

Dynamical approach to ballistic transport in graphene

H.C. Kao^a, M. Lewkowicz^{b,*}, Y. Korniyenko^c, B. Rosenstein^{b,c}

^a Physics Department, National Taiwan Normal University, Taipei, Taiwan, ROC

^b Applied Physics Department, Ariel University Center of Samaria, Ariel 40700, Israel

^c Electrophysics Department, National Chiao Tung University, Hsinchu 30050, Taiwan, ROC

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ABSTRACT

The process of the coherent creation of particle–hole excitations by an electric field in graphene is quantitatively described beyond linear response. We calculate the evolution of the current density and the number of pairs in the ballistic regime using the tight binding model. While for small electric fields the I–V curve is linear characterized by the universal minimal resistivity $\sigma = \pi/2(e^2/h)$, for larger fields, after a certain time interval, the linear regime crosses over to a quadratic one and finally at larger times Bloch oscillations set in.

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It became increasingly evident that electronic mobility in graphene is extremely large exceeding that in best semiconductor 2D samples. Since the system is so clean, the transport becomes ballistic especially in the suspended graphene samples [1]. The flight time can be estimated as $t_{bal} = L/v_g$, where $v_g = \frac{\sqrt{3}}{2} \frac{a\gamma}{\hbar}$ is the graphene velocity characterizing the “relativistic” spectrum of graphene near Dirac points and L is the length of the sample.

Electrons in graphene are described by the 2D tight binding model of nearest neighbor interactions:

$$\hat{H} = \sum_{\mathbf{k}} \begin{pmatrix} c_{\mathbf{k}}^{1\dagger} & c_{\mathbf{k}}^{2\dagger} \end{pmatrix} H_{\mathbf{p}} \begin{pmatrix} c_{\mathbf{k}}^1 \\ c_{\mathbf{k}}^2 \end{pmatrix}, \quad H_{\mathbf{p}} = \begin{pmatrix} 0 & h_{\mathbf{p}} \\ h_{\mathbf{p}}^* & 0 \end{pmatrix}, \quad (1)$$

where

$$h_{\mathbf{p}} = -\gamma \left[\exp\left(i \frac{ap_y}{\sqrt{3}}\right) + b \exp\left(-i \frac{ap_y}{2\sqrt{3}}\right) \right] \quad (2)$$

with γ being the hopping energy, a the distance between C atoms, $b = 2\cos(ak_x/2)$, and the sum is over the Brillouin zone. We consider the system in a constant and homogeneous electric field E along the y direction switched on at $t = 0$ described by the minimal substitution $\mathbf{p} = \hbar\mathbf{k} + \frac{e}{c}\mathbf{A}$, $\mathbf{A} = (0, -cEt)$. A convenient formalism to describe the pair creation is the “first quantized” formulation described in detail in [2,3]. To consider the ballistic transport at zero temperature, $T = 0$, one starts at time $t = 0$ from the zero field state in which all the negative energy one-particle states, $-|\hbar\mathbf{k}| \equiv -\varepsilon_{\mathbf{k}}$, are occupied. The second quantized state which evolves from it is uniquely characterized by the first quantized amplitude,

$$\psi_{\mathbf{k}}(t) = \begin{pmatrix} \psi_{\mathbf{k}}^1(t) \\ \psi_{\mathbf{k}}^2(t) \end{pmatrix}, \quad (3)$$

which is a “spinor” in the sublattice space. It obeys the matrix Schrödinger equation

$$i\hbar\partial_t \psi_{\mathbf{k}} = H_{\mathbf{p}} \psi_{\mathbf{k}}. \quad (4)$$

