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Disorder effect on the density of states in Landau quantized graphene

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We have studied the effect of gaussian potential (on-site) and unidirectional bond disorder on the density of states (DOS) of Landau quantized graphene. The broadening of the Landau levels weakly depends on energy and the symmetry of the disorder except at the Dirac point. There, bond disorder enhances significantly the peak in the DOS. For stronger disorder, Landau quantization becomes irrelevant, the discrete structures from Landau levels disappear, and we recover the zero field DOS.

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1. Introduction

The recent discovery of graphene has attracted a lot of interest due to its low energy excitations, being two-dimensional Dirac fermions [1–5]. These leave their strong fingerprints on transport properties such as the anomalous integer quantum Hall effect [4], which occurs at half-integer filling factors, and in the presence of universal minimal value of the conductance in the limit of vanishing carrier concentration. Its conductivity depends also linearly on the carrier concentration, a natural behaviour in Drude-like description of normal metals, which calls for more exotic explanation in graphene than simple potential scattering. Charged impurities as well as lattice corrugations or resonant scatterers can account for the observed behavior [6–8].

In order to understand the behavior of the conductivity, a natural starting point is the generalized Einstein relation, which is a generally valid relation of nonequilibrium statistical mechanics, first derived by Kubo [9], which avoids certain ambiguities hidden in the Kubo or Landauer formulation [10]. It states for the conductivity

$$\sigma = e^2 \rho D_{\rm diff}, \qquad (1)$$

where ρ is the density of states and $D_{\rm diff}$ is the diffusion coefficient, both at the Fermi energy E_F. Thus, this relation requires the knowledge of both the density of states and the diffusion coefficient. Here, we are going to address the behavior of the former in the presence of magnetic field, leaving the discussion of the diffusion coefficient and consequently the conductivity for a future publication. Recently, we have studied the conductivity through Eq. (1) without magnetic field [11].

Not surprisingly, Landau level formation in graphene is also unusual compared to normal metals. The resulting spectrum depends on the Landau level index n as $\sqrt{n}$ as opposed to the linear dependence in normal metals. This leads to many surprising phenomena in the magnetotransport properties, such as the violation of the Wiedemann-Franz law under certain conditions [12]. Due to Landau level formation, the density of states in the presence of quantizing magnetic field consists of Dirac delta peaks at the Landau level energies. In the presence of impurities, these peaks are expected to be broadened.

As a simple approximation, the broadening can be approximated by a finite, energy and magnetic field independent scattering time [13] in the spirit of the Drude theory. On the other hand, the self-consistent determination of the self-energy [12,14] reveals a complex dependence on the energy and magnetic field in the case of substitutional on-site (potential) disorder. The purpose of the present investigation is to extend this earlier analysis to the case of gaussian on-site and bond disorder, and concentrate on the resulting structures around Landau levels.

2. Formulation

The Hamiltonian of non-interacting quasiparticles living on a single graphene sheet is given by [14–16]:

$$H_0 = -v_F \sum_{j=x,y} \sigma_j(-i\partial_j + eA_j(\mathbf{r})), \tag{2}$$

where σ_j's are the Pauli matrices, and stand for Bloch states residing on the two different sublattices of the bipartite hexagonal lattice of graphene [14,17]. Strictly speaking, the Hamiltonian above describes quasiparticles around the K points of the Brillouin zone, where the spectrum vanishes. The vector potential for a constant, arbitrarily oriented magnetic field reads as $\mathbf{A(r)} = (-By\cos\theta, 0, B(y\sin\theta\cos\phi - x\sin\theta\sin\phi))$, where θ is the angle the magnetic field makes from the z-axis, and ϕ is the in-plane polar-angle measured from the x-axis. We have dropped the Zeeman term, its energy would be negligible with respect to energy of the Landau levels, Eq. (6), using $v_F \approx 10^6$ m/s, characteristic to graphene. Eq. (2) applies for both spin directions.

