(\frac{t_{\perp}}{t}\right)^{\frac{\eta}{1-\eta}} \equiv t^{*,\perp} \tag{23}$$

As the flow of the effective parameters corresponding to the relevant and marginal operators is bounded, the following bound is obtained, for $h \ge h_{\beta}$ (order by order in the renormalized expansion)

$$\frac{1}{\Lambda\beta} \int d\mathbf{\underline{x}} |W_{n,m}^{(h)}(\mathbf{\underline{x}})| \le C2^{h(3-n-m)}$$
(24)

We apply the above bound to the conductivity, which is given by

$$\sigma_{ii}(\omega) = -\frac{2}{3\sqrt{3}}\frac{1}{\omega}\int dx_0(e^{i\omega x_0} - 1)K_{i,i}(\mathbf{x})$$
(25)

We can decompose $K_{i,i}(\mathbf{x}) = K_{i,i}^{(a)}(\mathbf{x}) + K_{i,i}^{(b)}(\mathbf{x})$ where $K_{1,1}^{(a)}(\mathbf{x})$ is obtained from $K_{i,i}(\mathbf{x})$ setting $t^{\perp} = 0$ and, for any M

$$|K_{i,i}^{(a)}(\mathbf{x})| \leq \left[\frac{Z_h^{(i)}}{Z_h}\right]^2 \frac{2^{4h}}{1 + (2^h|\mathbf{x}|)^M} |K_{i,i}^{(b)}(\mathbf{x})| \leq \left[\frac{Z_h^{(i)}}{Z_h}\right]^2 \left[\frac{t_h}{2^h}\right]^2 \frac{2^{4h}}{1 + (2^h|\mathbf{x}|)^M}$$
(26)

The above estimates can be derived from the dimensional bound (24); roughly speaking there is, with respect to (24), an extra 2^{3h} due to a lacking integration and a decaying factor $\frac{1}{1+(2^{h}|\mathbf{x}|)^{M}}$ which can be extracted from the chain of propagators connecting the external fields. In the bound for $K_{i,i}^{(b)}(\mathbf{x})$ there are also two extra $\frac{t_{h}}{2^{h}}$. Therefore

$$\sigma_{ii}(\omega) = \sigma_{ii}(\omega)|_{t^{\perp}=0} + R_{ii}^{(b)}(\omega)$$
(27)

where

$$R_{ii}^{(b)}(\omega) = -\frac{2}{3\sqrt{3}} \frac{1}{\omega} \int dx_0 (e^{i\omega x_0} - 1) K_{i,i}^{(b)}(\mathbf{x})$$
(28)

so that for $t^{*.\perp} \leq \beta^{-1}$

$$\begin{aligned} |R_{ii}^{(b)}(\omega)| &\leq C \sum_{h=h_{\beta}}^{1} (t^{\perp})^{2} \int d\mathbf{x} \frac{2^{(2+2\eta)h}}{1+(2^{h}|\mathbf{x}|)^{5}} \\ &\leq \frac{C}{\omega} \sum_{h=h_{\beta}}^{1} (t^{\perp})^{2} 2^{h(-1+2\eta)} \leq C (\frac{t^{*,\perp}}{\omega})^{1-\eta} (t^{*,\perp}\beta)^{1-\eta} \end{aligned}$$

Therefore for $t^{*,\perp} \leq \beta^{-1} \ll \omega$ the conductivity is the one of a stack of independent layers plus a negligible corrections, in qualitative agreement with the observations in [1].

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