It is a peculiar property of the tight binding matrix Eq. (1) that the solution for an arbitrary k_y can be reduced to that for $k_y = 0$ and has the Fourier series:

$$\psi_{\mathbf{k}}^1(t) = \sum_{s=\pm 1} A^s \sum_{m=-\infty}^{\infty} p_m^s e^{-i\omega_m^s \tilde{t}},$$

$$\psi_{\mathbf{k}}^2(t) = - \sum_{s=\pm 1} A^s \sum_{m=-\infty}^{\infty} \frac{p_m^s + b p_{m-1}^s}{\omega_m^{-s}} e^{i\omega_m^{-s} \tilde{t}}, \quad (5)$$

where $\tilde{t} = t - \frac{\hbar}{eE} k_y$ and $\omega_m^s = \omega^s + 3\Omega m$ with the frequency $\Omega = \frac{ea}{2\sqrt{3}\hbar} E$. The recursion relation for the Fourier amplitudes p_m ,

$$p_m = \frac{\omega_m - 2\Omega}{b} \left[\omega_m - 3\Omega - \frac{1}{\omega_m - 5\Omega} - \frac{b^2}{\omega_m - 2\Omega} \right] p_{m-1} - \frac{\omega_m - 2\Omega}{\omega_m - 5\Omega} p_{m-2}, \quad (6)$$

has two solutions p^s , $s = \pm 1$, with two Floquet frequencies ω^s . The recursion is easily solved numerically. It turns out that the two Floquet frequencies obey the relation $\omega^+ = 2\Omega - \omega^-$, again peculiar to graphene, as can be checked by numerical results.

Evolution of the current density during the ballistic “flight time” t_{bal} is given by the integral over Brillouin zone (multiplied by factor 2 due to spin) [3]:

* Corresponding author.

E-mail address: vortexbar@yahoo.com (B. Rosenstein).

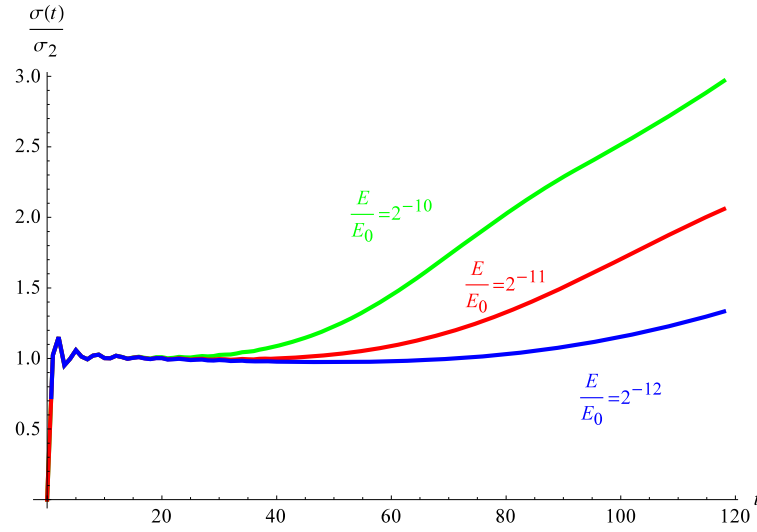


Fig. 1. The time evolution of the scaled current density (divided by electric field) for various values of the dimensionless electric field.

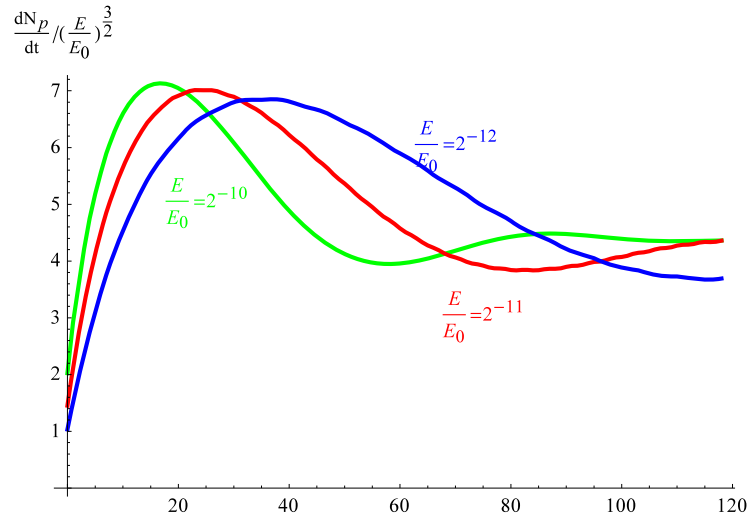


Fig. 2. The time evolution of the scaled pair creation rate for various values of the dimensionless electric field.

