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Suppression of Magnetotransport in Strongly Disordered Graphene

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A tight-binding model with randomly fluctuating atomic positions is studied to discuss the effect of strong disorder in graphene. We employ a strong-disorder expansion for the transport quantities and find a diffusive behavior, where the conductivity is decreasing with increasing disorder. For sufficiently strong disorder the magnetic field drops out of the diffusion coefficient and the conductivity. This signals a strong suppression of magnetotransport effects, a result which is consistent with recent experimental observations by Morozov *et al.*

Introduction.—Experimental studies on graphene revealed remarkable transport properties of this material [1–3]. There is a robust minimal conductivity in the absence of an external magnetic field and a quantum Hall effect in the presence of a strong magnetic field [1,2]. Morozov *et al.* found that also for weak magnetic fields unusual transport properties exist: The peak of the magnetoresistance at zero field, the hallmark of weak localization in two-dimensional systems [4], is strongly suppressed in graphene [3,5,6]. This suppression was attributed to disorder caused by ripples in the graphene sheet. When these ripples are removed, the quasiparticle mobility is significantly increased and a normal magnetoresistance peak appears [5]. The peak was also observed in multilayers of graphene, where ripples are less developed because of the higher rigidity of the material.

In this Letter we study the transport properties of graphene in terms of a tight-binding model for quasiparticles on a honeycomb lattice in the presence of a homogeneous magnetic field. Strong disorder is introduced by randomly fluctuating hopping rates. The study is restricted to a system without a gate (i.e., the system is at the Dirac point), where the model has a chiral symmetry.

The usual approximation by Dirac fermions is not applicable to strong randomness. Nevertheless, we find a qualitative agreement of the transport behavior between the tight-binding model and Dirac fermions with random vector potential [7] or random mass [8]. This indicates that the sublattice structure, and not the chiral symmetry, is responsible for the suppression of magnetoresistance peak.

Tight-binding model on a honeycomb lattice.—Hopping of quasiparticles on a honeycomb lattice is defined by the Hamiltonian

$$\mathcal{H} = -\sum_{R,R'} h_{R,R'} c_R^\dagger c_{R'} + \text{H.c.,} \qquad (1)$$

with quasiparticle creation (annihilation) operators $c_R^\dagger$ (c_R). The hopping rate $h_{R,R'}$ between lattice sites R and R' may fluctuate from bond to bond around the average value t due to ripples in the graphene sheet.

A nonorthogonal basis $\{a_1, a_2\}$ (cf. Fig. 1) is used to express the hopping rates in terms of the sublattice representation by writing $R = r$ ($= r + b_1$) if R on A (B). Now r can be expressed in the basis $\{a_1, a_2\}$, and $h_{R,R'}$ in Eq. (1) is replaced by the matrix

$$H = \begin{pmatrix} 0 & d + \Delta \\ d^T + \Delta^T & 0 \end{pmatrix}, \qquad d_{r,r'} = t \sum_{j=1,2,3} \delta_{r',r-c_j},$$
(2)

for $c_1 = 0$, $c_2 = a_2$, and $c_3 = a_1 + a_2$. $\Delta_{r,r'} = \sum_{j=1,2,3} t'_{r',r} \delta_{r',r-c_j}$ are random fluctuations of the hopping term with $\langle t'_{r',r} \rangle = 0$. We set $t = 1$ and keep in mind that t' and all other energies of the model are measured now in units of the hopping rate t.

Although curvature can have significant effects [9–11], it will be ignored here by assuming that the lattice is flat on length scales that are relevant for transport properties. Therefore, only fluctuations of the hopping rates between neighboring sites on the honeycomb lattice are considered.

The quasiparticle Hamiltonian H consists of a translational-invariant part $H_0 \equiv \langle H \rangle$ and a term that describes the random fluctuations. For the latter we assume that on large scales it can be approximated by on-site terms, provided there is only short-range disorder. Such a choice leads to a random vector potential, previously proposed for ripples in graphene by Morozov *et al.* [5] and derived for changes in the hopping due to hybridization between different orbitals in curved graphene sheets and due to elastic strain [9]:
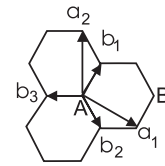

FIG. 1. Lattice vectors on the honeycomb lattice. The lattice is divided into sublattice A and B, where nearest neighbors of A belong to sublattice B.