In the absence of magnetic field, the energy spectrum of the system is given by

$$E(\mathbf{k}) = \pm v_F |\mathbf{k}|. \tag{3}$$

This describes massless relativistic fermions with spectrum consisting of two cones, touching each other at the endpoints. From this, the density of states per spin follows as

$$\rho(\omega) = \frac{1}{\pi}\sum_{\mathbf{k}} \delta(\omega - E(\mathbf{k})) = \frac{A_c}{2\pi^2}\int_0^{k_c} kdk\,\delta(\omega \pm v_F k) = \frac{2|\omega|}{D^2}, \tag{4}$$

where k_c is the cutoff, $D = v_F k_c$ is the bandwidth, and $A_c = 4\pi/k_c^2$ is the area of the hexagonal unit cell.

In the presence of magnetic field, the eigenvalue problem of this Hamiltonian ($H_0\Psi = E\Psi$) can readily be solved [14]. For the zero energy mode (E = 0), the eigenfunction is obtained as

$$\Psi_k(\mathbf{r}) = \frac{e^{ikx}}{\sqrt{L}}\begin{pmatrix} 0 \\ \phi_0(y - kl_B^2) \end{pmatrix}, \tag{5}$$

and the two components of the spinor describe the two bands. The energy of the other modes reads as

$$E(n,\alpha) = \alpha\omega_c\sqrt{n+1} \tag{6}$$

with $\alpha = \pm 1$, $n = 0, 1, 2, \ldots$, $\omega_c = v_F\sqrt{2e|B\cos(\theta)|}$ is the Landau scale or energy, but is different from the cyclotron frequency [18]. Only the perpendicular component of the field enters into these expressions, and by tilting the field away from the perpendicular direction corresponds to a smaller effective field. The sum over integer n's is cut off at N given by $N + 1 = (D/\omega_c)^2$, which means that we consider $2N + 3$ Landau levels altogether. For later convenience, we define a magnetic field B_0, whose Landau scale is equal to the bandwidth ($\omega_c = D$).

The corresponding wave function is

$$\Psi_{n,k,\alpha}(\mathbf{r}) = \frac{e^{ikx}}{\sqrt{2L}}\begin{pmatrix} \phi_n(y - kl_B^2) \\ \alpha\phi_{n+1}(y - kl_B^2) \end{pmatrix} \tag{7}$$

with cyclotron length $l_b = 1/\sqrt{eB}$. Here $\phi_n(x)$ is the nth eigenfunction of the usual one-dimensional harmonic oscillator. The electron-field operator can be constructed from these functions as

$$\Psi(\mathbf{r}) = \sum_k \left[\Psi_k(\mathbf{r})c_k + \sum_{n,\alpha}\Psi_{n,k,\alpha}c_{k,n,\alpha}\right]. \tag{8}$$

The Green's functions of these new operators do not depend on k, and read as

$$G_0(i\omega_n, k) = \frac{1}{i\omega_n}, \tag{9}$$

$$G_0(i\omega_n, k, n, \alpha) = \frac{1}{i\omega_n - E(n,\alpha)} \tag{10}$$

for c_k and $c_{k,n,\alpha}$, respectively, and ω_n is the fermionic Matsubara frequency.

3. Gaussian on-site and unidirectional disorder

To take scattering into account, we consider the mutual coexistence of both Gaussian potential (on-site) disorder (with matrix element $V_{o,r}$, satisfying $\langle V_{o,r}\rangle = 0$ and variance $\langle V_{o,r}V_{o,r'}\rangle = g_o\delta_{rr'}$) and bond disorder in only one direction (in addition to the uniform hopping with matrix element $V_{b,r}$, satisfying $\langle V_{b,r}\rangle = 0$ and variance $\langle V_{b,r}V_{b,r'}\rangle = g_b\delta_{rr'}$), which is thought to describe reliably the more complicated case of disorder on all bonds [19], and is shown in Fig. 1. In graphene, ripples can represent the main source of disorder, and are approximated by random nearest-neighbour hopping rates, while potential disorder might only be relevant close to the Dirac point [20]. The corresponding term in the Hamiltonian is

$$V = V_{o,r}\sigma_0 + V_{b,r}\sigma_1, \tag{11}$$

which results in $H = H_0 + V$. Due to the different structure of the eigenfunctions of the Landau levels in Eqs. (5), (7), the self energy due to impurity scattering is also expected to depend on the Landau level index, n. Moreover, the self energy is expected to depend on the symmetry of the disorder in the presence of magnetic field. By evaluating the lowest order correction, quasiparticles at the zero mode Landau level can only be scattered to a finite energy level for pure bond disorder, while scattering within the same level is possible for pure on-site disorder. Without mag-

