Physics Letters A 380 (2016) 2233–2236

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Singularity of density of states induced by random bond disorder in graphene

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ARTICLE INFO

Article history:
Received 19 February 2016
Accepted 29 April 2016
Available online 2 May 2016
Communicated by R. Wu

Keywords:
Density of states
Graphene
Chiral symmetry
Dirac point

ABSTRACT

We re-investigate the effect of random bond disorder on the density of states (DOS) in graphene. Our large-scale calculation supports that there exists a critical disorder value g_b^c dividing the DOS into two distinct structures. In the regime $g_b < g_b^c$ (g_b is randomness of bond disorder), the DOS away from the Dirac point behaves like a power-law with positive exponent ($\alpha > 0$): $\rho(E) \sim \rho_1 |E|^\alpha$ (E is Fermi energy with respect to the Dirac point, ρ_1 is a constant). In the regime $g_b > g_b^c$, it is observed that DOS develops a peak structure at the Dirac point $E = 0$. Through the finite-size scaling analysis, we elucidate that the DOS at the Dirac point diverges in the thermodynamics limit. Furthermore, it is found that the divergent behavior of DOS is sensitive to any on-site disorder which violates the chiral symmetry in graphene.

1. Introduction

Graphene, a single layer graphite, provides an interesting platform for studying the properties of Dirac-like fermions [1–3]. Recent experiments have revealed many interesting transport properties of disordered graphenes around and away from the charge-neutral Dirac point. Examples include the minimal conductivity [1], the absence of the weak localization effects [4], metal-to-insulator transition under a high magnetic field [5,6] and negative quantum capacitance [7,8]. These unusual phenomena indicate that the disorder effect plays a significant role on understanding the graphene physics near the Dirac point [6,8,9].

Our fundamental knowledge on the disordered systems is from the random matrix theory in which three universality classes were identified according to their respective symmetries [10–12]: orthogonal, unitary, and symplectic. In the last ten years, considerable research attentions have been focused on possible new universality class characterized by new additional symmetry such as the chiral or the particle-hole symmetry [13] related to the systems with some sublattice structures [14,15]. The previous study of chiral symmetry is mainly based on some specific lattice models. Recently, the discovery of graphene provides a wonderful experimental platform to study the effect of chiral symmetry. The chiral symmetry in graphene is conveniently stated as $\{H, \sigma_3\} = 0$, where H is the Hamiltonian describing the low-energy physics of electrons in graphene and σ_3 is a matrix which changes the sign of wave functions on one of the sublattices [9]. In other words, given an eigenstate ψ with energy E, $\sigma_3\psi$ is also an eigenstate with energy $-E$ [13]. Consequently, the energy spectrum is invariant under the transformation $E \to -E$. The chiral symmetry is destroyed by a potential disorder, while the random bond disorder preserves it. Note that the chiral symmetry implies that the eigenstates appear in chiral pairs, but not zero DOS at zero energy (the Dirac point) [16,17].

A long-standing puzzle in chiral system is the behavior of DOS near the zero energy. In the pioneering work of Gade [18], a divergent DOS of the form of $\rho(E) = \frac{1}{E} exp(-c(ln|E|)^{1/x})$ for both chiral unitary and chiral orthogonal systems was theoretically predicted for any randomness strength. Later, the exponent x of this divergent DOS form for the chiral orthogonal systems was corrected by the Motrunich et al. [19]. However, some other approaches showed a finite density of states at and near the Dirac point [16]. Recent studies [20,21] suggest a disorder-induced Kondo-like energy of $Q_0 \sim \Lambda exp(-const/c)$ (c is impurity concentration) separating high-energy from low-energy regime. Above this energy scale or away from the Dirac point, various approaches show that the DOS follows a power law behavior [21,22]. Below this energy scale or near the Dirac point, the behavior of DOS is still unclear. Although early numerical simulations on square lattice [22] observed the divergent DOS for strong enough disorder, it is believed that the result is inconclusive due to severe limits on the achievable energy resolution [23,24].

In this paper, an extensive numerical study of large system up to 8×10^6 atoms ($N_x \times N_y = 2000 \times 4000$) is carried out in order

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http://dx.doi.org/10.1016/j.physleta.2016.04.041
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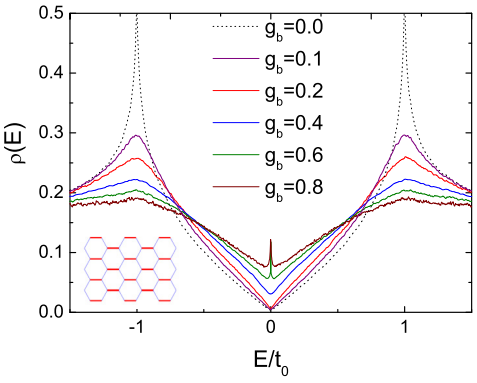

Fig. 1. (Color online.) Density of states of bond-disordered graphenes is shown for various g_b (in units of t_0^2) and $\gamma = 0.001$ (in units of t_0). Inset: The bond fluctuations on the red bonds.