$$H = H_0 + v_1\sigma_1 + v_2\sigma_2, \qquad (3)$$

with Pauli matrices σ_j. We introduce an uncorrelated Gaussian distribution for v with mean zero and variance g and write $v_1 = v\cos\alpha$, $v_2 = v\sin\alpha$ with a tunable parameter α. Similar models, based on Dirac fermions with a random vector potential, have been studied in the literature [7,12,13]. The seminal work by Ludwig *et al.* states that a random vector potential does not renormalize the variance g, and that (using a bosonization approach in replica space) the conductivity is not affected by this type of disorder [7]. The density of states, on the other hand, has a power law near the Dirac point with exponent $(\pi - g)/(\pi + g)$. This indicates that for strong disorder ($g > \pi$) the density of states diverges at the Dirac point, whereas it vanishes for weak disorder ($g < \pi$). The physical implications of this behavior can be discussed in terms of the Einstein relation, where the conductivity σ is given as the product of the density of states ρ and diffusion coefficient D as $\sigma \propto \rho D$. Then the nonzero conductivity at the Dirac point (minimal conductivity) would imply an infinite D for $g < \pi$ and $D = 0$ for $g > \pi$. In other words, these findings describe a transition at $g = \pi$ from ballistic transport directly to localization, without an intermediate diffusive regime.

For small g the exponent of the density of states can also be evaluated in perturbation theory as $1 - g/\pi$. However, in a recent work on the density of states a disorder created energy scale $\exp(-\pi/g)/g$ was detected, below which perturbation theory breaks down [14]. In other words, the assumption of a power law is invalid at the Dirac point and in its vicinity. The energy scale is similar to the Kondo scale of the Kondo effect [15] and was also found independently for the conductivity by Auslender and Katsnelson [16]. It implies a nonzero density of states at the Dirac point. A similar result was found for topological disorder [10]. In the following, it shall be discussed that the nonzero density of states is associated with spontaneous breaking of a symmetry which leads to diffusion of quasiparticles.

Magnetic field.—A magnetic field B perpendicular to the graphene plane enters the Hamiltonian through a Peierls phase; i.e., the hopping terms in H_0 are replaced by

$$d_{rr'}(B) = \sum_j e^{i\phi_{r,j}}\delta_{r',r-c_j}, \qquad \phi_{r,j} = \int_r^{r+b_j} A\,db_j, \quad (4)$$

where A is the vector potential of the magnetic field B. A homogeneous magnetic field creates additional terms to H that are periodic in one spatial direction and proportional to σ_1 and σ_2, respectively.

Symmetries.—H is invariant under the transformation $H \to e^{i\varphi\sigma_3}He^{i\varphi\sigma_3}$. This is related to the chiral symmetry discussed, for instance, in Refs. [17,18]. Here we are not so much interested in the symmetry of the Hamiltonian but in that of the two-particle Green function (2PGF) at the Dirac point

$$K(r, r'; \epsilon) = \langle \mathrm{Tr}_2[G(r, r'; i\epsilon)G(r', r; -i\epsilon)]\rangle. \qquad (5)$$

Tr_2 is the trace with respect to the spinor structure, $G(i\epsilon) \equiv (H + i\epsilon)^{-1}$ is the one-particle Green function, and $\langle \cdots \rangle$ is the average with respect to the random term of the Hamiltonian. The second Green function in Eq. (5) can be replaced by $-\sigma_3 G(r', r; i\epsilon)\sigma_3$, because it obeys the relation $G(-i\epsilon) = -\sigma_1 G(i\epsilon)\sigma_1$. Within a linear-response approach, $K(r, r'; \epsilon)$ gives the transport properties: The dc conductivity at zero temperature is [7,19–23]

$$\sigma_{jj} \propto \epsilon^2 \sum_r r_j^2 K(r, 0; \epsilon)|_{\epsilon=0}. \qquad (6)$$

For localized states the 2PGF decays exponentially on the localization length for which this expression gives a vanishing dc conductivity.