$$J_y(t) = -2e \sum_{\mathbf{k}} \psi_{\mathbf{k}}^\dagger(t) \frac{\partial H_{\mathbf{p}}}{\partial p_y} \psi_{\mathbf{k}}(t). \quad (7)$$

The current density divided by electric field, $\sigma(t) \equiv J_y(t)/E$, is shown in Fig. 1 for various values of the dimensionless electric field $\mathcal{E} = E/E_0$. Here the (microscopic) unit of electric field is $E_0 = \frac{\gamma}{ea}$, so that at realistic fields $\mathcal{E} \ll 1$. After an initial fast increase on the microscopic time scale t_γ , $\sigma(t)$ approaches the universal value $\sigma_2 = \frac{\pi}{2} \frac{e^2}{\hbar}$ and settles there, as was shown, using linear response, in [3]. This is clearly seen for electric fields much smaller than E_0 , $\mathcal{E} = 2^{-11}$ – 2^{-9} , shown (up to $120t_\gamma$, $t_\gamma = \hbar/\gamma$) in Fig. 1. Then at

$$t_{nl} = \frac{4}{3\sqrt{\mathcal{E}}} t_\gamma \quad (8)$$

the current rises linearly with time above the constant “universal” value σ_2 :

$$J(t) = \sigma_2 \frac{3}{4} E_0 \mathcal{E}^{3/2} \frac{t}{t_\gamma}. \quad (9)$$

This linear increase regime can be considered as a precursor of the Bloch oscillations.

The number of pairs [4] is

$$N_p(t) = 2 \sum_{\mathbf{k}} |A_{\mathbf{k}}|^2 = 2 \sum_{\mathbf{k}} \left| \psi_1^* + \frac{\hbar_{\mathbf{k}}}{\varepsilon_{\mathbf{k}}} \psi_2^* \right|^2, \quad (10)$$

and the rate $\frac{d}{dt} N_p$ is shown in Fig. 2 as function of time for fields $\mathcal{E} = 2^{-11}$ – 2^{-9} . Immediately after the switching on of electric field (times of order t_γ) the rate behaves as t^3 and approaches the “Schwinger” limit [5] after t_{nl} , when the rate stabilizes approximately at

$$\frac{d}{dt} N_p = 3.5 v_g^{-1/2} \left(\frac{eE}{\hbar} \right)^{3/2} \quad (11)$$

and scales as the power $E^{3/2}$.

It is not surprising since the power $E^{3/2}$ is dictated by dimensionality assuming ultra-relativistic approximation is valid. However the physical meaning is somewhat different. We have used here a definition of the pairs number with respect to Fermi level of the system before the electric field is switched on. This is different not only from the Schwinger’s path integral definition in which the Fermi level is “updated” along the work of electric field and from the definition proposed recently in [6] in connection with graphene also shown in Fig. 2. The two have the same continuum limit (at $t \gg t_\gamma$).

At finite temperature, described by dimensionless parameter $\theta = \frac{L}{\hbar v_g} k_B T$, the conductivity is

$$\sigma_D = \sigma_2 \left[1 + 4 \log(2)\theta + \frac{2i}{\pi} \log \frac{\Gamma(1 + i\theta/2)\Gamma((1 - i\theta)/2)}{\Gamma(1 - i\theta/2)\Gamma((1 + i\theta)/2)} \right]. \quad (12)$$

If in addition the chemical potential is nonzero an additional contribution appears

$$\Delta\sigma = \sigma_2 \frac{1}{\pi} \left[4\theta \log[\cosh(Q/\theta)] - \int_{q=0}^Q \frac{\tanh(q/(2\theta))}{q} \sin(q) \right] \quad (13)$$

where $Q = \frac{\mu L}{\hbar v_g}$. Details of the calculation will be published elsewhere.

To conclude, we have investigated the ballistic transport in graphene using the dynamical approach beyond linear response theory and found that there exists a novel time scale of transition to a nonlinear regime which is within reach of current experimental techniques. On the other hand, the influence of temperature and nonzero chemical potential in the nonlinear regime are expected to be similar to those in the linear response studied in [3].

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