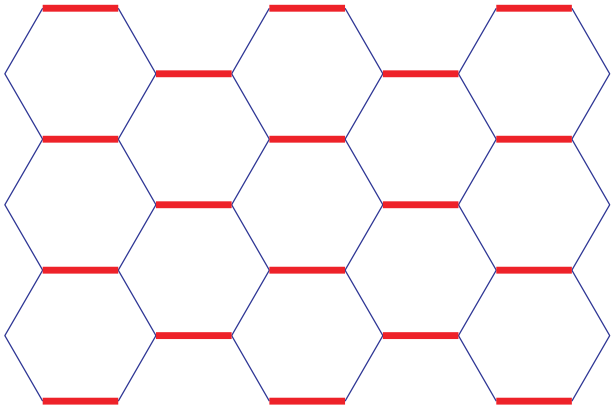

Fig. 1. A small fragment of the honeycomb lattice is shown. The thick lines denote the uni-directional bond disorder, on-site disorder acts on the lattice points.

netic field, pure on site or bond disorder leads to the same self energy [11].

Before going into the details of the calculation, we conjecture that disorder washes out the presence of Landau levels, when its strength is larger than the distance between two adjacent levels. Then for $\omega < \omega_c^2 / 2\sqrt{g_{o,b}}$, the distinct Landau level structure in the density of states is visible, while for higher energies, the zero field DOS is recovered.

In the presence of magnetic field, two self-energies appear belonging to the zero mode and all other Landau levels with non-zero energy, respectively. The general structure of the resulting Green's function reads as

$$G(i\omega_n, k, n, \alpha) = \frac{1}{i\omega_n - E(n,\alpha) - \Sigma_1(i\omega_n)}, \qquad (12)$$

$$G(i\omega_n, k) = \frac{1}{i\omega_n - \Sigma_0(i\omega_n)}, \qquad (13)$$

where the self-energies obey to the following self-consistency equations:

$$\Sigma_0(i\omega_n) = \sum_{x,y=\pm 1} \frac{\beta_0(x,y)}{4}, \qquad (14)$$

$$\Sigma_1(i\omega_n) = \sum_{x,y=\pm 1} \frac{\beta_1(x,y)}{4}, \qquad (15)$$

where

$$\beta_0(x,y) = -\frac{2xV_o + g_c S(i\omega_n) yV_b (xV_o + yV_b)}{\Lambda}, \qquad (16)$$

$$\beta_1(x,y) = -\frac{(1 + g_c G(i\omega_n, k) yV_b)(xV_o + yV_b)}{\Lambda} + \frac{1}{2/(V_o + V_b) - g_c S(i\omega_n)}, \qquad (17)$$

$$\Lambda = (xV_o + yV_b) g_c S(i\omega_n)(yV_b g_c G(i\omega_n, k) + 1) + 2(xV_o g_c G(i\omega_n, k) - 1), \qquad (18)$$

where $g_c = 1/(N+1)$ is the degeneracy of a Landau level per unit cell, $V_o = \sqrt{g_o}$ and $V_b = \sqrt{g_b}$. The resulting self energies are symmetric with respect to $\omega = 0$, since the gaussian nature of the disorder with zero mean does not allow for particle-hole symmetry breaking [21]. Eqs. (14) and (15) are the generalisation of previous results [12] with inclusion of bond disorder. By restricting the sums in Eqs. (14) and (15) to the $x = y = 1$ terms, we get back the results obtained for substitutional disorder [22].