To analyze the 2PGF in detail, we follow Ref. [24] and write it, before averaging, as a Gaussian functional integral with two independent Gaussian fields, a boson (complex) field χ_{rk} and a fermion (Grassmann) field Ψ_{rk} ($k = 1, 2$):

$$G_{jj'}(r, r'; i\epsilon)G_{k'k}(r', r; i\epsilon) = \int \chi_{r'j'}\bar{\chi}_{rj}\Psi_{rk}\bar{\Psi}_{r'k'}$$
$$\times \exp(-S_0)\mathcal{D}\Psi\mathcal{D}\chi. \qquad (7)$$

S_0 is a quadratic form of the four-component field $\phi_r = (\chi_{r1}, \chi_{r1}, \Psi_{r2}, \Psi_{r2})$:

$$S_0 = -i\sum_{r,r'}\phi_r \cdot (\mathbf{H} + i\epsilon)_{r,r'}\bar{\phi}_{r'}(\epsilon > 0). \qquad (8)$$

The use of the mixed field ϕ_r avoids an extra normalization factor for the integral. (The replica trick, used in Ref. [10], is an alternative to avoid this extra normalization factor.) The extended Hamiltonian $\mathbf{H} = \mathrm{diag}\,(H, H)$ of S_0 acts in the boson and in the fermion sector separately. It is invariant under the transformation

$$\mathbf{H} \to \mathbf{UHU} = \mathbf{H} \quad \text{with} \quad \mathbf{U} = \exp\begin{pmatrix} 0 & \psi\sigma_3 \\ \bar{\psi}\sigma_3 & 0 \end{pmatrix} \quad (9)$$

for Grassmann variables ψ and $\bar{\psi}$, whereas $i\epsilon$ in Eq. (8) causes a symmetry breaking. This symmetry is central for the transport properties, because it determines the large-scale properties of the 2PGF by creating a massless mode. The latter is a consequence of a possible spontaneous symmetry breaking at the Dirac point $\epsilon \to 0$ [8]. This indicates that transport at the Dirac point is *qualitatively* different from transport away from the Dirac point, where this symmetry is explicitly broken by the Fermi energy. An important question in this context is how the symmetry affects average quantities, and whether spontaneous symmetry breaking occurs. The signature of the latter is a nonzero density of states at the Dirac point [25]. (The method of Ref. [25] can be applied to the present model to prove that the average density of states is nonzero.)

Averaging the 2PGF over the Gaussian distribution of v_r means replacing $\exp(-S_0)$ by $\langle\exp(-S_0)\rangle$ on the right-hand side of Eq. (7). The average quantity can be written again as an exponential function $\langle\exp(-S_0)\rangle = \exp(-S_1)$, where the new function S_1 contains also quartic terms of the field ϕ, a consequence of the Gaussian distribution. Then it is convenient to transform the integration variables as

$$\begin{pmatrix} \chi_r\bar{\chi}_r & \chi_r\bar{\Psi}_r \\ \Psi_r\bar{\chi}_r & \Psi_r\bar{\Psi}_r \end{pmatrix} \rightarrow \mathbf{Q}_r = \begin{pmatrix} Q_r & \Theta_r \\ \bar{\Theta}_r & -iP_r \end{pmatrix}, \quad (10)$$

where Q_r, P_r are symmetric 2×2 matrices, and Θ_r, $\bar{\Theta}_r$ are 2×2 matrices whose elements are independent Grassmann variables. The average 2PGF now reads as a correlation function in the new field $\mathbf{Q}_r$:

$$\begin{aligned} K(r, r'; \epsilon) = &-\frac{1}{g^2} \int \text{Tr}_2(\Theta_{r'}[\sigma_1 \cos\alpha + \sigma_2 \sin\alpha]) \\ &\times \text{Tr}_2(\bar{\Theta}_r[\sigma_1 \cos\alpha + \sigma_2 \sin\alpha]) \\ &\times \exp(-S_2)\mathcal{D}[\mathbf{Q}], \end{aligned} \quad (11)$$

with

$$S_2 = \sum_{r,r'} \frac{1}{g} \text{Trg}(\mathbf{Q}_r^2) - \ln[\text{detg}[H_0 + i\epsilon - 2\gamma\mathbf{Q}]]. \quad (12)$$