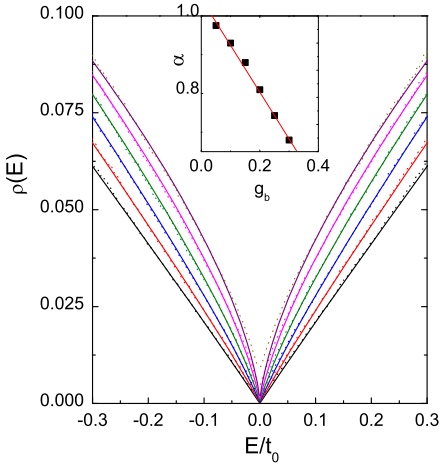

Fig. 2. (Color online.) The low energy DOS for $g_b = 0.04, 0.10, 0.16, 0.20, 0.25, 0.30, 0.36$ (dotted lines from the bottom to the top) and $\gamma = 0.001$. The solid lines follow the power-law as $\rho(E) = \rho_1|E|^\alpha$. Inset: The exponent α is a function of the variance of disorder. The fitting line stands for the relationship $\alpha = 1.05 - 1.24 g_b$.

to resolve the discrepancies mentioned earlier. We calculate the DOS of graphene near and away from the Dirac point by a recursive method with the bond disorder. We find that, in the disorder regime $g_b < g_b^c$, DOS behaves like a non-universal power-law away form the Dirac point, whose exponent depends on the strength of disorder. In the disorder regime $g_b > g_b^c$, on the other hand, DOS at Dirac point has a divergence behavior which implies a Anderson transition from diffusive regime to localization [25].

2. Model and method

The low energy physics of graphene comes from its π-electrons that can be modeled by a tight-binding Hamiltonian on a honeycomb lattice

$$H = \sum_{<ij>} t_{ij} c_i^\dagger c_j + h.c. \tag{1}$$

where $c_i^\dagger$ (c_j) creates (annihilates) a π-electron at site i (j). The hopping energy between two nearest neighboring sites is $t_{ij} = t_0 + \delta t_{ij}$ where energy unit $t_0 = 1.0$ is the hopping coefficient for the pure graphene and δt_{ij} is a real random variable originated from the fluctuation of bond length or angles between the p_z orbits [9]. In this study, δt_{ij} is assumed to have a Gaussian distribution $P[\delta t] \propto exp[-\delta t^2/2g_b]$, and only one of the three types of bonds is disordered, say vertical ones as shown in inset of Fig. 1 [21]. Indeed, we have tested that all of results are qualitatively unchanged when taking into account fluctuations in all three carbon–carbon bonds. The reason is that the critical behavior only depends on the symmetry of the system. Therefore, how to choose the disorder does not affect our qualitative results as long as we keep the same symmetry. In this paper, a graphene with only unidirectional bond disorder belongs to the chiral orthogonal symmetry class since time-reversal symmetry is preserved [15].

The averaged DOS of Hamiltonian (1) can be evaluated by

$$\rho(E) = -\frac{1}{\pi} \overline{< \psi | \frac{1}{E - H + i\eta} | \psi >}, \tag{2}$$

where η is an infinitesimal positive number. In this paper, the accurate averaged DOS is studied using the well developed Lanczos recursive method [6,8,26]. To remove the influence of edge effect, periodic boundary conditions are used. A large enough supercell up to 2000×4000 carbon atoms has been used to remove the finite size effect. In this approach, we have to introduce a small artificial parameter γ to simulate the infinitesimal imaginary energy η. The relationship between proper γ and system size L^2 (L is the typical length of system) has been studied systematically before [27]. γ decreases very slowly with L and the relation $\gamma \sim 1/L$ approximately holds within $L < 5000$ [28]. Physically, γ can be viewed as the energy scale averaged over the energy interval of $\rho(E)$. Thus, we may use this property to detect the divergence in DOS. Due to the finite size calculation, the divergence behavior in DOS just behaves as a peak structure for a given γ. With decreasing γ, that the peak structure becomes sharper indicates a divergent behavior. We can also scale the results to $\gamma \to 0$ to estimate the DOS in the thermodynamic limit (see Fig. 3).

3. Results and discussion

Fig. 1 is the DOS of both pure and disordered graphenes over a wide energy range. The DOS for the pure graphene (doted line in Fig. 1) is linear in the vicinity of the Dirac point ($E = 0$). Two Van Hove singularities at $E = \pm t_0$ are present. The two Van Hove singularities are smoothened in the presence of disorder ($g_b \neq 0$), similar to the previous results with Anderson on-site disorder [29]. Interestingly, the DOS at the Dirac point behaves very differently for weak and strong disorder. Dip appears for a finite value at $E = 0$ and a small g_b. Peak develops when disorder strength is larger than a critical value ($g_b^c \simeq 0.4$), $g_b > g_b^c$.

Fig. 2 plots the DOS $\rho(E)$ away from the Dirac point or above the Kondo-like energy Q_0 for weak disorder. The symbols are numerical results, but the solid lines fit the power-law form

$$\rho(E) = \rho_1 |E|^\alpha \tag{3}$$

where ρ_1 and α are fitting parameters. It is found that ρ_1 is almost a constant in our simulations, and α decreases as disorder strength g_b increases. Our results support the power-law behavior of $\rho(E)$ with a positive exponent α. The inset of Fig. 2 is α versus g_b. The numerical data well fit $\alpha = 1.05 - 1.24 g_b$ (solid line). This linear relationship is consistent with the perturbation theory [21]. It also agrees with the previous numerical simulations using the π-flux model [30,31] on square lattices with random hopping coefficients.

As shown in Fig. 1, the DOS at the Dirac point will change from a dip in the weak disorder to a sharp peak in the strong disorder. In the following, we will elucidate the γ-dependent behavior of the sharp peak indicates the divergence of the DOS at the Dirac point. Noted that if the system size L is large enough and the corresponding positive broadening width γ is reasonably small, the relationship between DOS and γ can be viewed as the calculated results dependence on system size L. In Fig. 3(a), the DOS