These equations describe impurity effects for arbitrary scattering potential $V_{o,b}$ within the self-consistent non-crossing approximation. The summation over Landau levels can be performed to yield

$$S(i\omega_n) = \sum_{n,\alpha} G(i\omega_n, k, n, \alpha) = 2\frac{z}{\omega_c}[\Psi(1 - z^2) - \Psi(N + 2 - z^2)], \qquad (19)$$

where $z = (i\omega_n - \Sigma_1(i\omega_n))/\omega_c$, $\Psi(z)$ is the digamma function.

The density of states (DOS) is determined from

$$\rho(\omega) = -\frac{1}{\pi} \mathrm{Im} \sum_k \left(G(\omega + i\varepsilon, k) + \sum_{n,\alpha} G(\omega + i\varepsilon, k, n, \alpha) \right) \qquad (20)$$

with $\varepsilon \to 0^+$, and is shown in Fig. 2. In the limit of pure on-site disorder ($V_b = 0$), the residual DOS is given by

$$\rho(0) = \frac{1}{\pi} \sqrt{\frac{B}{g_o B_0}} \qquad (21)$$

for weak disorder and field. In general, the expansion of the self energy proceeds in integer powers of g_o due to the gaussian nature of the disorder. Terms containing $\sqrt{g_o}$ originate from the self consistency condition, Eqs. (14) and (15).

The broadening of the levels is almost symmetric for weaker disorder, but is far from being Lorenztian [23]. Also the level position is modified in the presence of impurities due to the finite real part of the self energies, and this shift increases with the variance. This was also found in a similar treatment [14].

On the other hand, the residual DOS becomes more divergent with disorder in the pure bond-disorder limit ($V_o = 0$) as

$$\rho(0) = \frac{D}{g_b \pi} \sqrt{\frac{2B}{B_0 \ln(B_0/B)}}. \qquad (22)$$

The divergence of these residual DOS follows naturally from the fact, that in the limit of zero disorder, the