Trg is the graded trace, detg the graded determinant [24], and γ is a 4×4 matrix, consisting of the linear combination $\gamma_1 \cos\alpha + \gamma_2 \sin\alpha$, where $\gamma_j = \text{diag}(\sigma_j, \sigma_j)$. The integration over $\mathbf{Q}$ can be performed in a saddle-point (SP) approximation, where the SP satisfies the extremal condition $\delta_{\mathbf{Q}}S_2 = 0$, which reads explicitly

$$\mathbf{Q}_r^{\text{SP}} = 2g[H_0 + i\epsilon - 2\gamma\mathbf{Q}^{\text{SP}}]_{rr}^{-1}\gamma. \quad (13)$$

A consequence of the symmetry (9) is that with $\mathbf{Q}^{\text{SP}}$ also $\mathbf{UQ}^{\text{SP}}\mathbf{U}^\dagger$ is a solution of the SP equation at the Dirac point $\epsilon = 0$.

The right-hand side of Eq. (13) is translational invariant in the absence as well as in the presence of a homogeneous magnetic field. This is a consequence of the fact that the diagonal Green function G_{rr} describes closed loops of quasiparticles. These loops depend only on the flux which they enclose. The translational-invariant G_{rr} has a constant SP solution $\mathbf{Q}^{\text{SP}} = -i(\eta/2)\gamma$ which satisfies

$$\eta = 4ig(H_0 + i\epsilon + i\eta)_{rr}^{-1}. \quad (14)$$

η can be interpreted as a self-energy of the average one-particle Green function $(H_0 + i\epsilon + i\eta)^{-1}$ [26]. Then the average density of states at the Dirac point is $\rho = \eta/g$. A SP solution $\eta > 0$ exists even in the limit $\epsilon \rightarrow 0$, which reflects spontaneous symmetry breaking. η increases with g and reaches for large g, the asymptotic regime with $\eta \sim 2\sqrt{g}$, where the density of states decays like $\rho \sim g^{-1/2}$.

The invariance of the SP equation requires the integration over all SPs and their vicinities. This leads to a SP

manifold, generated by the symmetry transformation in form of the nonlinear field

$$\mathbf{Q}'_r = -i\frac{\eta}{2}\mathbf{U}_r^\dagger \gamma \mathbf{U}_r = -i\frac{\eta}{2}\gamma\mathbf{U}_r^2. \quad (15)$$

$\mathbf{U}_r$ is the matrix $\mathbf{U}$ of Eq. (9) with space-dependent Grassmann fields ψ_r and $\bar{\psi}_r$. The integration with respect to the chiral symmetry is not taken into account here because the corresponding fields are perpendicular to the Grassmann fields in leading order. Thus they do not contribute to the average 2PGF.

Replacing $\mathbf{Q}_r$ by $\mathbf{Q}'_r$ in S_2 provides two major simplifications: (i) The first term in expression (12) vanishes, because $\mathbf{Q}'^2_r$ is proportional to the 4×4 unit matrix. (ii) The second term becomes

$$-\ln\text{detg}(\mathbf{U}^{-1}(\mathbf{H}_0 + i\epsilon)\mathbf{U}^{-1} + i\eta), \quad (16)$$

because $\text{detg}\mathbf{U} = 1$. This expression can be expanded either in powers of η^{-1} or in powers of η. The problem of the latter case is that at low energies, which are relevant at the Dirac point, the expansion terms $(\mathbf{H}_0 + i\epsilon)^{-l}$ are arbitrarily large. Consequently, this expansion cannot be controlled. The expansion in powers of η^{-1}, on the other hand, has always small terms for a smoothly varying $\mathbf{U}^{-1}$, provided η is not too small in comparison with energies of these modes. The expansion in powers of η^{-1} can also be justified by using large values of η formally, and then continue it down to physically reasonable values of η. Because no singularity appears, this extrapolation is at least qualitatively correct. Thus the second-order term is a good approximation for low energies. It gives for the expression in Eq. (16)

$$S_2 = -\frac{8}{\eta}\sum_{r,r'}(\epsilon\delta_{rr'} + C_{rr'})\psi_r\bar{\psi}_{r'} + o(\eta^{-3}), \quad (17)$$

where $C_{rr'}$ is

$$\frac{1}{2\eta}\left(\sum_{\bar{r}}\text{Tr}_2[H_{0,\bar{r}r'}H_{0,r'\bar{r}}]\delta_{r,r'} - \text{Tr}_2[H_{0,rr'}H_{0,r'r}]\right). \quad (18)$$

The average 2PGF of Eq. (11) then reads

$$K(r, r'; \epsilon) \approx \frac{\eta^3}{2g^2}(\epsilon + C)_{rr'}^{-1}. \quad (19)$$

This is the main result of our SP calculation. It means that details of the transport properties depend only on the SP solution η and the average Hamiltonian H_0 in the correlation C. A similar expression was found for the 2PGF of weakly disordered Dirac fermions [8].