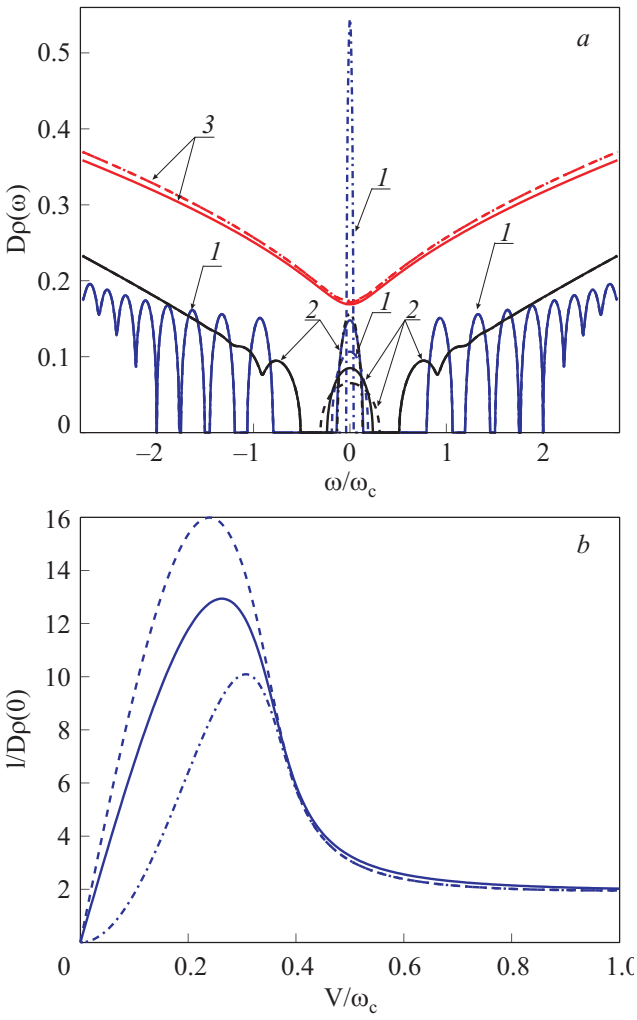

Fig. 2. The density of states is shown for on-site and/or unidirectional bond disorder for $N = 1000$, $V/\omega_c = 0.1$ (*1*), 0.2 (*2*), 0.4 (*3*). The solid line represents the coexisting bond and potential disorder with $V_o = V_b = V/\sqrt{2}$, the dashed/dashed-dotted denotes the on-site/bond disorder (*a*). The inverse of the residual density of states for $N = 1000$ with on-site ($V_o = V$, dashed line), bond disorder ($V_b = V$, dashed-dotted line) with strength V and for their coexistence with $V_o = V_b = V/\sqrt{2}$ (solid line) (*b*).

DOS consists of Dirac-delta peaks at the Landau level energies including zero energy, which should be recovered when $V_{o,b} \to 0$. Here B_0 represents the bandwidth, i.e. a magnetic field scale, when the first Landau level equals to the cutoff energy.

The density of states at the Dirac point first increases with disorder, because of the broadening of the Landau levels. After reaching a minimum, it increases and saturates to a finite value: due to the renormalization of Landau level energies, E_0 moves closer to zero, and at the same time, the broadening continuously increases with disorder. Therefore, the levels merge together, and the presence of the field does not play a role any more, as is seen in Fig. 2.

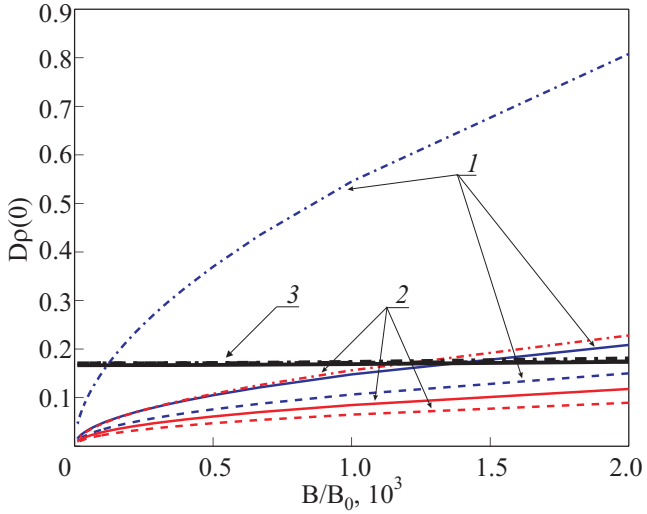

Fig. 3. The density of states is shown as a function of magnetic field for $V/\omega_c = 0.1$ (*1*), 0.2 (*2*), 0.4 (*3*) from top to bottom. The solid line represents the coexisting bond and unidirectional bond disorder with $V_o = V_b = V/\sqrt{2}$, the dashed/dashed-dotted denotes the on-site/bond disorder.

The difference in the DOS for various disorders in magnetic field is the most visible at small energies, close to the zeroth Landau level. There, as suggested by Eqs. (21), (22), the contribution of bond disorder is most pronounced for weak scatterers. For stronger scatterers, as is seen in Fig. 2, they are very close to each other, which is compatible with Ref. 11.

In Fig. 3 the magnetic field dependence of the DOS at the Dirac point is shown. The bond disorder increases it more efficiently with magnetic field than on-site disorder. With increasing variance, the DOS at $B = 0$ enhances, and for large disorder, neither the symmetry of the disorder, nor the explicit value of the field matters, the various curves fall on top of each other.

4. Conclusions

We have studied the effect of gaussian on-site and unidirectional bond disorder in the density of states in graphene in the presence of quantizing magnetic field. Due to the different symmetry of the disorder, distinct density of states characterizes the pure on-site and bond disorder case in the self-consistent non-crossing approximation, in contrast to the zero magnetic field case [11]. These differences become less relevant for higher energies $\omega > \omega_c^2/2\sqrt{g_{o,b}}$ or stronger disorder. The Landau level energies are strongly renormalized by the disorder toward lower energies. The broadening of the levels is not Lorentzian, but remains almost symmetric.

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