Discussion.—(i) $B = 0$: Translational invariance of $C_{rr'}$ suggests to study its Fourier components

$$C(q) = \frac{1}{\eta}(2 - \cos q_2 - \cos[(\sqrt{3}q_1 + q_2)/2]), \quad (20)$$

or for the more general case (e.g., for a low-energy ap-

proximation of H_0 by Dirac fermions), the Fourier components

$$C(q) = \frac{1}{2\eta} \int_k [\mathrm{Tr}_2(h_k^2) - \mathrm{Tr}_2(h_{k+q/2} h_{k-q/2})].$$

Here h_k are the Fourier components of H_0; i.e., for Dirac fermions we have $h_k = k_1 \sigma_1 + k_2 \sigma_2$. $C(q)$ vanishes at $q = 0$ and describes the dispersion of the two-particle excitations. In contrast to quasiparticles with Hamiltonian H_0, which have low-energy excitations near the Dirac nodes $k \neq 0$, the two-particle excitations at low energies appear around $q = 0$. This implies that $K(q; \epsilon)$ is a diffusion propagator with diffusion tensor

$$D_{ij} = \frac{1}{2} \frac{\partial^2 C(q)}{\partial q_i \partial q_j} \bigg|_{q=0} = \frac{2}{\eta} \int_k \mathrm{Tr}_2\left(\frac{\partial h_k}{\partial k_i} \frac{\partial h_k}{\partial k_j}\right). \quad (21)$$

Then the main contribution to diffusion comes from the vicinities of the Dirac points, where the slope of h_k is the strongest. This would justify an approximation of h_k by Dirac fermions. Furthermore, in agreement with physical intuition, D is monotonically decreasing with increasing disorder. Finally, the dc conductivity σ can be evaluated via the Kubo formula as

$$\sigma_{jj} \propto -\epsilon^2 \frac{\partial^2}{2q_j^2} K(q; \epsilon)|_{q=0, \epsilon=0} \propto \frac{\eta^2}{g^2} \quad (22)$$

in units of e^2/h. This result indicates that the minimal conductivity is not constant but decreases with increasing disorder. For the regime of strong disorder the conductivity is proportional to g^{-1}, which was also found for topological disorder [10].

(ii) $B \neq 0$: The Hamiltonian H_0 appears in $C_{rr'}$ only as

$$\mathrm{Tr}_2[H_{0,rr'} H_{0,r'r}] = |d_{rr'}(B)|^2 + |d_{r'r}(B)|^2.$$

For a given pair of nearest neighbors (r, r') we have only one contribution for each pair, namely, $|e^{i\phi_{r,j}} \delta_{r', r \pm c_j}|^2$, such that the Peierls phase drops out: $|d_{rr'}(B)|^2 = |d_{rr'}(0)|^2$. Thus, the magnetic-field dependence of the average 2PGF in Eq. (19) is due to the SP solution η. The latter can be evaluated from Eq. (14) by expanding the right-hand side in powers of η^{-1}:

$$\eta^2 = 4g - \frac{4g}{\eta^2} \sum_{r'} \mathrm{Tr}_2[H_{0,rr'} H_{0,r'r}] + o(\eta^{-3}). \quad (23)$$

Again, the B dependence appears only in higher orders of the expansion. While η increases monotonically with g, its B dependence is suppressed.

Disorder due to potential scattering by impurities has been ignored in our approach. Including it in the calculation would affect transport properties at low temperatures significantly, because it causes localization [27]. It is not clear, however, whether this type of disorder is relevant in graphene at the Dirac point.

We conclude that quasiparticles on the honeycomb lattice with random bonds are subject to diffusion. The diffusion coefficient as well as the conductivity decrease with increasing disorder. For sufficiently strong disorder the magnetic-field dependence drops out of the transport quantities. This reflects the suppression of an external magnetic field by disorder, which is consistent with experimental observations of magnetotransport in graphene [5,6].

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